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# AI-Driven PFAS Monitoring for Sustainable Water Quality Management

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**Abstract**

Per- and polyfluoroalkyl substances (PFAS), which are extremely persistent in the environment and bioaccumulate in humans and animals, have become a serious threat to the environment and human health. Traditional analytical and biochemical techniques, such as chromatographic and mass spectrometric methods, are characterized by high accuracy but are associated with high costs and low feasibility for continuous real-time monitoring. Recent advances in artificial intelligence (AI), machine learning (ML), internet of things (IoT) technologies, smart and biosensors enable novel approaches for the rapid and economic detection of PFAS and assessment of water quality. The current review focuses on recent advances in AI-assisted PFAS detection and monitoring through the use of intelligent sensors, IoT-based water monitoring systems, optical and electrochemical biosensors, and machine learning algorithms. The potential of the discussed approaches for the prediction of PFAS sources and contamination fates, as well as the implementation of smart water management systems for sustainable development, are evaluated. Particular attention is paid to the critical challenges associated with the creation of novel PFAS monitoring concepts, including the availability of high-quality data sets, sensor validation and calibration, issues of cybersecurity and data privacy, and the feasibility of implementing AI-driven approaches in practice. The research directions related to explainable AI, edge intelligence, and digital twins, which can be employed for developing autonomous monitoring systems for smart water management, are highlighted. Overall, the present review aims to provide an insight into the intelligent technologies that support the needs of PFAS recognition, monitoring, and management and promote sustainable development.

**Keywords:** Per- and Polyfluoroalkyl Substances; Artificial Intelligence; Machine Learning; Internet of Things; Water Quality Monitoring.

## 1. Introduction

Per- and polyfluoroalkyl substances (PFAS), also known as forever chemicals, have become one of the most dangerous environmental threats due to their outstanding stability, resistance, and versatility. PFAS have been used in various products such as firefighting foams, non-stick cookware, waterproof clothing, food packaging, cosmetics, and semiconductor devices since the 1940s. Their unique carbon–fluorine bonds make PFAS resistant to degradation processes, threatening surface water, groundwater, soils, and biota. In addition, chronic exposure to PFAS may lead to immune deficiencies, hormone abnormalities, developmental defects, liver damage, and cancer. Therefore, PFAS monitoring and management are becoming an urgent and important challenge that requires an effective and reliable solution. Advanced analytical methods, such as liquid chromatography–mass spectrometry, allow for reliable and sensitive detection of PFAS in the environment. However, their use in practice is limited by high costs, required equipment, and professional skills. Thus, there is a growing need to develop and apply innovative monitoring technologies and systems that can be used in practice to provide consistent and reliable water surveillance data.

Today, a wide range of emerging and transformative technologies, including artificial intelligence (AI), machine learning (ML), the Internet of Things (IoT), smart sensors, and biosensors, enable new ways of environmental monitoring and management. AI technologies allow detecting contamination patterns, estimating pollution levels, predicting pollution spread, and supporting decision-making based on data acquired from the IoT infrastructure. At the same time, biosensors, including optical and electrochemical sensors, offer new opportunities to ensure timely and affordable PFAS monitoring through rapid on-site toxicity detection and preliminary screening. Overall, AI, IoT, and smart sensors can help create an innovative water quality monitoring system for sustainable PFAS management. At the same time, there is a need for further research to consider such factors as reliability, scalability, and cost-effectiveness.

Various studies reported substantial progress in PFAS monitoring using AI technologies. Recent research studies described and analyzed emerging solutions and evaluated their performance to identify the advantages and disadvantages of different technologies and approaches. However, the majority of studies focus on particular aspects of the problem, such as ML-based analysis or sensor development, while multiple factors, including smart sensors, AI-driven monitoring, decision support systems, and management solutions, should be considered together. Therefore, it is important to review and systemize the existing knowledge on the topic to obtain a deeper understanding of the current possibilities and limitations of AI technologies and solutions in PFAS monitoring and create a reliable water safety management infrastructure.

This article will present a comprehensive overview and discussion of recent advances in AI-driven PFAS monitoring for sustainable water quality management. The review will focus on emerging intelligent sensing technologies and solutions, including IoT-based environmental monitoring systems, ML-based approaches, and advanced biosensors for PFAS detection and assessment. Moreover, the article will discuss existing challenges and research gaps and explore innovative opportunities for improving water safety management and sustainable PFAS monitoring using AI, IoT, and smart sensors.

## 2. Literature Review

### 2.1. Conventional PFAS Detection Methods

Per- and polyfluoroalkyl substances (PFAS) are typically detected using laboratory-based analytical techniques like liquid chromatography–mass spectrometry (LC–MS/MS) and gas chromatography–mass spectrometry (GC–MS). These methods are known for their sensitivity, selectivity, and accuracy in identifying and quantifying PFAS, but they come with limitations such as high costs and the need for specialized equipment and expertise [4]. There is a growing interest in alternative methods that can be used to supplement traditional approaches for more efficient PFAS monitoring.

### 2.2. Artificial Intelligence and Machine Learning for PFAS Monitoring

Artificial Intelligence (AI) and Machine Learning (ML) have been implemented to analyze and predict environmental data sets. Supervised machine learning techniques, including deep learning algorithms, have been explored for PFAS prediction and pollution source identification to improve environmental decision-making processes. Overall, AI has proven to be a valuable tool in accelerating data analysis; however, there is a risk of reduced accuracy due to the complexity of the algorithms, requiring careful consideration of model interpretation and validation.

### 2.3. IoT-Based Smart Water Monitoring

The Internet of Things (IoT) has played a critical role in advancing environmental monitoring capabilities by enabling interconnected sensors that facilitate the continuous collection and transmission of data to cloud-based systems for advanced data analytics. IoT-based water quality monitoring systems offer tremendous potential in detecting and analyzing contamination sources with automated alerts. Nonetheless, there are several challenges associated with the technology, including issues with calibration, connectivity, energy consumption, and security.

### 2.4. Biosensors and Intelligent Sensing Technologies

Biosensors represent a promising alternative to conventional analytical techniques such as LC–MS/MS and GC–MS for detecting PFAS contamination in the environment. These sensors utilize electrochemical or optical mechanisms to identify target molecules with good accuracy and relatively short response times. Although biosensors have been recognized for their potential in PFAS monitoring, most of the current research is still in pre-validation stages and needs to be tested in practical applications before deployment .

### 2.5. Research Gap

The reviewed articles have made significant contributions towards understanding PFAS monitoring and detection. However, the overall body of work lacks a comprehensive study that brings together AI-based approaches, IoT, machine learning, biosensors, edge intelligence, and digital twins to create a robust PFAS monitoring framework. Additionally, there is a need for more research on addressing the issues mentioned in this paper, including issues with the standardization of data sets, model interpretation, and security in developing a PFAS monitoring framework.

## 3. Methodology

This study adopts a systematic literature review methodology to examine recent advances in Artificial Intelligence (AI)-driven PFAS monitoring for sustainable water quality management. The review aims to identify, evaluate, and synthesize published research on intelligent sensing technologies, machine learning models, Internet of Things (IoT)-based monitoring systems, biosensors, and data-driven decision-support frameworks for PFAS detection.

Relevant articles were collected from well-established scientific databases, including Scopus, Web of Science, IEEE Xplore, ScienceDirect, and Google Scholar. The search focused on peer-reviewed journal articles published between 2020 and 2026 using keywords such as PFAS, Artificial Intelligence, Machine Learning, Internet of Things, Smart Sensors, Biosensors, and Water Quality Monitoring. Duplicate records, non-English publications, conference abstracts, and studies unrelated to PFAS monitoring were excluded.

The selected articles were analyzed based on several criteria, including the monitoring technology used, detection approach, AI or ML techniques, sensor type, application domain, reported advantages, limitations, and future research directions. The findings from different studies were compared and organized into thematic categories to identify current trends, research gaps, and emerging opportunities in intelligent PFAS monitoring.

**Table I. Summary of the Literature Review Methodology**

| Parameter | Description |
|---|---|
| Review Type | Systematic Literature Review |
| Database | Scopus, Web of Science, IEEE Xplore, ScienceDirect, Google Scholar |
| Publication Period | 2020–2026 |
| Language | English |
| Document Type | Peer-reviewed journal articles and review papers |
| Research Focus | AI, ML, IoT, Biosensors, PFAS Monitoring, Water Quality |

## 4. Results

The literature review indicates that using Artificial Intelligence (AI), Machine Learning (ML), the Internet of Things (IoT), and smart sensing contributes to more effective PFAS monitoring than traditional laboratory analyses. AI allows for faster data processing, thus enabling quicker assessments and decisions in relation to pollution foci. IoT enables the creation of monitoring systems that allow for real-time information gathering. Smart biosensors enable faster, more transportable, and therefore more effective ways of detecting contaminants. Thus, although traditional analytical methods are more accurate, innovative smart technologies offer more opportunities for cost-effective and large-scale water monitoring

**Table II. Comparison of PFAS Monitoring Technologies**

| Technology | Advantages | Limitations | Typical Application |
|---|---|---|---|
| LC–MS/MS | High sensitivity and accuracy | Expensive equipment; laboratory-based | PFAS identification and quantification |
| AI/Machine Learning | Rapid data analysis; contamination prediction | Requires high-quality datasets | Pollution prediction and decision support |
| IoT Monitoring | Continuous real-time monitoring | Connectivity and cybersecurity challenges | Smart water quality monitoring |
| Smart Biosensors | Portable; rapid detection | Calibration and validation required | On-site PFAS screening |
| Edge AI | Low latency; reduced cloud dependence | Limited processing capability | Remote environmental monitoring |

The comparison of the reviewed technologies shows that each approach offers unique strengths for PFAS monitoring. Conventional laboratory methods provide superior analytical accuracy, whereas AI- and IoT-based systems improve monitoring efficiency through automation and real-time data analysis. Smart biosensors enable rapid field detection, while Edge AI enhances remote monitoring by reducing processing delays. These findings suggest that combining conventional analytical techniques with intelligent monitoring technologies can provide a more efficient and sustainable framework for water quality management.

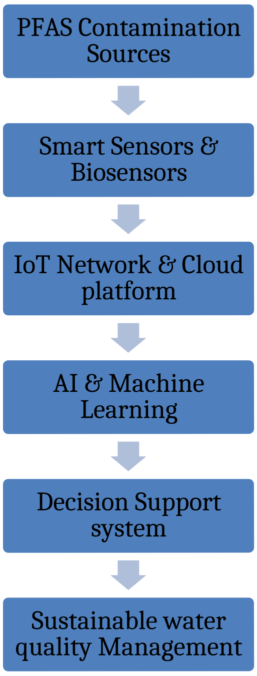


*Figure 1.Framework for AI-driven PFAS Monitoring and Sustainable Water Quality Management.*

## 5. Discussion

The results of this review demonstrate that applying Artificial Intelligence, Machine Learning, the Internet of Things, and smart sensing technologies can make a significant difference in achieving efficient PFAS monitoring and water quality management. Compared to traditional laboratory testing, such approaches can provide faster results and better support the management decisions. The combination of AI technologies with IoT-based sensor equipment can enable real-time monitoring of water quality and support timely response to possible contamination incidents.

However, most of such models are based on limited data sets, which affects their ability to generalize and work with different sources of information. Moreover, the quality of results strongly depends on the characteristics of the monitoring equipment, and there may be significant differences between trials using various sensors. Other limitations include cybersecurity threats and high costs of implementing such an approach, which decreases the possibility of its rapid adoption.

The reviewed articles confirm that AI, biosensors, IoT, and cloud technologies can be used in combination with conventional methods to achieve faster and more efficient monitoring. Nevertheless, most of the studies analyze the performance of individual models, while the interactions between them are rarely considered. More research is needed to fully incorporate AI-driven approaches into existing systems and benefit from synergistic effects. The current state of research highlights the importance of multidisciplinary studies that consider the perspectives of environmental monitoring, AI, sensor technology, and water management.

Therefore, future studies should focus on addressing the existing limitations and achieving the benefits suggested by the researchers. It is essential to collect comprehensive PFAS data sets to allow such models to be used in different settings. It is also critical to increase the accuracy of biosensors and apply novel approaches, such as edge computing and digital twins, in developing monitoring systems. These improvements will allow creating a sustainable system that continuously monitors the environment in real time and supports managers in making better decisions.

## 6. Conclusion

This review aimed to present recent advances in Artificial Intelligence (AI)-based PFAS monitoring for sustainable water quality management by exploring the use of AI, Machine Learning (ML), Internet of Things (IoT), smart sensors, and biosensing technologies. The reviewed articles demonstrated that such technologies as AI, IoT, and smart sensors may be applied for PFAS detection and monitoring to ensure faster and more efficient response and management decisions compared to traditional laboratory analyses.

Nevertheless, multiple challenges and limitations were identified, including the availability of high-quality data, calibration and standardization of sensors, model interpretability, cybersecurity, and the adoption of AI-based monitoring systems in practice. These barriers should be addressed to ensure that emerging PFAS monitoring technologies meet all requirements and serve as valuable tools for water quality management.

The future of PFAS monitoring and management will be driven by addressing these limitations and barriers. Particular attention should be paid to creating standardized environmental datasets, developing explainable AI, and improving biosensors. Moreover, there is a need for considering such concepts as edge computing, digital twins, and cloud analytics in PFAS monitoring. Finally, multidisciplinary collaboration will be critical to ensure that scientists, engineers, policymakers, and other stakeholders work together to turn recent innovations into reality.

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This research received no external funding.

## Conflict of Interest

The authors declare no conflict of interest.

## Data Availability Statement

No new data were created or analyzed in this study. The findings of this review are based on previously published literature, and all sources cited are included in the References section.

## AI Usage Disclosure

Generative AI tools were used only for minor language editing and improving clarity. All ideas, analysis, and conclusions are the authors' own.

## Author Contributions

Conceptualization: Kavya M M and Anakha.P.P.; Methodology: Anagha.V.S. and Niranjana.A.P.; Investigation: Kavya.M.M., Anakha.P.P., and Anagha.V.S.; Formal Analysis: Niranjana.A.P. and Krishna Madhu; Writing—Original Draft Preparation: Kavya.M.M. and Anakha.P.P.; Writing—Review and Editing: Anagha.V.S., Krishna Madhu, and Niranjana.A.P.; Visualization: Anagha.V.S.; Supervision: Kavya.M.M and Krishna Madhu .All authors contributed substantially to this work, participated in the preparation and revision of the manuscript, and have read and agreed to the published version of the manuscript.

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