A Survey of PFAS Migration Pathways, Transformation Mechanisms, Monitoring and Prediction in Water Contamination, Environmental Remediation and Analytical Techniques

Abstract

Per- and polyfluoroalkyl substances (PFAS) present significant environmental and health challenges due to their persistence, bioaccumulation, and resistance to degradation. This survey synthesizes current knowledge on PFAS, focusing on their migration pathways, transformation mechanisms, monitoring, prediction, and remediation strategies. The study highlights the complexity of PFAS contamination, exacerbated by their widespread distribution across environmental media such as water, soil, and air. The survey underscores the critical need for standardized detection methods and enhanced regulatory frameworks to manage PFAS effectively. Advances in analytical techniques, such as mass spectrometry and innovative sensor technologies, are essential for improving PFAS detection and monitoring. Furthermore, the development of predictive models and novel remediation technologies, including electrochemical degradation and metamaterials, shows promise in addressing PFAS contamination. The survey emphasizes the importance of interdisciplinary collaboration and data transparency to inform regulatory decisions and foster the development of sustainable remediation strategies. Future research should prioritize the exploration of environmentally friendly materials, comprehensive health impact assessments, and optimization of existing technologies to mitigate the adverse effects of PFAS on ecosystems and public health. By integrating advanced computational tools and innovative monitoring approaches, the scientific community can enhance the understanding and management of PFAS, ultimately contributing to more effective environmental protection strategies.

1 Introduction

1.1 Significance of PFAS in Environmental Science

Per- and polyfluoroalkyl substances (PFAS) are persistent environmental pollutants, widely used in industrial applications, leading to global contamination and significant health risks [1]. Their resistance to degradation and bioaccumulation in food chains pose substantial challenges for environmental management, particularly as PFAS can persist in ecosystems for extended periods, impacting both human and wildlife health. The application of PFAS-laden biosolids to agricultural soils further intensifies these risks by potentially contaminating food sources [2].

A major hurdle in addressing PFAS contamination is the lack of standardized detection methods and the variability of regulatory frameworks across regions, complicating the establishment of effective management strategies [3]. With over 4700 known PFAS compounds, individual testing becomes impractical, necessitating the development of grouping strategies to protect human and environmental health [4]. The widespread presence of PFAS, particularly in drinking water, underscores the urgent need for improved removal technologies and robust regulatory measures.

§1. Introduction

§2. Background and Definitions

§3. PFAS Migration Pathways

3.1 Environmental Media and PFAS Distribution

3.2 Mechanisms of PFAS Migration

3.3 Sources and Environmental Transport Pathways

3.4 Implications for Environmental Contamination

§4. Transformation Mechanisms of PFAS

§5. Monitoring and Prediction of PFAS Contamination

5.1 Current Monitoring Technologies

5.2 Challenges in Monitoring and Data Collection

5.3 Predictive Models for PFAS Distribution

5.4 Innovative Monitoring Approaches

5.5 Future Directions in PFAS Monitoring and Prediction

§6. Analytical Techniques for PFAS Detection

6.1 Advanced Mass Spectrometry Techniques

6.2 Innovative Sensor Technologies

6.3 Novel Separation and Detection Methods

6.4 Biosensing Platforms

6.5 Data-Driven Detection Approaches

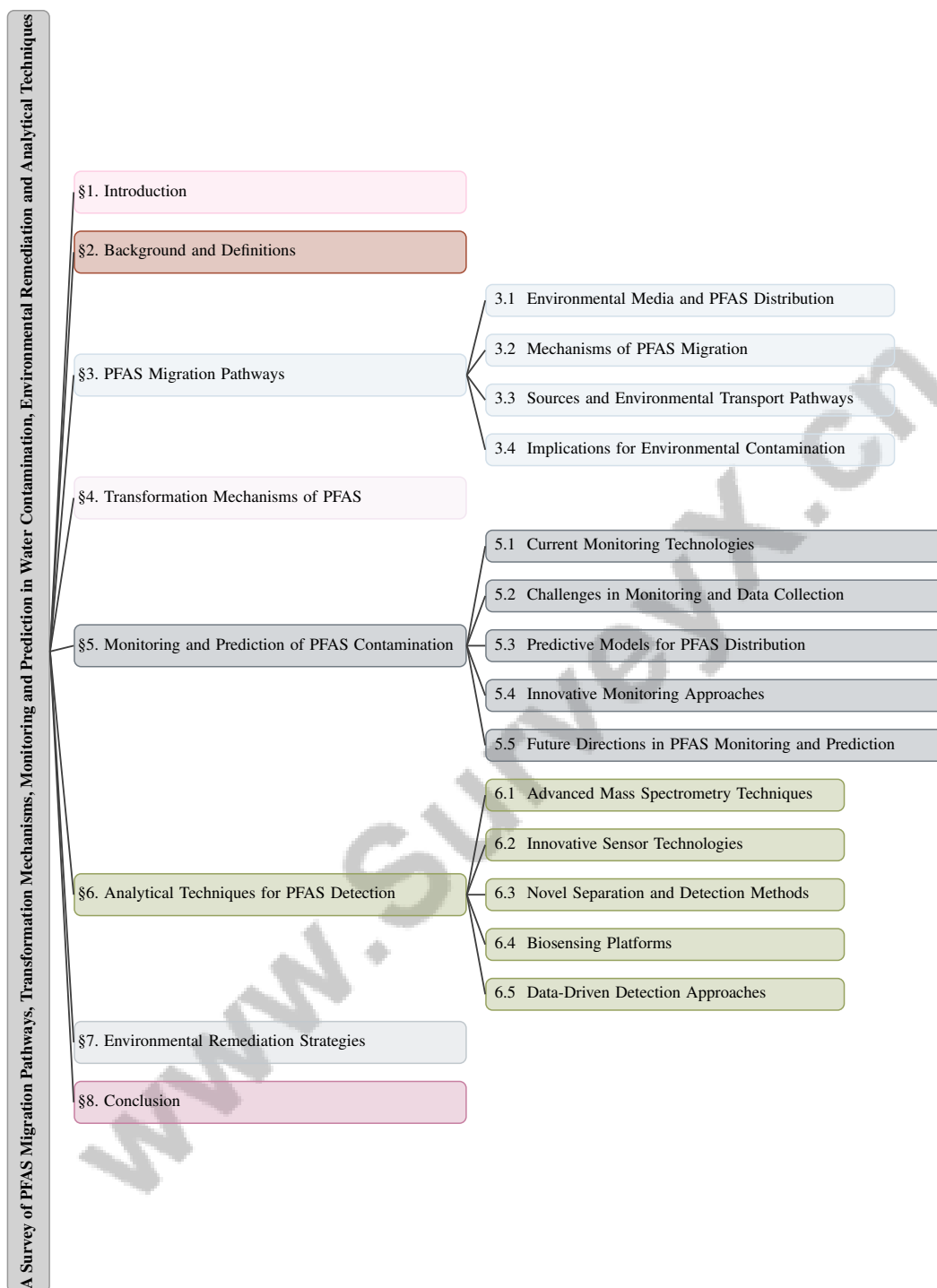§7. Environmental Remediation Strategies

§8. Conclusion

Figure 1: chapter structure

The global challenge of ensuring access to safe drinking water highlights the transformative potential of reliable detection methods for contaminants, including PFAS [5]. This survey aims to bridge critical knowledge gaps in PFAS research, focusing on global production, environmental hotspots, measurement accessibility, waste management, health effects, and economic implications. Understanding these facets is vital for formulating effective management strategies to mitigate PFAS's adverse impacts on the environment and public health.

1.2 Structure of the Survey

This survey offers a comprehensive synthesis of current knowledge regarding the migration pathways, transformation mechanisms, monitoring, prediction, and remediation of PFAS in the environment. The paper is organized into several key sections, each addressing critical aspects of PFAS research and management.

The introductory section establishes the significance of PFAS in environmental science and outlines the challenges associated with their contamination. Following this, a background section defines key terms such as migration pathways and transformation mechanisms while providing an overview of PFAS's chemical properties and environmental persistence.

Subsequent sections explore specific topics, beginning with an analysis of PFAS migration pathways, detailing their distribution across various environmental media—water, soil, and air—and identifying sources and transport pathways that contribute to environmental contamination.

The survey also examines PFAS transformation mechanisms, focusing on the influence of microbial activity and environmental conditions on these processes. Innovative analytical techniques, such as microbiome-omics and nanoparticle-based sensors, are highlighted for their role in enhancing our understanding of pathogen suppression and biodegradation [6, 7, 4].

Monitoring and prediction of PFAS contamination are addressed through a review of current methods and technologies for tracking PFAS in water sources, alongside predictive models for forecasting their distribution and innovative monitoring approaches that outline future research directions.

The evaluation of analytical techniques for detecting PFAS is comprehensive, emphasizing advanced mass spectrometry, innovative sensor technologies, and cutting-edge separation techniques. This review discusses the strengths and limitations of methodologies such as liquid chromatography-mass spectrometry (LC-MS), nanoparticle-based sensors, and smartphone applications, as well as essential tools like the total oxidizable precursor assay (TOPA) and total organic fluorine (TOF) content for quantifying PFAS precursors and conducting mass balance analyses across diverse environmental matrices [8, 6, 9]. Data-driven approaches for enhancing detection capabilities are also explored.

The survey concludes with an evaluation of environmental remediation strategies for PFAS, detailing the effectiveness of current technologies and investigating innovative approaches, including advanced analytical methods and regulatory frameworks aimed at addressing pervasive PFAS contamination and mitigating its harmful impacts on human health and ecosystems [8, 9, 6]. Regulatory and policy considerations, alongside future research needs, are discussed to inform effective management strategies.

Throughout the survey, emphasis is placed on synthesizing current understanding and identifying key knowledge gaps that hinder informed regulatory decisions, as highlighted by recent studies [10].The following sections are organized as shown in Figure 1.

2 Background and Definitions

2.1 Chemical Properties and Environmental Persistence of PFAS

Per- and polyfluoroalkyl substances (PFAS) are characterized by robust carbon-fluorine (C-F) bonds, contributing to their persistence and categorization as persistent organic pollutants. Their structural stability complicates environmental degradation, as elucidated by Graph Convolutional Networks (GCN) modeling, which reveals their binding affinities with biological molecules [1]. The hydrophobic and lipophobic nature of PFAS facilitates their extensive distribution in water, soil, and air, earning them the moniker 'forever chemicals' due to their environmental stability and remediation challenges [11]. Since their introduction in the 1950s, PFAS have become ubiquitous in the environment [11].

The accumulation of PFAS in water sources poses ecological and human health risks through persistence and bioaccumulation, inducing oxidative stress and toxic effects in organisms [12]. The application of PFAS-laden biosolids in agriculture exacerbates contamination risks, affecting soils, groundwater, and food chains [2]. Research on PFAS categorization underscores the importance of understanding their properties and persistence [4]. Traditional models fall short in predicting biodegradability and toxicity, necessitating advanced approaches to link PFAS structures with properties [13]. The computational demands of the electronic Schrödinger equation for PFAS further

3

complicate modeling efforts [14]. These challenges highlight the need for effective remediation and advanced analytical techniques to mitigate PFAS's environmental impact.

2.2 Defining Key Terms: Migration Pathways and Transformation Mechanisms

Understanding PFAS migration pathways and transformation mechanisms is crucial for evaluating their environmental and health impacts. Migration pathways describe the routes PFAS take through environmental media, influenced by their hydrophobicity and lipophobicity, which aid in their distribution and persistence [15]. Categorizing PFAS research into intrinsic properties and risk assessment methods emphasizes the significance of these pathways for estimating cumulative exposure and effects [4].

Transformation mechanisms involve chemical and biological processes that alter PFAS, including biodegradation by microbes and the compounds' toxicity to organisms [13]. The diverse range of PFAS compounds, each with unique chemical behaviors, complicates these transformations. Recent studies highlight ineffective management of human excrement as a key issue in public health crises and environmental degradation, underscoring the need for comprehensive management of PFAS migration and transformation [7]. This survey aims to establish a foundational understanding essential for developing strategies to mitigate PFAS's environmental and health impacts.

2.3 Historical Context and Current State of PFAS Research

PFAS research began with enthusiasm for their resistance to heat, water, and oil, leading to widespread industrial and consumer use since the mid-20th century. However, concerns about their environmental persistence and bioaccumulation have grown, highlighting potential health and ecological impacts [16]. Early research focused on compounds like perfluorooctanoic acid (PFOA) and perfluorooctanesulfonic acid (PFOS), which are well-studied due to their prevalence and persistence [11].

Recent research has expanded to newer compounds like ADONA and GenX, which require tailored treatment approaches [11]. Despite advancements, significant gaps remain in understanding PFAS applications and impacts, particularly in emerging industries [16]. The lack of comprehensive data on most PFAS compounds limits regulatory framework effectiveness [4]. Research focuses on occurrence studies and treatment technologies, emphasizing PFAS presence in drinking water due to public health implications [3]. The absence of historical data on PFAS in biosolids complicates assessments of temporal changes, hindering understanding of long-term impacts [2].

Current PFAS research emphasizes developing innovative analytical and computational methods to overcome traditional technique limitations. The challenge of calculating large PFAS molecules' electronic structures, due to the exponential scaling of computational resources needed for full configuration interaction (FCI) methods, remains a significant hurdle [14]. As the scientific community addresses these challenges, developing effective remediation strategies and enhanced regulatory measures is crucial to mitigating PFAS's environmental and public health risks.

In recent years, the study of per- and polyfluoroalkyl substances (PFAS) has garnered significant attention due to their persistent nature and widespread environmental impact. Understanding the pathways through which PFAS migrate is crucial for assessing their risks and developing effective remediation strategies. As illustrated in Figure 2, the hierarchical categorization of PFAS migration pathways provides a comprehensive overview of this complex issue. This figure highlights the distribution of PFAS across various environmental media, the mechanisms of their migration, and the sources from which they originate. Furthermore, it delineates the transport pathways and the implications these have for environmental contamination. Each section of the figure delves into specific aspects, including PFAS characteristics, their environmental impact, and the challenges associated with contamination, while also proposing innovative solutions for monitoring and remediation efforts. This structured approach not only enhances our understanding of PFAS dynamics but also underscores the urgency of addressing their environmental footprint.
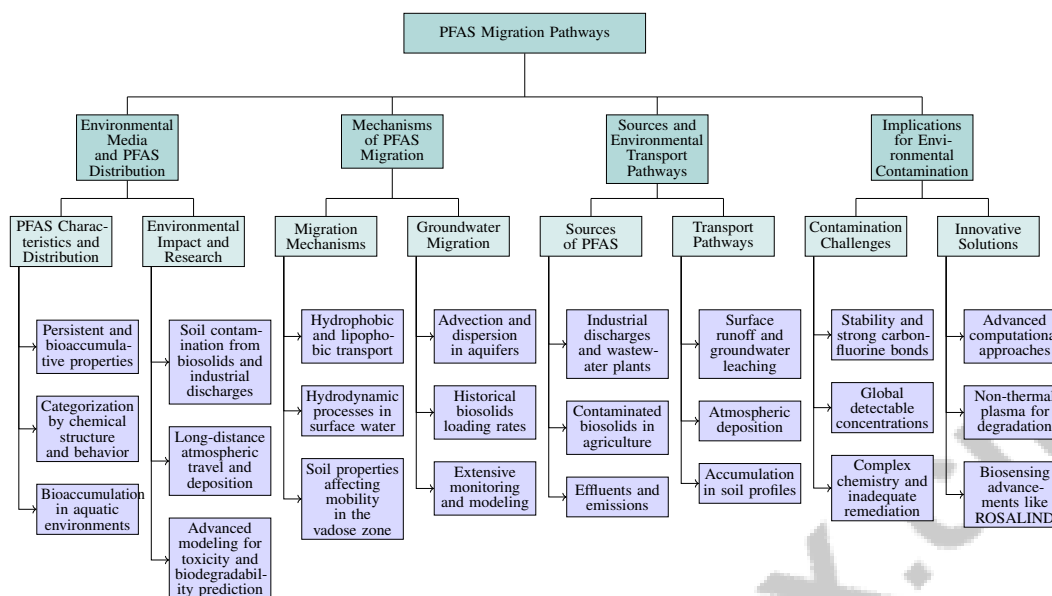
4

Figure 2: This figure illustrates the hierarchical categorization of PFAS migration pathways, highlighting environmental media distribution, migration mechanisms, sources and transport pathways, and implications for environmental contamination. Each section delves into specific aspects such as PFAS characteristics, environmental impact, migration mechanisms, transport pathways, contamination challenges, and innovative solutions for remediation and monitoring.

3 PFAS Migration Pathways

3.1 Environmental Media and PFAS Distribution

PFAS are pervasive in water, soil, and air due to their persistent and bioaccumulative properties. Categorizing PFAS by chemical structure and environmental behavior aids in understanding distribution and health impacts [8, 12]. In aquatic environments, PFAS bioaccumulate in organisms, posing ecological and health risks. Organic matter complicates PFAS adsorption, necessitating research on short-chain PFAS for effective remediation [15]. Soil contamination from biosolids and industrial discharges leads to groundwater pollution, threatening drinking water and agriculture. Understanding global PFAS production is crucial for tracking impacts and developing management strategies [17]. PFAS can travel long distances atmospherically, entering ecosystems via deposition. Advanced modeling, like MULTIMODAL-MOLFORMER, integrates chemical language with physicochemical features to predict PFAS toxicity and biodegradability, enhancing understanding of environmental interactions [13]. The widespread distribution of PFAS necessitates comprehensive monitoring and innovative analytical techniques to assess and mitigate health and ecological impacts. Collaboration among researchers, regulators, and industries is vital to address data gaps and improve understanding of PFAS health effects and waste management [6, 17].

3.2 Mechanisms of PFAS Migration

PFAS migration is governed by chemical properties and interactions, with hydrophobic and lipophobic characteristics facilitating transport through surface water, the vadose zone, and groundwater [2]. Understanding these mechanisms is crucial for identifying high-concentration areas for targeted remediation [17]. In surface water, hydrodynamic processes and organic matter affect PFAS sorption and desorption. In the vadose zone, soil properties like porosity and moisture impact PFAS mobility. Johnson et al. highlight the differential behavior of short- and long-chain PFAS based on soil depth, crucial for understanding persistence and groundwater contamination [2]. Groundwater migration involves advection and dispersion, influenced by aquifer properties and PFAS characteristics. Historical biosolids loading rates are key for assessing PFAS presence and mobility, providing insights into

5

long-term impacts [2]. These mechanisms necessitate extensive monitoring and modeling to predict distribution and develop effective remediation strategies [8, 9, 6, 17].

(a)   Perfluorooctanesulfonic Acid[18]

(b) Veneto Region Contaminated Area Map[12]
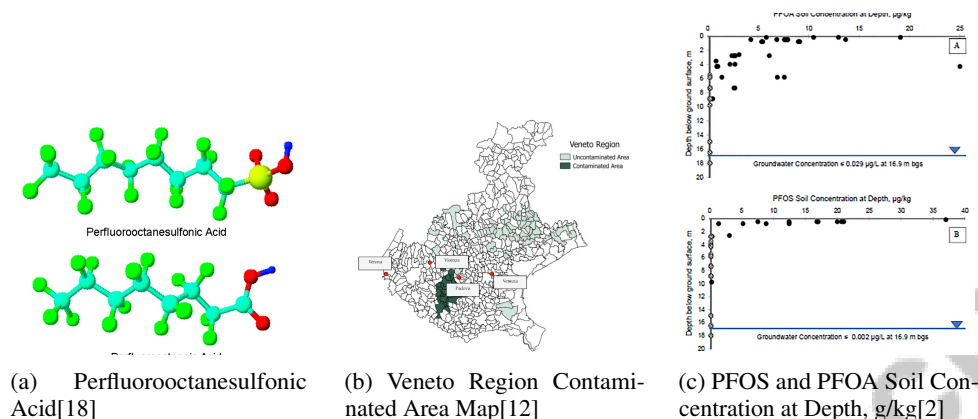
(c) PFOS and PFOA Soil Concentration at Depth, g/kg[2]

Figure 3: Examples of Mechanisms of PFAS Migration

As depicted in Figure 3, understanding PFAS migration involves recognizing environmental movement pathways and mechanisms. The first image shows PFOS's molecular structure, emphasizing persistence. The second image maps Veneto Region contamination, highlighting geographical scope. The third image illustrates PFOS and PFOA soil concentrations at depth, indicating vertical migration. These visuals underscore PFAS migration's complexity and the need for comprehensive understanding to develop mitigation strategies [18, 12, 2].

3.3   Sources and Environmental Transport Pathways

PFAS transport pathways are linked to sources like industrial discharges, wastewater plants, and contaminated biosolids in agriculture. Industrial activities contribute significantly to environmental contamination through effluents and emissions, leading to widespread distribution [10]. In water networks, PFAS contamination from accidental or intentional events requires optimal sensor placement for rapid detection to protect water quality [19]. The complexity of PFAS transport is compounded by inadequate population surveys and analytical methods, hindering exposure quantification and risk assessment [10]. PFAS migrate via surface runoff, groundwater leaching, and atmospheric deposition, with high persistence allowing significant distance migration, evidenced by detection in remote soils and groundwater. PFAS accumulation in soil profiles, with some compounds at depths up to 9 meters, indicates long-term persistence and risks to water resources. Biosolid application further contributes to distribution, raising public health and ecological concerns [18, 9, 17, 2]. Understanding these mechanisms is essential for developing management and remediation strategies to mitigate impacts.

3.4   Implications for Environmental Contamination

PFAS migration across media presents significant contamination implications. Their stability, due to strong carbon-fluorine bonds, challenges degradation and removal from sites [20]. This persistence results in detectable concentrations globally, even in remote regions [9]. PFAS chemistry complexity requires advanced computational approaches for behavior simulation and analysis, as existing remediation methods are often inadequate [21]. Integrating effect-based tools and monitoring strategies is critical for ecological impact assessment and regulatory framework development [22]. Innovative technologies, like non-thermal plasma (NTP), show promise for degrading PFAS in water, allowing treatment efficiency evaluations across compounds and matrices [11]. Advancements in biosensing, like ROSALIND, facilitate rapid detection without viable cells, addressing traditional method limitations and enhancing PFAS monitoring [5]. The pervasive presence and potential health impacts of PFAS necessitate a multifaceted strategy integrating innovative remediation, computational modeling, and monitoring frameworks to manage migration, understand behavior, and mitigate ecosystem and public health effects, as highlighted by PFAS concentrations in soils and potential leaching into water [9, 17].

6

4 Transformation Mechanisms of PFAS

4.1 Chemical Processes in PFAS Transformation

The transformation of per- and polyfluoroalkyl substances (PFAS) involves intricate chemical processes crucial for their degradation. The cleavage of the robust carbon-fluorine (C-F) bonds is a primary challenge in PFAS remediation. Recent advancements in electrochemical methods, such as boron-doped reduced graphene oxide sponge anodes, have shown promise in promoting defluorination [20]. Advanced computational techniques, like the QPFAS hybrid quantum-classical workflow, utilizing the Variational Quantum Eigensolver (VQE) algorithm, enhance our understanding of PFAS electronic structures, revealing potential degradation pathways [21].

Adsorption mechanisms are pivotal for optimizing PFAS removal, with research focusing on identifying physicochemical characteristics that influence PFAS-adsorbent interactions [15]. The causal multi-stage feature selection method aids in targeting remediation strategies by identifying relevant characteristics [13]. Research on newer PFAS compounds emphasizes elucidating specific degradation pathways and byproducts, addressing emerging contaminants for effective environmental management [11].

4.2 Biological Processes and Microbial Activity

Microbial activity plays a significant role in PFAS transformation, though complete mineralization is hampered by strong C-F bonds. Certain microbial communities can partially degrade PFAS through enzymatic pathways, producing intermediate products [13]. The effectiveness of microbial degradation depends on environmental conditions such as pH, temperature, and co-substrates that enhance microbial activity. Specific bacterial strains, capable of both anaerobic and aerobic degradation, can initiate PFAS breakdown under optimized conditions, though rates vary among compounds [7].

Innovative approaches integrating computational models with experimental data identify effective microbial species and enzymes for PFAS transformation, elucidating interactions between PFAS and microbial pathways [13]. Exploring microbial consortia and their synergistic interactions offers promising avenues for enhancing PFAS degradation in contaminated environments [7].

4.3 Environmental Conditions Influencing PFAS Transformation

PFAS transformation is significantly influenced by environmental conditions, including soil composition, moisture, and microbial activity, which affect their chemical stability and degradation pathways. These conditions are crucial for predicting PFAS fate and transport in ecosystems and developing remediation strategies [8, 18, 9]. Factors such as pH, temperature, and co-contaminants can alter reaction rates and microbial activity, impacting PFAS degradation [2]. Organic matter and co-contaminants can influence PFAS sorption and microbial degradation [9].

Advanced computational methods, such as the QPFAS workflow, simulate molecular interactions during PFAS bond-breaking experiments, providing insights into transformation pathways [21]. Applying complex network theory optimizes sensor placement in water distribution networks, enhancing PFAS contamination monitoring and informing on environmental conditions affecting transformation [19].

Understanding the interplay between environmental factors and PFAS behavior is vital for developing regulatory measures and remediation technologies to mitigate contamination [8]. Leveraging computational tools and environmental data improves predictions of PFAS behavior and facilitates targeted remediation strategies.

4.4 Innovative Analytical Techniques for Studying Transformation Mechanisms

Innovative analytical techniques have advanced the study of PFAS transformation mechanisms, crucial for elucidating degradation pathways and assessing environmental impacts. Graphene-based materials have demonstrated efficacy in PFAS electrosorption and electrooxidation, offering efficient removal without harmful byproducts [20]. Metamaterials, utilizing super-hydrophobicity and strong capillary effects, enhance PFAS removal efficiency from contaminated water [23].

7

Computational models, such as the Graph Convolutional Network (GCN), improve understanding of PFAS transformation by predicting hepatotoxicity and binding mechanisms [1]. These models complement experimental techniques, providing deeper insights into molecular interactions and transformation pathways.

Biosensing platforms like ROSALIND enhance PFAS detection, enabling rapid RNA-level output generation, streamlining monitoring processes [5]. Continued research on PFAS impacts underscores the importance of developing effective remediation technologies and innovative analytical methods [8]. Future efforts should focus on identifying alternatives for high-use PFAS applications and improving regulatory frameworks for better management and reduction of PFAS in the environment [16]. Advanced analytical techniques play a pivotal role in enhancing our understanding of PFAS risks and informing regulatory actions [4].

5 Monitoring and Prediction of PFAS Contamination

5.1 Current Monitoring Technologies

Monitoring PFAS is crucial for mitigating their ecological and health impacts. Recent advancements in detection technologies emphasize the need for standardized methods to understand PFAS-related health risks [18]. However, PFAS's chemical stability complicates their removal [3]. Developing accessible measurement methods across environmental media is essential for effective monitoring and regulatory compliance [2]. Innovative approaches, such as non-thermal plasma technologies, show promise for treating PFAS-contaminated water [11]. In water distribution networks, sensor placement using complex network theory enhances contamination detection [19]. Affordable online sensors support extensive real-time data collection [24]. Advanced technologies like the QPFAS workflow simulate PFAS degradation, highlighting quantum computing's potential in environmental monitoring [21]. The ROSALIND biosensing platform efficiently detects water contaminants [5]. The current landscape of PFAS monitoring technologies reflects efforts to improve detection and address the challenges posed by these pollutants, with ongoing research essential for bridging knowledge gaps [8].

5.2 Challenges in Monitoring and Data Collection

PFAS monitoring faces challenges that hinder understanding their environmental and health impacts. A significant issue is the lack of comprehensive eco-toxicological data, limiting insights into PFAS effects [12]. Insufficient monitoring complicates risk assessments [22]. Limitations in studies, such as small sample sizes, obscure true associations between PFAS exposure and health outcomes [25]. The absence of data on emerging PFAS compounds leads to underestimations of exposure risks [10]. Sensor deployment struggles with optimizing placement for maximum coverage, diminishing monitoring efficacy [19]. High false alarm rates in event detection further complicate monitoring [24]. Current detection methods often suffer from complexity and high costs, making them impractical for real-time applications [26]. Addressing PFAS contamination challenges requires enhancing monitoring capabilities through optimal sensor placement and innovative detection technologies leveraging complex network theory [19].

5.3 Predictive Models for PFAS Distribution

Predictive models for PFAS distribution are essential for understanding their environmental persistence and health risks [18, 9]. A primary challenge is the limited availability of binding affinity data, which constrains model accuracy [1]. Advancements in simulation models enhance contamination event detection, with performance evaluated based on sensor coverage [19]. Integrating multiple algorithms in event detection systems improves monitoring and classification, providing timely alerts for unusual events [24]. Advanced computational approaches, including chemical language methods, show promise in predicting PFAS toxicity and distribution [13]. Quantum chemistry techniques contribute to understanding PFAS behavior at the molecular level, providing insights into degradation pathways [14]. Future research should focus on optimizing materials for simultaneous detection and removal of PFAS contaminants [26].

5.4 Innovative Monitoring Approaches

Innovative technologies have significantly advanced PFAS monitoring. EventDetectR, an open-source R package, detects events in water quality data, providing timely alerts [24]. Novel sensor technologies, such as an optical microresonator sensor, have demonstrated successful PFAS detection in water, achieving low detection limits [26]. These approaches highlight the importance of integrating advanced technologies into PFAS monitoring frameworks. Combining software tools with sensor technologies enhances detection accuracy and efficiency, contributing to effective environmental management. Prioritizing scalable and cost-effective monitoring solutions is critical to address challenges such as identifying unknown hotspots and managing PFAS-containing waste [8, 9].

5.5 Future Directions in PFAS Monitoring and Prediction

Benchmark	Size	Domain	Task Format	Metric
NTP-APPJ[11]	1,000	Water Treatment	Degradation Measurement	Removal Efficiency

Table 1: Summary of key benchmark datasets for water treatment applications, highlighting the size, domain, task format, and metric used for evaluating performance. This table specifically focuses on the NTP-APPJ dataset, which is utilized for assessing removal efficiency in plasma-based water treatment processes targeting PFAS degradation.

Future research in PFAS monitoring should prioritize comprehensive sampling, especially in industrialized regions, to facilitate accurate assessments of PFAS distribution [9]. Investigating factors influencing PFAS retention and migration is critical for developing effective management strategies. Advancements in event detection algorithms should be pursued to improve accuracy in differentiating false alarms from contamination events [24]. The development of innovative sensor technologies will play a pivotal role in advancing PFAS monitoring and prediction. Addressing critical research needs, such as understanding global PFAS production and evaluating health impacts, will enhance knowledge and management of PFAS contamination. Table 1 presents a representative benchmark dataset utilized in the domain of water treatment, providing insights into the task format and metric employed for evaluating PFAS degradation efficiency. Collaborative efforts among scientists, regulatory bodies, and industries are essential for filling data gaps and implementing regulatory measures [8, 9].

6 Analytical Techniques for PFAS Detection

Category	Feature	Method
Novel Separation and Detection Methods	Graph-Based Models	GCN[1]
	Material-Based Innovations	MS[23]
Biosensing Platforms	RNA-Based Detection	ROSALIND[5]

Table 2: This table provides a summary of novel methods and platforms for the separation and detection of per- and polyfluoroalkyl substances (PFAS). It categorizes the methods into novel separation and detection techniques and biosensing platforms, highlighting specific features and associated methods such as Graph-Based Models and RNA-Based Detection.

The detection and analysis of per- and polyfluoroalkyl substances (PFAS) are crucial due to their pervasive environmental presence and associated health risks. Researchers have developed various analytical techniques, each addressing specific challenges in PFAS detection. Advanced mass spectrometry, particularly liquid chromatography-mass spectrometry (LC-MS), is the gold standard for quantifying a broad range of PFAS across diverse matrices [6]. However, traditional methods often entail complexity and high costs, prompting the exploration of more efficient approaches [26]. Table 2 presents a comprehensive overview of innovative methods and platforms developed for the efficient separation and detection of PFAS, underscoring their significance in advancing analytical techniques for environmental monitoring. Additionally, Table 4 offers a detailed comparison of these methods, emphasizing their significance in advancing analytical techniques for environmental monitoring.

Recent advancements in mass spectrometry focus on enhancing detection capabilities while reducing operational costs. Innovations such as nanoparticle sensors and smartphone applications offer promising solutions for on-site PFAS detection, enabling rapid and cost-effective analysis without extensive

9

laboratory infrastructure [6]. These developments complement existing LC-MS methodologies, facilitating real-time PFAS monitoring.

Ongoing research aims to refine mass spectrometry methods and explore innovative approaches like nanoparticle-based sensors and smartphone applications. These efforts are crucial for effectively monitoring persistent contaminants that pose significant risks to environmental quality and human health [6, 7, 4]. By leveraging advanced mass spectrometry and integrating novel detection technologies, researchers aim to establish comprehensive frameworks for effective PFAS monitoring and management.

6.1 Advanced Mass Spectrometry Techniques

Advanced mass spectrometry techniques are pivotal for PFAS detection, offering exceptional sensitivity and specificity. LC-MS is widely recognized for accurately quantifying a wide range of PFAS compounds across various environmental matrices [6]. However, the complexity and costs of traditional methods have led to the exploration of more efficient detection strategies [26].

Recent innovations focus on enhancing detection capabilities while reducing costs. The integration of nanoparticle sensors and smartphone applications offers promising avenues for on-site PFAS detection, facilitating rapid and cost-effective analyses without extensive laboratory infrastructure [6]. These developments aim to augment existing LC-MS methodologies by providing accessible solutions for real-time PFAS monitoring.

Research continues to address the limitations of traditional analytical techniques, particularly in detecting PFAS across various environmental matrices. By refining mass spectrometry methods and exploring innovative approaches, scientists aim to enhance sensitivity and selectivity in PFAS analysis, which is vital for monitoring these persistent contaminants that pose significant environmental and health risks [6, 7, 4]. Leveraging advanced mass spectrometry and integrating novel detection technologies will enable the development of comprehensive frameworks for effective PFAS management.

6.2 Innovative Sensor Technologies

Innovative sensor technologies have emerged as essential tools in detecting and managing PFAS contamination, addressing the limitations of traditional analytical methods. Recent advancements have prioritized the development of highly sensitive detection systems for real-time monitoring of PFAS across various environmental media, utilizing methods such as nanoparticle-based sensors and smartphone applications. These systems respond to the critical need for effective detection of persistent contaminants, which pose significant risks to human health and ecosystems [26, 6].

One notable advancement is the optical microresonator sensor, which utilizes the unique optical properties of microresonators to achieve high sensitivity and specificity in PFAS detection, capable of identifying PFAS at concentrations as low as 1 part per billion (ppb) for perfluorobutanesulfonic acid (PFBS) and 10 ppb for perfluorooctanoic acid (PFOA) [26]. Integrating these sensors into water monitoring systems enhances detection capabilities and provides timely alerts for contamination events, contributing to effective environmental management.

Additionally, the development of metamaterials with super-hydrophobic properties has opened new avenues for PFAS separation and detection. These materials rapidly absorb organic compounds while repelling water, offering a novel approach to PFAS separation that contrasts with traditional methods [23]. This innovation improves the efficiency of PFAS removal from contaminated water sources and highlights the potential of advanced material science in addressing environmental challenges.

The exploration of sensor technologies continues to evolve, focusing on optimizing performance for real-time detection and analysis. Integrating these innovative technologies into existing monitoring frameworks can enhance the accuracy and efficiency of PFAS detection, ultimately contributing to effective environmental management and public health protection. Prioritizing scalable and cost-effective solutions that address the persistent challenges posed by PFAS contamination requires a collaborative effort among scientific, regulatory, and industry stakeholders [8, 6, 9].

10

Method Name	Methodological Innovations	Technological Integration	Environmental Applications
MS[23]	New Analytical Techniques	Metamaterials And Optical	Environmental Remediation Efforts
GCN[1]	Gcn Framework Integration	-	-

Table 3: Comparison of methodological innovations, technological integration, and environmental applications of novel PFAS separation and detection methods. The table highlights the use of metamaterials and optical sensors in environmental remediation and the integration of advanced computational models for predicting PFAS interactions.

6.3 Novel Separation and Detection Methods

Recent advancements in the separation and detection of PFAS have focused on developing innovative analytical methodologies that significantly improve efficiency and accuracy across various matrices. These methodologies address the critical need for precise detection of trace amounts of PFAS, a class of chemicals known for their environmental persistence. Techniques such as the total oxidizable precursor assay (TOPA) and total organic fluorine (TOF) analysis enhance our understanding of PFAS contamination and its implications for human health and environmental safety [18, 6]. While traditional separation techniques like liquid chromatography are effective, they often require sophisticated equipment and are limited by complexity. Emerging methods aim to simplify detection processes and reduce reliance on extensive laboratory infrastructure. Table 3 presents a detailed comparison of recent methodological advancements and technological integrations in PFAS separation and detection, underscoring their applications in environmental remediation efforts.

One promising approach utilizes metamaterials with super-hydrophobic properties, facilitating rapid absorption of PFAS from aqueous solutions while repelling water. This innovative separation technique capitalizes on the unique capillary effects of metamaterials, providing a more efficient means of isolating PFAS from environmental samples [23]. The ability of these materials to selectively absorb organic compounds underscores their potential in improving PFAS remediation processes.

In addition, the integration of optical microresonator sensors has been explored as a novel detection method. These sensors leverage the optical properties of microresonators to achieve high sensitivity and specificity, enabling the detection of PFAS at low concentrations in environmental samples [26]. Deploying such sensors in water monitoring systems significantly enhances detection capabilities, providing real-time data crucial for effective environmental management.

Furthermore, advanced computational models, such as the Graph Convolutional Network (GCN), facilitate the prediction of PFAS interactions with biological molecules, offering insights into their binding mechanisms and potential environmental impacts [1]. These models complement experimental techniques by providing a deeper understanding of the molecular dynamics involved in PFAS separation and detection.

As research in PFAS continues to advance, prioritizing the optimization of innovative analytical methods for enhanced scalability and cost-effectiveness is essential. This focus will facilitate their integration into comprehensive environmental monitoring frameworks, addressing the urgent need for effective detection and management of these persistent contaminants across diverse environmental matrices [6, 22, 19]. By advancing PFAS separation and detection, these innovative approaches contribute to a more comprehensive understanding of their distribution and impact, ultimately informing more effective regulatory and remediation strategies.

6.4 Biosensing Platforms

The development of biosensing platforms has emerged as a promising approach for detecting PFAS, offering a rapid and efficient means of monitoring these persistent environmental pollutants. Biosensing technologies utilize biological recognition elements, such as enzymes and nucleic acids, to achieve highly sensitive detection of PFAS in various environmental matrices. Recent advancements include the development of nanoparticle-based sensors and innovative cell-free systems like ROSALIND, which leverage RNA output sensors to detect a range of water contaminants, including PFAS [6, 5].

The ROSALIND platform, a cell-free biosensing technology, utilizes RNA output sensors activated by ligand induction for PFAS detection. This platform streamlines the detection process by circumventing complex protein translation processes, enabling rapid identification of PFAS contaminants in water samples [5]. The efficiency and simplicity of the ROSALIND platform make it valuable for real-time

11

PFAS monitoring, particularly in resource-limited settings where traditional analytical methods may be impractical.

Biosensing platforms present significant opportunities for enhancing PFAS detection by enabling integration with advanced detection technologies, including optical and electrochemical sensors. This integration can improve sensitivity and specificity, which is crucial given the environmental persistence of these contaminants. Recent advancements in methodologies, such as nanoparticle-based sensors and smartphone applications, support the development of more effective monitoring systems for PFAS, addressing urgent environmental and health concerns [26, 6]. Combining the unique capabilities of biosensors with advanced signal transduction mechanisms can lead to hybrid systems that provide comprehensive monitoring solutions for PFAS contamination.

Ongoing research and development of biosensing platforms aim to address the limitations of current detection methods, such as high costs and the need for specialized equipment. By optimizing performance and scalability, biosensing platforms can significantly enhance the accessibility and effectiveness of PFAS monitoring efforts. Prioritizing the enhancement of robustness and versatility in biosensing technologies will facilitate their deployment in critical areas, particularly in environmental monitoring and safeguarding public health through rapid and reliable detection of water contaminants. Improving these platforms ensures their widespread adoption and utility in addressing pressing global challenges related to environmental quality and health protection [5, 27, 6, 4].

6.5 Data-Driven Detection Approaches

Data-driven detection approaches have become increasingly important for enhancing the detection of PFAS, particularly given the complexity and diversity of these compounds. Future research should focus on developing methodologies capable of analyzing a broader spectrum of PFAS, including short-chain variants and precursors, to address current detection limitations [6]. These advancements are crucial for improving the comprehensiveness of PFAS monitoring and ensuring effective identification and management of emerging contaminants.

One promising innovation is the utilization of whispering gallery mode (WGM) microresonators for optical PFAS detection in aqueous solutions, providing enhanced sensitivity and real-time monitoring capabilities essential for assessing PFAS contamination [26]. Integrating WGM microresonators with data-driven analytical frameworks significantly improves detection limits and specificity, offering a robust approach to environmental surveillance.

Moreover, sophisticated computational models and machine learning algorithms can enhance data-driven detection strategies. For instance, the MULTIMODAL-MOLFORMER combines chemical language representation with physicochemical features for improved molecular property prediction, while the EventDetectR system employs multiple algorithms to identify unexpected water quality events by modeling relationships among multivariate signals [13, 24]. These advanced methodologies improve predictive accuracy and facilitate the identification of critical features, advancing detection systems' effectiveness in complex scenarios. By leveraging large datasets and sophisticated analytical techniques, researchers can develop predictive models that identify patterns in PFAS distribution, informing targeted remediation efforts and regulatory actions.

As the field of PFAS research progresses, enhancing data-driven detection methodologies for scalability, accuracy, and accessibility is essential. This emphasis is vital for effectively identifying PFAS in diverse environmental matrices and addressing critical gaps in understanding their prevalence and impact. Recent developments in analytical techniques, including advanced instrumentation and innovative sensor technologies, underscore the need for comprehensive approaches that facilitate widespread monitoring of these persistent contaminants [6, 1, 9]. Addressing these challenges will improve overall effectiveness in PFAS monitoring efforts and contribute to ecosystem and public health protection.

7 Environmental Remediation Strategies

Addressing the challenges of environmental contamination, particularly from per- and polyfluoroalkyl substances (PFAS), necessitates a comprehensive exploration of diverse remediation strategies. These strategies aim to reduce the presence of these persistent pollutants and enhance treatment methodologies. This section examines current remediation technologies, their operational mechanisms,

Feature	Advanced Mass Spectrometry Techniques	Innovative Sensor Technologies	Novel Separation and Detection Methods
Detection Sensitivity	Exceptional Sensitivity	High Sensitivity	Low Concentration Detection
Technological Integration	Nanoparticle Sensors	Optical Microresonators	Metamaterials
Cost Efficiency	High Operational Costs	Cost-effective	Reduces Lab Reliance

Table 4: This table provides a comparative analysis of three cutting-edge methodologies for PFAS detection: Advanced Mass Spectrometry Techniques, Innovative Sensor Technologies, and Novel Separation and Detection Methods. It highlights key features such as detection sensitivity, technological integration, and cost efficiency, showcasing the strengths and limitations of each approach in advancing environmental monitoring and analysis.

effectiveness, and limitations in PFAS removal, providing a foundation for evaluating their applicability in real-world scenarios and informing future innovations.

7.1 Current Remediation Technologies

Remediation of PFAS-contaminated environments is challenging due to the chemical stability and persistence of these compounds. Current technologies include activated carbon, anion exchange resins, and high-pressure membranes, each with unique advantages and limitations. Anion exchange resins and high-pressure membranes often demonstrate superior removal efficiencies for specific PFAS compared to activated carbon [3]. However, the effectiveness of these methods varies based on the PFAS compounds targeted, particularly newer compounds like ADONA and GenX, for which non-thermal plasma technology has shown promise [11].

Electrochemical degradation techniques, such as those utilizing boron-doped reduced graphene oxide (BRGO) anodes, have been explored, achieving removal efficiencies of 16.7

Modified nanoclays have been investigated for their biocompatibility and effectiveness in PFAS remediation, yet concerns regarding environmental compatibility and potential toxicity necessitate careful consideration [27]. Additionally, the low adsorption capacity of short-chain PFAS compared to long-chain PFAS presents challenges for adsorption-based technologies, highlighting the need for improved adsorbents and regeneration methods [15].

Emerging technologies, such as metamaterials for separation processes, offer innovative solutions for PFAS remediation. Characterized by super-hydrophobic properties and low energy consumption, these materials facilitate efficient separation without extensive infrastructure [23]. Nonetheless, gaps in understanding the overall effectiveness and scalability of these technologies underscore the need for ongoing research and collaboration among stakeholders [8].

7.2 Innovative Approaches and Emerging Technologies

Significant advancements in PFAS remediation have emerged through innovative technologies, including advanced analytical methods for detecting PFAS in environmental matrices, nanoparticle-based sensors, and smartphone applications for real-time monitoring [6]. These innovations aim to enhance the effectiveness of PFAS removal from contaminated environments.

Electrochemical degradation using BRGO anodes has demonstrated scalability and adaptability across various PFAS-contaminated waters, showcasing its versatility in remediation efforts [20]. Additionally, the development of biocompatible nanoclays focuses on synthesis, toxicity assessment, and application, although further research is essential to understand their long-term impacts [27].

Metamaterials have emerged as groundbreaking solutions for PFAS separation, enabling efficient organic compound separation from water while minimizing energy consumption [23]. Future research should enhance the scalability and durability of these materials in practical applications.

Advanced computational techniques, such as the QPFAS workflow, offer potential for refining PFAS degradation pathways through improved error mitigation strategies [21]. These advancements can inform the development of more effective remediation technologies by elucidating molecular interactions and transformation processes of PFAS.

The exploration of innovative technologies is crucial for advancing PFAS remediation efforts. Future research should prioritize standardized detection methods, understanding long-term health impacts of PFAS exposure, and exploring novel treatment solutions to mitigate contamination [18]. Leveraging

13

these technologies can enhance environmental management and inform more effective remediation strategies [6].

7.3 Regulatory and Policy Considerations

The regulatory landscape surrounding PFAS is complex and evolving, significantly impacting remediation efforts. A primary challenge is the toxic effects associated with conventional surfactants used in modifying nanoclays for PFAS remediation. The limited research on the biocompatibility of these materials complicates their regulatory approval and implementation in environmental applications [27]. Establishing clear guidelines and standards for their safe use is essential.

Furthermore, the study by Johnson et al. highlights the need for regulatory updates regarding biosolids application, as it characterizes PFAS across multiple soil depths and groundwater [2]. Policymakers must consider the long-term environmental impacts of biosolids to protect soil and water quality.

Determining financial responsibility for PFAS contamination is another critical regulatory aspect. Allocating costs associated with remediation is vital for accountability and securing necessary funding [17]. Policymakers must navigate the complexities of liability and funding mechanisms to support comprehensive remediation strategies.

The regulatory framework for PFAS remediation must address the urgent challenges of widespread contamination and potential health impacts while adapting to emerging technologies. Collaboration among scientists, regulatory bodies, and industry stakeholders is essential to address knowledge gaps, such as identifying PFAS hotspots and managing PFAS waste. This collaborative effort is crucial for developing effective and adaptable regulatory measures in response to the evolving landscape of PFAS research and remediation technologies [8, 18, 9, 17].

7.4 Future Directions and Research Needs

Future research in PFAS remediation should prioritize key areas to address the ongoing challenges posed by these substances. Enhancing microbiome technologies to improve composting efficiency and develop targeted inoculants, alongside exploring socio-cultural factors influencing composting adoption, could yield novel insights into microbial communities' bioremediation potential [7].

Longitudinal studies are essential for assessing health impacts of PFAS exposure over time, aiming to develop effective regulatory measures and clarify the relationship between PFAS exposure and cancer risk through robust cohort designs [8, 18, 17, 4]. This research is vital for shaping public health policies and regulatory frameworks.

Developing environmentally friendly surfactants and improving nanoclay biocompatibility are critical for advancing remediation technologies. Future studies should assess the long-term ecological effects of these materials to ensure safe application [27]. Standardized methodologies for monitoring PFAS, coupled with enhanced data collection and modeling, will be necessary to predict risks associated with chemical contamination [22].

Advancements in treatment technologies for short-chain PFAS, understanding co-adsorption dynamics, and optimizing regeneration processes remain vital research areas. Investigating advanced adsorbents and the role of organic matter in adsorption processes is crucial for improving remediation strategies aimed at addressing the pervasive environmental contamination caused by PFAS [15, 17, 23, 9, 4].

The application of the Graph Convolutional Network (GCN) method to predict PFAS toxicity and integrating iFCI with other computational tools for predicting reaction pathways are promising avenues for future research. Enhancing model robustness against outliers and exploring additional features will be essential for ongoing innovation in PFAS remediation strategies [13]. Addressing these research needs will significantly advance the understanding and management of PFAS contamination, contributing to more effective environmental protection and public health outcomes.

8   Conclusion

The pervasive nature of per- and polyfluoroalkyl substances (PFAS) presents multifaceted challenges, primarily due to their persistent environmental presence, diverse migration pathways, and complex

transformation mechanisms. These substances are increasingly recognized for their potential neuro-toxic effects, which include disrupting calcium homeostasis and neurotransmitter functions, thereby necessitating a more profound investigation into their health implications. The demand for advanced analytical techniques and comprehensive studies is critical to accurately evaluate PFAS exposure, informing risk assessments and regulatory frameworks.

Exploration of PFAS remediation strategies reveals the absence of a universally applicable solution, largely due to regional regulatory differences, thus advocating for a multi-faceted approach to effective management. The current regulatory structures are insufficient to address the intricacies of PFAS contamination, highlighting the pressing need for reform. It is imperative that scientific, regulatory, and industrial entities collaborate to enhance data transparency and propel regulatory advancements, which are crucial for the development of effective remediation technologies.

Future research should focus on advancing innovative analytical methods, refining sensor technolo-gies, and creating scalable, sustainable remediation approaches. Continued efforts in research and innovation are vital to addressing the PFAS challenge, with an emphasis on interdisciplinary collab-oration to close knowledge gaps and guide policy-making. As scientific understanding progresses, integrating state-of-the-art technologies and comprehensive monitoring systems will be essential in mitigating the environmental and health impacts of PFAS, ultimately safeguarding ecosystems and public health.

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