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Machine Learning–Enhanced PFAS Contaminant Fate and Transport Modeling for Optimized Groundwater Remediation Strategies at Industrial Sites

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Abstract

This study investigates the persistent challenge of accurately modeling per and polyfluoroalkyl substances (PFAS) fate and transport in groundwater at industrial sites, where heterogeneous geology, variable groundwater flow, mixed PFAS chemistries, and uncertain source zones often weaken remediation planning and delay effective intervention. The purpose of the research was to examine whether machine learning enhanced PFAS fate and transport modeling can improve the optimization of groundwater remediation strategies in complex industrial settings. The study adopted a quantitative, cross sectional, case-based design and drew on a purposive sample of 120 professionals from cloud and enterprise style environmental decision contexts, including environmental engineers, hydrogeologists, remediation specialists, consultants, industrial site managers, and regulatory professionals. The key variables were PFAS transport complexity, machine learning modeling capability, machine learning predictive trust, PFAS predictive modeling quality, and optimized groundwater remediation strategies. Data were collected through a structured 5-point Likert scale questionnaire and analyzed using descriptive statistics, Cronbach's alpha, Pearson correlation, and multiple regression in SPSS. Reliability was strong across all constructs, with Cronbach's alpha values ranging from 0.82 to 0.89 and an overall instrument reliability of 0.86. Descriptive findings showed high mean scores for PFAS transport complexity (M = 4.21, SD = 0.61), machine learning modeling capability (M = 4.08, SD = 0.66), predictive trust (M = 3.94, SD = 0.70), predictive modeling quality (M = 4.12, SD = 0.63), and remediation optimization (M = 4.18, SD = 0.59). Correlation analysis revealed that predictive modeling quality had the strongest association with optimized remediation strategies (r = 0.76, p < .01). Regression results showed that the model explained 68.4% of the variance in remediation optimization (R² = 0.684, F = 49.87, p < .001), with predictive modeling quality emerging as the strongest predictor (β = 0.38, p < .001), followed by machine learning capability (β = 0.29, p = .001), PFAS transport complexity (β = 0.24, p = .003), and predictive trust (β = 0.21, p = .006). The study concludes that machine learning enhanced modeling offers a practically significant pathway for improving PFAS remediation decision quality, plume control, treatment prioritization, and cost-efficient groundwater cleanup planning at industrial sites.

Keywords

INTRODUCTION

Per- and polyfluoroalkyl substances (PFAS) are a large class of synthetic organofluorine chemicals characterized by carbon–fluorine bonds with exceptional bond strength, chemical stability, and resistance to thermal and biological degradation. In environmental research, PFAS are commonly defined as amphiphilic compounds containing fluorinated carbon chains attached to functional groups such as carboxylates or sulfonates, properties that explain their surface activity, mobility in aqueous systems, and persistence in soils, sediments, groundwater, and biota (Ambaye et al., 2022). This chemical class gained global policy and scientific prominence because the same structural durability that made PFAS useful in firefighting foams, metal plating, textile treatment, paper coating, polymer processing, semiconductor production, and many other industrial applications also underlies their long-term environmental recalcitrance and broad human exposure potential. International significance arises from the fact that PFAS contamination is not restricted by local hydrogeologic boundaries or national regulatory regimes; once released, many PFAS species can migrate through vadose zones, aquifers, rivers, estuaries, food webs, and water reuse systems, creating transboundary environmental burdens and long-lived remediation liabilities (Brusseau, 2018; Brusseau et al., 2021). The issue is especially acute at industrial sites because these settings frequently involve repeated source loading, mixed PFAS chemistries, legacy operations, precursor compounds, co-contaminants, and engineered or disturbed subsurface conditions that complicate contaminant distribution and cleanup. Early sorption studies established that PFAS behavior differs systematically by chain length and functional group, showing stronger retention for longer-chain compounds and distinct interactions with organic matter and mineral surfaces (Lyu et al., 2022; Sharifan et al., 2021; Sunderland et al., 2019). Later reviews and field investigations expanded this understanding by documenting widespread occurrence in aquatic environments and by linking production, disposal, and use histories to persistent groundwater contamination near industrial and AFFF-associated sites. Within this context, groundwater remediation is not simply a localized engineering task; it is part of a broader international environmental protection agenda that intersects drinking-water security, industrial accountability, public health protection, and sustainable site management. A rigorous introduction to PFAS fate and transport modeling therefore begins with definition, chemistry, and global relevance because those elements frame why industrial-site groundwater contamination remains one of the most technically demanding and societally consequential challenges in contemporary environmental science.

A second foundational issue concerns the environmental behavior of PFAS once they enter subsurface systems. Traditional groundwater contamination research often relies on assumptions developed for chlorinated solvents, hydrocarbons, metals, or nutrients, yet PFAS display a more complex set of partitioning and retention mechanisms because they interact not only with solid phases but also with air–water interfaces, nonaqueous phases, dissolved organic matter, and variable geochemical conditions (Brusseau, Khan, et al., 2019). The literature demonstrates that PFAS fate and transport are governed by advection, dispersion, sorption, interfacial adsorption, retardation, mass transfer limitations, and in some cases precursor transformation, with the relative importance of each process varying by compound class, concentration, porewater chemistry, saturation state, and porous-medium properties. Research on unsaturated and variably saturated systems has been especially important because vadose zones can function as long-term secondary sources that slowly release PFAS mass to groundwater over extended periods, even after original source inputs are reduced or physically removed. Column studies and modeling analyses have shown that adsorption at air–water interfaces can markedly increase retardation, particularly for certain long-chain compounds, and this process cannot be neglected when estimating travel time, leaching potential, and plume persistence (Ellis et al., 2023). Investigations into nonideal transport further indicate that elution tailing, rate-limited desorption, and multiprocess retention can sustain downgradient loading even when dissolved concentrations in source zones appear to decline, thereby complicating remediation endpoint evaluation and risk communication. Reviews focused on groundwater occurrence and transformation reinforce that short-chain substitutes and replacement chemistries often exhibit greater aqueous mobility and can travel farther from industrial release areas, which alters the spatial logic of exposure assessment and plume management. Accordingly, PFAS contamination in groundwater is not adequately described as a simple dissolved-phase problem (Li et al., 2023; Li & MacDonald Gibson,

2022). It is a coupled hydrogeologic and physicochemical problem in which concentration profiles reflect the interplay of source history, subsurface architecture, compound-specific interfacial behavior, and delayed mass transfer. For industrial sites, this complexity enlarges uncertainty in plume delineation, temporal forecasting, and remedy selection, making fate and transport modeling central to any serious remediation strategy (Rafiei & Nejadhashemi, 2023).

Figure 1: Industrial PFAS Contamination Cycle: From Source Generation to Environmental and Biological Accumulation
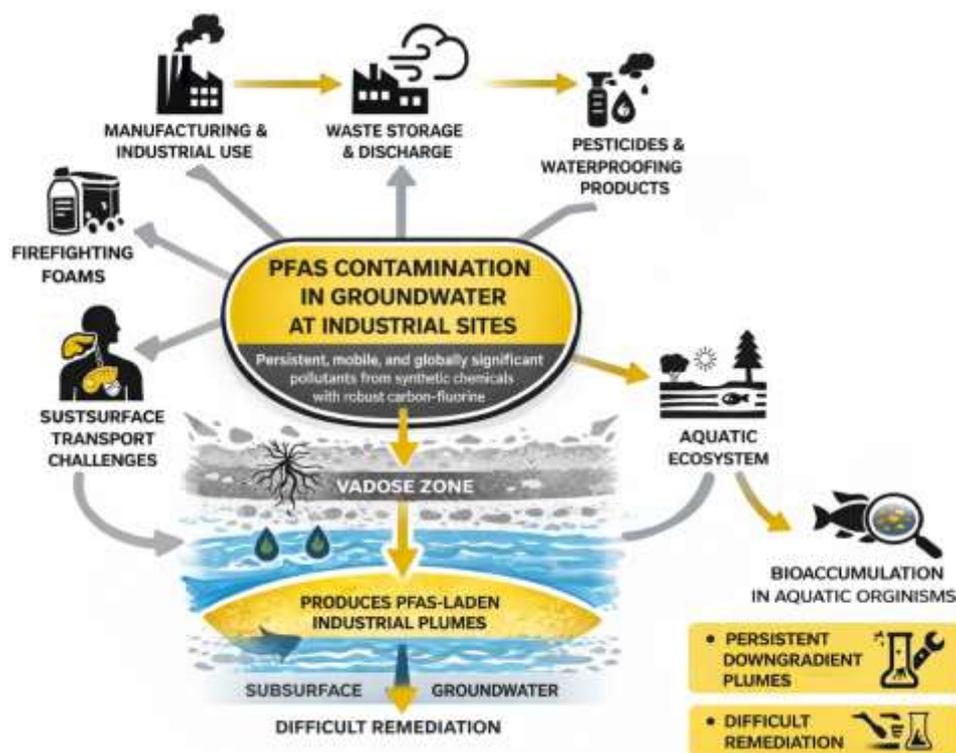
The international significance of PFAS groundwater contamination also becomes clearer when industrial release settings are examined more closely. Industrial sites are not homogeneous sources; they involve manufacturing footprints, disposal units, firefighting infrastructure, wastewater discharges, storage areas, land-applied residuals, and legacy operational zones that may have generated multiple release episodes over long periods (Hisham & Robel, 2022; Siddique & Amin, 2022). Field-based research at AFFF-impacted and industrially influenced locations has shown that source-zone mass can remain distributed across soils, shallow groundwater, deeper groundwater, and precursor reservoirs, producing persistent downgradient plumes that are difficult to characterize using sparse monitoring networks alone. High-resolution investigations have revealed that site-specific fate and transport processes differ markedly from one location to another according to lithologic heterogeneity, infiltration history, hydraulic gradients, co-contaminant presence, and local PFAS composition, all of which affect whether retention, leaching, and plume elongation are dominated by solid-phase interactions, air–water interfacial adsorption, dissolved transport, or mixed controls (Md & Islam, 2022; Mehedi & Md, 2022; Sit et al., 2020). This site specificity matters because remediation design depends on identifying where the major retained mass resides, how rapidly it is released, and whether hydraulic containment, pump-and-treat, sorptive barriers, excavation, monitored attenuation, or hybrid systems can address the dominant transport regime. A field-scale mass-based study of AFFF-associated source areas demonstrated that retained PFAS mass within source zones can be substantial, confirming that dissolved plume concentrations alone may underrepresent the persistence of the contamination problem (Mainuddin & Chandra, 2022; Shahinur & Sultan, 2022). Complementary characterization work across multiple AFFF sites documented that relevant transport processes are not uniform across facilities, reinforcing the need for models capable of integrating local subsurface

conditions with compound-specific behavior. Reviews of groundwater occurrence and remediation similarly emphasize that industrial and commercial PFAS sources continue to shape contamination patterns worldwide and that short-chain and emerging PFAS complicate management because they are often more mobile and less amenable to assumptions developed for PFOS and PFOA (Mostafa & Tohidul, 2022; Oyetade et al., 2018; Khatun & Morshedul, 2022). In this sense, industrial PFAS contamination is both a local hydrogeologic phenomenon and an international environmental management problem. It requires analytical frameworks that can connect heterogeneous source architecture with transport uncertainty, monitoring data, and remedy optimization in a scientifically defensible manner (Islam & Aditya, 2023; Zakia & Nahar, 2022).

A major challenge in this research area lies in the limitations of conventional fate and transport modeling when applied to PFAS-contaminated industrial groundwater systems. Mechanistic groundwater models remain indispensable because they encode governing transport processes, permit scenario testing, and support hydrogeologic interpretation. At the same time, the PFAS literature shows that model reliability is heavily dependent on parameterization of adsorption, interfacial partitioning, retardation, source loading, infiltration, precursor contributions, and uncertainty in subsurface structure (Adamson et al., 2020; Ahrens, 2011; Oyetade et al., 2018). Several studies have shown that advanced mathematical models can represent PFAS-specific processes in the vadose zone and aquifers, including nonlinear and rate-limited adsorption at solid–water and air–water interfaces, surfactant-induced flow effects, and sensitivity to porewater chemistry. Yet the same studies also show that these models can become data intensive, computationally demanding, and sensitive to uncertain field inputs, particularly when applied to long-term leaching or mixed PFAS source conditions (Ahmed & Hasan Or, 2021; Md & Mehedi, 2021). At watershed and regional scales, integrated hydrogeochemical models have improved source identification and management support by linking topography, soil-water retention, and adsorption behavior, but these frameworks still depend on adequate field data and careful calibration to local conditions (Aditya & Chandra, 2022; Anick & Tasnim, 2022). Reviews focused on vadose-zone and groundwater dynamics underline that mechanistic formulations are strongest when physicochemical parameters are well characterized, whereas practical site management often proceeds with incomplete source inventories, uneven monitoring coverage, and mixtures of legacy and replacement compounds. For industrial sites, this means that traditional modeling alone can struggle to capture nonlinear relations among hydrogeologic features, land use, release history, analytical datasets, and remediation performance indicators (Huang et al., 2022; Lau et al., 2007). The modeling problem is therefore not a rejection of physics-based approaches; it is a recognition that PFAS remediation planning takes place under substantial parameter uncertainty, sparse or irregular sampling, and multiscale environmental interactions. Under such conditions, the value of complementary data-driven methods becomes increasingly evident because they can detect hidden structure in complex datasets, supplement mechanistic understanding, and strengthen site-specific prediction where direct parameter measurement is incomplete (Lei et al., 2023; Lyu et al., 2018).

This is the point at which machine learning becomes especially relevant to PFAS contaminant fate and transport research. In environmental systems, machine learning refers to a family of computational methods that learn patterns, dependencies, and predictive relationships from observed data rather than relying solely on explicitly specified physical equations. In groundwater and hydrologic studies more broadly, machine learning has been used for classification, regression, anomaly detection, ensemble prediction, spatiotemporal interpolation, and feature importance analysis, often performing well in contexts where interactions are nonlinear, high dimensional, or partially observed. Reviews of machine learning in groundwater quality modeling describe rapid growth in supervised, unsupervised, semi-supervised, and ensemble methods for predicting water quality parameters and contamination states, emphasizing their value in extracting predictive structure from heterogeneous hydrogeologic and monitoring datasets. Broader reviews of hydrology and water-resources applications similarly show that deep learning and ensemble learning have expanded the analytical capacity available for forecasting and environmental pattern recognition where classical assumptions of linearity or stationarity are weak. Within PFAS research specifically, machine-learned Bayesian networks have already demonstrated strong predictive performance for estimating the occurrence of short-chain PFAS in groundwater by combining monitoring records with explanatory variables linked to source

proximity, hydrogeology, soil properties, and land use (Xu et al., 2021; Kermani et al., 2021). That study is notable not only because of its high predictive accuracy but also because it shows how data-driven models can remain interpretable enough to identify important predictors relevant to environmental decision-making. The significance of this literature for the present study lies in the bridging function of machine learning. It offers a way to complement mechanistic transport understanding with empirical pattern discovery, thereby improving screening, prioritization, and predictive confidence under complex industrial-site conditions. In other words, machine learning enters PFAS groundwater research not as a generic technological addition, but as an analytical response to multidimensional uncertainty, incomplete field characterization, and the practical need to optimize remediation decisions using every available signal embedded in environmental data (Anderson et al., 2016; Brusseau, Yan, et al., 2019).

Another critical dimension of the introduction concerns remediation, because the value of fate and transport modeling is ultimately tied to how well it supports remedy design, implementation, and optimization (Khaled & Mosheur, 2023; Shahab & Aditya, 2023). PFAS remediation in groundwater remains technically demanding because many established treatment technologies are better suited to phase transfer or sequestration than to complete destruction, and because treatment performance varies by compound class, influent chemistry, competing ions, concentration ranges, and operational design (Higgins & Luthy, 2006; Hasan Or et al., 2023; Mehedi & Nahar, 2023; Zeng et al., 2021). Reviews of PFAS removal from contaminated soil and water identify adsorption, ion exchange, membrane separation, electrochemical methods, advanced oxidation and reduction pathways, and emerging hybrid systems as major intervention categories, while also documenting trade-offs in cost, waste generation, selectivity, and field scalability. Groundwater-focused reviews likewise emphasize that short-chain compounds and replacement chemistries complicate remediation because their mobility can reduce capture efficiency and shift performance expectations for activated carbon and related sorbents (Sultan & Anick, 2023; Mostafa, 2023). Recent life-cycle and cost analyses comparing anion exchange and granular activated carbon systems for PFAS-contaminated groundwater show that remedy evaluation increasingly depends on integrated metrics that include environmental footprint, media usage, waste handling, and long-term treatment economics, not only removal efficiency at a single point in time (Ratul & Aditya, 2023; Tasnim & Zaheda, 2023). This places additional pressure on predictive modeling, because design decisions about capture zones, media changeout frequency, barrier placement, source treatment priority, and monitoring intensity are only as good as the site conceptualization and transport forecasts on which they are based. Field and laboratory studies on PFAS retention, interfacial adsorption, and source-zone mass distribution confirm that remediation planning must account for delayed mass release and compound-specific behavior, otherwise operational systems may underperform or produce misleading expectations about cleanup timescales (Haggerty et al., 2023; Iftekhar & Tohidul, 2024; Towhidul & Uddin, 2024). The remediation challenge therefore cannot be separated from the modeling challenge. Groundwater cleanup strategy for PFAS at industrial sites depends on understanding which compounds move fastest, which mass fractions remain retained in source media, how local hydrogeology alters release pathways, and how predictive accuracy influences selection among competing remedial options. A study focused on optimized remediation strategies must therefore situate modeling as a decision-support instrument embedded within technical, environmental, and economic dimensions of site management.

Taken together, the literature establishes a clear intellectual basis for a study on machine learning–enhanced PFAS contaminant fate and transport modeling for optimized groundwater remediation strategies at industrial sites (Guo et al., 2022; Haggerty et al., 2023). PFAS are globally significant industrial contaminants because of their persistence, mobility, and health relevance; their transport in the subsurface is controlled by interacting processes that extend beyond conventional dissolved-phase assumptions; industrial sites generate heterogeneous source architectures and long-lived plume behavior; mechanistic models provide essential scientific structure but face parameter, data, and uncertainty constraints; machine learning offers flexible predictive capacity in complex groundwater settings; and remediation optimization depends on robust, site-specific forecasting rather than generic assumptions (Mushfequr & Aditya, 2024; Sakib, 2024). Existing studies have addressed important pieces of this problem, including sorption and sediment interactions, occurrence and fate in aquatic

systems, source-zone distribution at AFFF-impacted sites, multiprocess transport and retardation in subsurface media, vadose-zone retention and leaching, groundwater occurrence and remediation reviews, machine-learned prediction of short-chain PFAS in groundwater, and broad assessments of machine learning for groundwater quality modeling. What emerges from this body of scholarship is a need for an integrated quantitative perspective that connects PFAS transport complexity, predictive modeling quality, and remediation decision optimization within an industrial-site framework (Guo et al., 2022). Such a perspective is well aligned with a quantitative, cross-sectional, case-study-based design using structured Likert-scale evidence, descriptive statistics, correlation analysis, and regression modeling, because it allows technical knowledge, practitioner judgment, and decision-oriented variables to be examined within a coherent empirical structure. In that context, the present study is positioned within the intersection of contaminant hydrogeology, environmental informatics, and remediation engineering, with emphasis on how machine learning can strengthen the analytical basis for understanding PFAS fate and transport and for selecting groundwater remediation strategies under real industrial conditions (Adamson et al., 2022; Brusseau, 2018).

Background of the Study

The background of this study is rooted in the growing environmental and operational challenge posed by per- and polyfluoroalkyl substances in groundwater systems surrounding industrial sites. PFAS are a large group of synthetic chemicals widely used in industrial manufacturing and commercial processes because of their heat resistance, water repellency, and chemical stability. These same properties have made them persistent contaminants that can remain in subsurface environments for long periods, migrate through soil and aquifer systems, and create serious remediation difficulties once released. Industrial facilities such as chemical plants, metal finishing operations, textile treatment plants, electronics manufacturing sites, and locations with historical firefighting foam usage have become important points of concern because they often generate repeated or long-term PFAS discharge into surrounding land and water systems. Groundwater contamination at such sites is especially problematic because aquifers serve as critical sources of drinking water, industrial process water, and ecological support, meaning that contamination can produce broad environmental, economic, and public health consequences. A major scientific difficulty in managing PFAS contamination lies in understanding how these compounds move, persist, accumulate, and interact within complex subsurface conditions. Their fate and transport behavior is influenced by a wide range of variables, including soil composition, hydraulic conductivity, porosity, groundwater flow direction, chemical structure, chain length, sorption behavior, source history, and site-specific hydrogeologic heterogeneity. As a result, conventional contaminant transport models often struggle to capture the full complexity of PFAS movement across different industrial settings. At the same time, remediation decision-making increasingly requires precise and adaptive modeling tools capable of supporting plume delineation, risk estimation, treatment selection, and long-term management planning. In this context, machine learning has emerged as a promising analytical approach because it can identify hidden relationships in complex environmental data, improve predictive performance under uncertainty, and strengthen decision support in technically challenging contamination scenarios. The present study is therefore grounded in the need to understand whether machine learning–enhanced PFAS fate and transport modeling can provide more reliable and practically useful guidance for optimizing groundwater remediation strategies at industrial sites where contamination behavior is variable, uncertain, and strongly dependent on local site conditions.

Problem Statement

The problem addressed in this study arises from the increasing difficulty of accurately understanding and managing PFAS contamination in groundwater at industrial sites. PFAS contamination is not a simple pollution issue that can be explained by one transport pathway or one remediation method. It is a highly complex environmental management problem shaped by the interaction of contaminant chemistry, subsurface geology, groundwater flow behavior, historical release patterns, and differences in industrial site conditions. In many industrial settings, PFAS are released over long periods through manufacturing activities, waste handling, storage areas, accidental spills, or firefighting foam use, creating contamination plumes that are difficult to detect, predict, and control. The main challenge is that PFAS do not always behave like conventional groundwater contaminants. Their persistence,

mobility, and varying interaction with soil, water, and porous media make their fate and transport behavior uncertain across different sites. As a result, remediation teams often face serious limitations when trying to estimate plume movement, identify high-risk zones, select the most effective treatment strategies, and determine the likely duration and cost of remediation. Conventional contaminant transport models remain useful, but they often struggle to fully capture the nonlinear, site-specific, and multidimensional behavior of PFAS in industrial groundwater systems. These limitations reduce predictive confidence and may lead to delayed responses, inefficient remediation investments, weak prioritization of treatment zones, and uncertainty in long-term cleanup planning. At the same time, machine learning has emerged as a potentially valuable tool for improving environmental prediction because it can process complex datasets, identify hidden relationships among variables, and improve model adaptability under uncertain conditions. Even so, there remains insufficient quantitative evidence showing how machine learning–enhanced PFAS fate and transport modeling can directly support optimized groundwater remediation strategies in industrial environments. A clear research gap therefore exists in linking PFAS transport complexity, machine learning modeling capability, predictive trust, and remediation decision quality within one integrated empirical framework. This study is designed to address that problem by examining whether machine learning–enhanced modeling can improve the analytical basis of groundwater remediation strategy selection and optimization at industrial sites affected by PFAS contamination.

Objective-Based Paragraph

The objective of this study is to examine how machine learning–enhanced PFAS contaminant fate and transport modeling can contribute to more effective and optimized groundwater remediation strategies at industrial sites. The study is designed to move beyond general discussions of PFAS contamination and focus directly on the practical decision-making value of improved predictive modeling in real industrial contexts. More specifically, the first objective is to identify and evaluate the major site-specific factors that influence PFAS fate and transport behavior in groundwater systems, including hydrogeological variability, source-zone characteristics, contaminant complexity, and uncertainty in plume migration. Understanding these factors is essential because remediation planning begins with an accurate interpretation of how contamination behaves under different industrial conditions. The second objective is to assess the role of machine learning in enhancing the quality of PFAS transport prediction by improving the ability to interpret complex environmental relationships and support better site characterization. The study also seeks to determine whether machine learning capability is associated with stronger predictive confidence and more reliable support for remediation decisions. A third objective is to analyze the relationship between predictive modeling quality and the optimization of groundwater remediation outcomes, including treatment prioritization, plume control planning, cost-efficiency, and decision effectiveness. This means the study is not only interested in whether machine learning can improve prediction in a technical sense, but also whether that improved prediction translates into better remediation strategy selection in practice. Another objective is to investigate the level of trust that environmental professionals place in machine learning–based PFAS prediction and how such trust shapes the usability of data-driven models in industrial groundwater management. Overall, the study aims to build an integrated empirical understanding of how PFAS transport complexity, machine learning modeling capability, predictive trust, and remediation optimization relate to one another. By doing so, the research intends to provide a structured basis for evaluating whether machine learning–enhanced modeling can serve as a more practical and effective tool for supporting groundwater remediation planning at industrial sites affected by persistent PFAS contamination.

Research Hypotheses

The research hypotheses of this study are developed from the central assumption that improved understanding and prediction of PFAS contaminant behavior can strengthen groundwater remediation planning at industrial sites. Since the study is quantitative, cross-sectional, and case-study based, the hypotheses are intended to test measurable relationships among the key variables identified in the conceptual structure of the research. The first hypothesis proposes that PFAS transport complexity across industrial site conditions has a significant effect on groundwater remediation strategy optimization. This hypothesis is based on the idea that the more difficult it is to understand

contaminant movement under variable hydrogeological and source-related conditions, the more important accurate modeling becomes for effective remediation planning. The second hypothesis proposes that machine learning modeling capability has a significant positive relationship with PFAS predictive quality. This reflects the view that stronger data-processing ability, better pattern recognition, and greater adaptability to nonlinear environmental conditions can improve the quality of PFAS fate and transport prediction. The third hypothesis states that machine learning predictive trust has a significant positive relationship with remediation decision effectiveness. This hypothesis is important because even when a predictive model is technically strong, its practical value depends on whether professionals are confident enough to use its outputs in site management and treatment planning. The fourth hypothesis proposes that PFAS predictive modeling quality significantly predicts the optimization of groundwater remediation strategies at industrial sites. In this study, remediation optimization includes clearer treatment prioritization, better plume control decisions, stronger confidence in remedial design, and improved efficiency in resource allocation. Together, these hypotheses form a connected structure that allows the study to test whether site complexity influences remediation challenges, whether machine learning strengthens predictive quality, whether predictive trust supports decision effectiveness, and whether modeling quality ultimately contributes to more optimized remediation strategies. These hypotheses therefore provide the statistical foundation for examining the broader argument of the research, which is that machine learning–enhanced PFAS fate and transport modeling can play a meaningful role in improving groundwater remediation performance in complex industrial settings.

Significance of the Research

The significance of this research can be explained through several important contributions to knowledge, practice, and environmental management:

i. Academic significance: This study contributes to the growing body of knowledge on PFAS contamination by connecting contaminant fate and transport modeling with machine learning and remediation strategy optimization in a single research framework. It expands the academic discussion beyond general contamination assessment and places stronger emphasis on predictive decision support within industrial groundwater systems.

ii. Methodological significance: The research offers value by applying a quantitative, cross-sectional, case-study–based design to a topic that is often discussed in highly technical or purely experimental terms. By using descriptive statistics, correlation analysis, regression modeling, and Likert-scale measurement, the study creates a structured empirical basis for examining professional judgment and decision-oriented modeling outcomes.

iii. Practical significance for environmental professionals: The study is significant for hydrogeologists, remediation engineers, environmental consultants, and industrial site managers because it focuses on how improved modeling quality can support better treatment selection, plume control planning, and prioritization of contaminated zones. This makes the study directly relevant to real-world environmental problem solving.

iv. Significance for industrial site management: Industrial facilities facing PFAS contamination often need reliable tools to reduce uncertainty in site characterization and cleanup planning. This research provides insight into whether machine learning–enhanced models can strengthen management confidence and improve the efficiency of remediation decision-making.

v. Significance for policy and regulatory understanding: The findings of this study may be useful for regulators and environmental oversight bodies that require stronger analytical justification for groundwater remediation actions. The study supports a more evidence-based perspective on how predictive tools can inform remediation planning under complex site conditions.

vi. Significance for environmental protection: Groundwater is an essential resource for drinking water, industrial use, and ecosystem stability. Any improvement in the ability to understand and remediate PFAS contamination has wider significance for protecting water quality, reducing contamination risks, and supporting more responsible industrial environmental management.

vii. Interdisciplinary significance: This study strengthens the connection between environmental science, hydrogeology, machine learning, and remediation engineering. It shows how different fields can be integrated to address persistent contamination problems through more adaptive and data-

informed approaches.

LITERATURE REVIEW

The literature review for this study is grounded in the need to understand the scientific, technical, and analytical foundations of PFAS contaminant fate and transport modeling and its relationship to groundwater remediation strategy optimization at industrial sites. PFAS contamination has emerged as a major topic in environmental research because these substances are persistent, mobile, and difficult to remediate once they enter soil and groundwater systems. The complexity of PFAS behavior has led scholars to investigate not only their sources and occurrence but also the processes that govern their movement through subsurface environments, their interaction with geological materials, and the long-term consequences of their presence in industrial and mixed-use settings. At the same time, the literature has shown that remediation planning for PFAS requires more than contamination detection alone; it requires reliable analytical frameworks that can predict plume development, support treatment decisions, and reduce uncertainty in site management. This has made contaminant fate and transport modeling an essential topic in both hydrogeology and remediation engineering. Alongside this, the rapid growth of machine learning in environmental science has introduced new possibilities for interpreting large and complex datasets, identifying nonlinear relationships, and improving predictive performance where traditional models may be limited by uncertainty or data gaps. As a result, the present review must bring together several related bodies of scholarship, including PFAS contamination in groundwater, PFAS fate and transport processes, machine learning applications in environmental contaminant modeling, the theoretical foundation that explains interconnected site and decision systems, and the conceptual structure that links the study variables. The purpose of this literature review is therefore not only to summarize previous studies, but also to establish the intellectual basis for the current research by identifying what is already known, where the main gaps remain, and how this study is positioned within the broader academic conversation. In doing so, the review provides a foundation for understanding why an integrated study of PFAS transport complexity, machine learning modeling capability, predictive trust, and remediation optimization is both relevant and necessary in the context of industrial groundwater contamination.

PFAS Contamination in Groundwater at Industrial Sites

Per- and polyfluoroalkyl substances have become a defining groundwater contamination issue at industrial and fire-training locations because their release histories, chemical diversity, and subsurface persistence combine to produce plumes that are unusually durable and difficult to characterize. The literature shows that groundwater contamination at these sites is rarely limited to one compound or one release mechanism (Sazzadul & Rebeka, 2024; Tasnim & Anick, 2024). Instead, industrial facilities and aqueous film-forming foam use areas often generate mixtures of perfluoroalkyl acids, precursor compounds, and transformation products that enter soil and aquifer systems through repeated operational losses, disposal practices, surface infiltration, and subsurface leaching over long periods. A foundational study demonstrated that the transport potential of perfluoroalkyl acids at AFFF-impacted sites is strongly influenced by carbon-chain length, sediment properties, and co-contaminant conditions, which means that contamination behavior at industrial sites cannot be understood through a single generic assumption about plume migration (Guelfo & Higgins, 2013). Another study strengthened this perspective by showing that precursor compounds remain present in AFFF-impacted groundwater and associated solids, indicating that measured terminal PFAS concentrations may represent only part of the subsurface contamination burden (Houtz et al., 2013). This is important for industrial sites because historical source zones may continue to release additional PFAS mass long after initial site operations have changed or ceased. Another important investigation added a further layer of complexity by documenting that remediation activities themselves can alter the subsurface distribution of PFAS, which means that groundwater contamination at such sites is not static but can be reshaped by engineering interventions, hydraulic disturbances, and site management decisions (McGuire et al., 2014; Md, 2025; Zaheda & Hamidur, 2024). At a broader scale, a global synthesis of groundwater data showed that PFAS concentrations span many orders of magnitude across source types and geographic settings, confirming that industrial and source-zone conditions create highly variable contamination signatures (Johnson et al., 2022). Taken together, these studies establish that PFAS contamination in groundwater at industrial sites is best understood as a heterogeneous, source-

dependent, and chemically evolving problem that requires detailed site characterization and a strong awareness of how historical releases, compound mixtures, and subsurface conditions interact to control plume behavior over time.

Figure 2: Major Pathways and Processes Governing PFAS Contamination at Industrial Sites
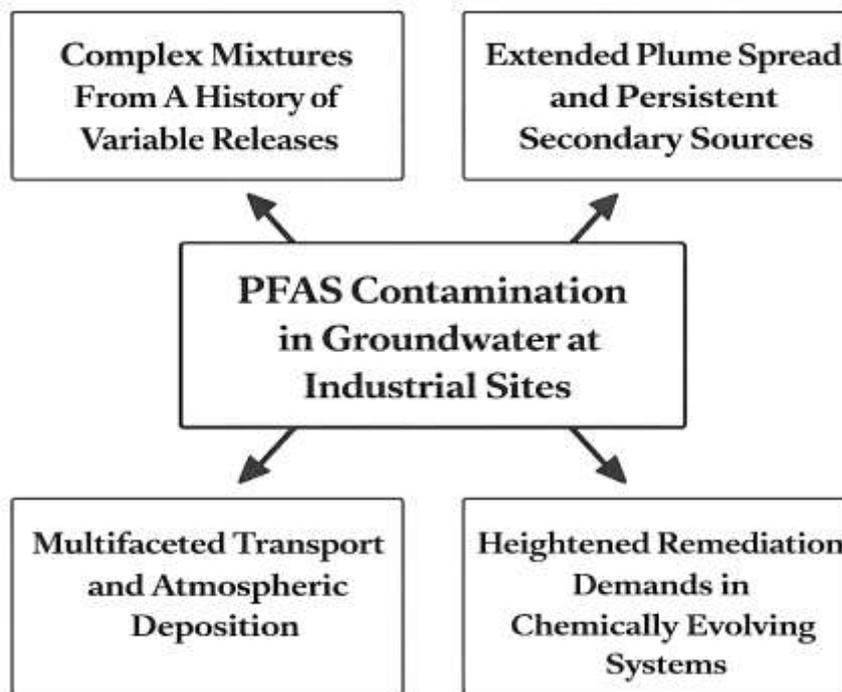
A second major theme in the literature is that industrial PFAS contamination often extends farther and persists longer than traditional site investigation logic would suggest. One reason is that PFAS movement is not governed solely by saturated-zone advection and dispersion. Industrial settings may contain unsaturated soils, buried source materials, low-permeability strata, preferential pathways, and long operational histories that permit gradual mass transfer into groundwater over extended timescales. Field evidence for this point was provided through research documenting deep seepage of PFAS through the soil profile at a firefighter training site and subsequent contamination of groundwater, illustrating how contaminants can migrate vertically through subsurface layers and reach aquifers even when source behavior appears superficially contained (Dauchy et al., 2019; Md Shahab, 2025; Mostafa, 2025). These findings are especially relevant for industrial and mixed-use sites because they show that PFAS source control cannot be separated from vadose-zone understanding. Another study broadened the source discussion by demonstrating that groundwater contamination may also arise from industrial airborne emissions followed by land deposition, with contaminated groundwater detected at locations downwind and topographically elevated relative to the manufacturing source . This finding is highly significant for industrial-site studies because it challenges the narrow assumption that PFAS risks are confined to areas immediately downgradient of known discharge points. In practical terms, the contamination footprint may reflect atmospheric transport, land deposition, and diffuse recharge, not just direct liquid-phase disposal or spills. The global groundwater synthesis similarly reported that PFAS are present even in locations apparently removed from identifiable sources, supporting the view that industrial contamination can be spatially extensive and operationally misleading when site investigations rely on simplified source models(Sazzadul, 2025). Earlier studies also reinforce this interpretation by showing that transport and persistence are shaped by compound-specific mobility and precursor behavior, so contamination at industrial sites may remain active even when monitoring focuses on a narrower subset of analytes. As a result, PFAS groundwater contamination at industrial sites must be framed as a multidimensional occurrence problem involving direct releases, retained precursors, vertical migration, atmospheric deposition, and

long-lived secondary sources rather than a short-term plume problem with a clearly bounded source area (Schroeder et al., 2021).

The literature also makes clear that the seriousness of PFAS contamination at industrial sites lies not only in its occurrence but also in what that occurrence implies for monitoring, risk evaluation, and remediation planning. When contamination consists of mixed PFAS classes, includes hidden precursor reservoirs, and spreads through multiple pathways, groundwater assessment becomes more demanding than standard contaminant mapping. One important study showed that precursor compounds can account for a substantial share of total PFAS burden in AFFF-impacted groundwater and solids, meaning that analytical programs focused only on a small set of terminal compounds may underestimate future mass loading and plume persistence. Another study showed that site interventions can redistribute PFAS in the subsurface, which suggests that remediation design and monitoring must account for the possibility that contaminant patterns observed at one stage of site management may not remain stable after active engineering measures begin. Research on firefighter training areas demonstrated that substantial vertical penetration can occur through soils, highlighting the importance of depth-resolved sampling and the danger of treating shallow observations as representative of the whole site. Another industrial perspective indicated that atmospheric emission and deposition can create contamination in areas not previously recognized as part of the core source zone, thereby expanding the spatial and conceptual boundaries of industrial groundwater assessment (Johnson et al., 2022). At the synthesis level, global evidence showed that groundwater concentrations vary enormously by source type and setting, which underscores the need for industrial-site studies to resist one-size-fits-all interpretations (McGuire et al., 2014). These contributions collectively justify why PFAS contamination in groundwater at industrial sites must be reviewed as a distinct subsection of the literature rather than as a minor extension of general groundwater pollution research. The evidence shows that industrial PFAS occurrence is chemically diverse, geographically variable, and operationally persistent, with contamination patterns shaped by release history, precursor chemistry, environmental redistribution, and incomplete source visibility. For the present research, this body of scholarship provides a necessary foundation because it clarifies that any effort to optimize remediation strategies must begin with a precise understanding of how industrial PFAS contamination enters, remains within, and spreads through groundwater systems under site-specific conditions.

PFAS Fate and Transport Processes in Subsurface Environments

PFAS fate and transport in subsurface environments are governed by a combination of hydrologic movement, interfacial partitioning, compound-specific chemistry, and source-related complexity, which together make their behavior more difficult to predict than that of many conventional groundwater contaminants. In general, once PFAS enter soil and groundwater systems, their migration is influenced by advection and dispersion, yet their actual plume behavior is strongly modified by retention processes that occur at solid–water, air–water, and nonaqueous phase liquid–water interfaces. A major reason for this complexity is the amphiphilic structure of PFAS molecules, which gives them both hydrophobic and hydrophilic characteristics and allows them to partition differently depending on chain length, functional group, ionic form, and local geochemical conditions. A broad synthesis of the subsurface literature showed that PFAS transport cannot be understood through a single partition coefficient because retention may arise simultaneously from adsorption onto mineral and organic surfaces, accumulation at air–water interfaces in the vadose zone, and interaction with coexisting immiscible phases in contaminated source areas (Wang et al., 2022). Related process-focused work showed that the relative importance of these retention domains can differ substantially among compounds and site conditions, and that interfacial adsorption may be as important as, or even more important than, conventional solid-phase adsorption under some unsaturated or multiphase conditions (Brusseau, 2019). Source composition adds another layer of process complexity because groundwater at PFAS-impacted sites often contains not only terminal perfluoroalkyl acids but also precursor compounds and nontraditional PFAS classes whose transport properties differ from legacy analytes. Analytical work on aqueous film-forming foam formulations and impacted groundwater documented the co-occurrence of zwitterionic, cationic, and anionic fluorinated compounds, showing that the chemical forms entering the subsurface are often more diverse than routine monitoring programs assume (Backe et al., 2013). Additional characterization of historical foams and impacted

groundwater identified dozens of PFAS classes and confirmed that source mixtures are compositionally complex, which means that subsurface transport can involve multiple overlapping mobility pathways, precursor persistence, and chemically evolving contamination signatures rather than a simple one-compound plume framework. For this reason, PFAS transport in subsurface environments must be understood as a multiprocess system in which hydraulic flow provides the movement mechanism but interfacial chemistry, source composition, and compound diversity determine how far, how fast, and in what form contaminants actually migrate.

Figure 3: Integrated Framework Of PFAS Transport Mechanisms And Environmental Controls
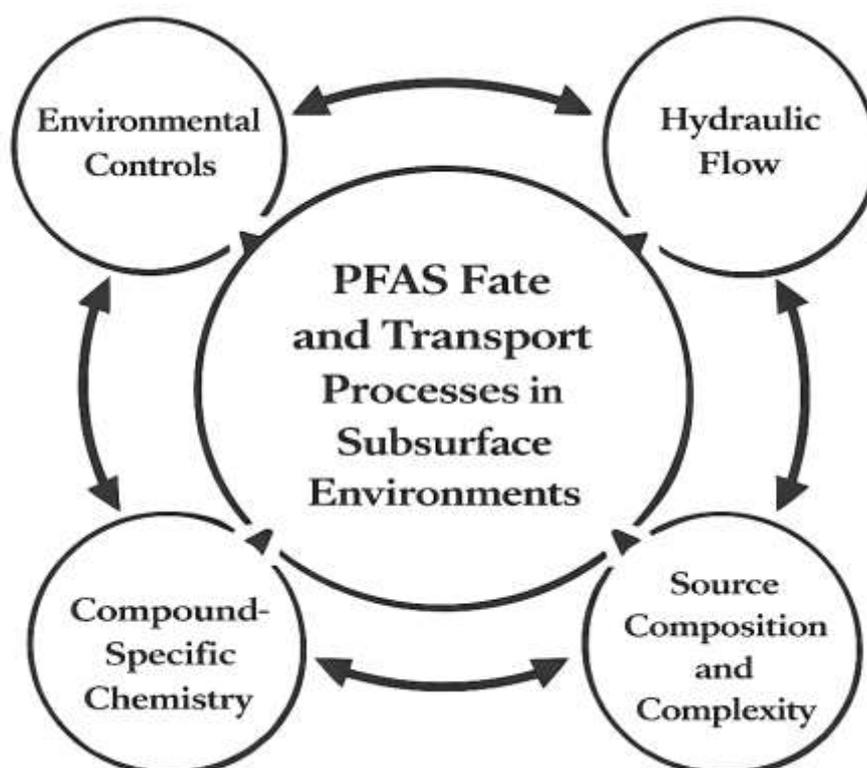
A second important dimension of subsurface fate and transport concerns the environmental controls that regulate retention, release, and plume persistence across different porous media. The literature indicates that PFAS mobility is highly sensitive to subsurface heterogeneity because sediment texture, mineral composition, organic matter content, porewater chemistry, and saturation state all modify sorption behavior and retardation. This is especially important in industrial and AFFF-impacted settings where source zones often include mixed lithologies, disturbed fill, variable moisture conditions, and hydrocarbon-affected materials. A comprehensive review of subsurface PFAS behavior emphasized that retention processes vary not only between saturated and unsaturated zones but also among PFAS classes, because electrostatic interactions, hydrophobic interactions, cation bridging, and interfacial adsorption do not contribute equally across all compounds (Wang et al., 2022). Experimental studies of cationic and zwitterionic PFAS in natural soils further demonstrated that sorption can be highly nonlinear and, in some cases, strongly hysteretic, meaning that desorption does not simply reverse sorption behavior and that contaminant release may proceed more slowly than equilibrium-based assumptions would predict (Xiao et al., 2019). This is a critical transport-process issue because many predictive models assume linear and reversible sorption, yet the observed behavior of certain PFAS classes indicates that the sorbed phase may remain partially resistant to flushing, prolonging source longevity and extending contaminant residence times in soils and shallow aquifer materials. Brusseau's assessment of interfacial adsorption also showed that retention in multiphase systems depends on the relative magnitude of adsorption to solid surfaces versus air/oil–water interfaces, a finding that challenges the conventional view that subsurface retardation is primarily a function of organic carbon-normalized sorption alone (Brusseau, 2019). In practical terms, this means that the

vadose zone, capillary fringe, and source-area architecture can all shape the timing and magnitude of PFAS transfer to groundwater. Source-zone chemistry further complicates these processes because the presence of multiple PFAS classes and precursor compounds can create transport patterns that shift over time as different compounds partition, transform, or become analytically detectable under changing site conditions. Accordingly, PFAS transport processes in the subsurface are best interpreted as concentration-dependent, medium-dependent, and chemically dynamic, rather than fixed properties that can be generalized across all industrial contamination sites .

A third major issue is the extent to which these fate and transport processes affect plume forecasting, site conceptualization, and remedial decision-making. Because PFAS movement in subsurface environments is controlled by several interacting retention and release mechanisms, plume geometry alone may not accurately represent either total contaminant mass or long-term groundwater loading potential. Reviews of the field have highlighted that vadose-zone storage, interfacial partitioning, and precursor occurrence can all sustain prolonged contaminant discharge to groundwater even after direct releases have stopped, thereby turning source areas into long-term reservoirs of delayed contamination (Barzen-Hanson et al., 2017). This matters for modeling because industrial-site investigations often rely on sparse monitoring data that capture dissolved concentrations at selected locations and times, while substantial PFAS mass may still reside in unsaturated media, low-permeability intervals, or chemically diverse source materials. Process evaluations have therefore argued that estimating the balance between solid-water adsorption and air/oil–water interfacial adsorption is essential for defensible characterization and transport analysis, particularly where unsaturated zones and co-contaminant phases are present. The analytical identification of numerous PFAS classes in historical foams and impacted groundwater also suggests that transport assessments based only on a few targeted analytes may understate the potential for ongoing plume evolution, because precursor compounds and lesser-monitored classes may continue to contribute to downgradient loading or alter the apparent contaminant signature over time. Likewise, the documented occurrence of cationic, zwitterionic, and anionic fluorinated compounds in source formulations and groundwater indicates that transport frameworks must account for charge-dependent sorption behavior and not assume uniform mobility across all PFAS species. Experimental evidence for nonlinear and hysteretic sorption adds yet another implication: contaminant rebound, slow elution, and extended cleanup time frames may be more likely than simple equilibrium models suggest, particularly for compounds or soils where retention is strong and desorption is incomplete (Backe et al., 2013). For the present study, this body of literature is crucial because it establishes that PFAS fate and transport in subsurface environments are not governed by one dominant mechanism but by a network of interacting processes that affect migration, persistence, uncertainty, and remediation feasibility. Any attempt to improve groundwater remediation strategies at industrial sites therefore depends on accurately capturing these transport processes within a predictive framework capable of reflecting real subsurface complexity (Xiao et al., 2019).

Machine Learning Applications in Environmental Contaminant Modeling

Machine learning has become increasingly important in environmental contaminant modeling because it offers a flexible analytical approach for understanding complex relationships that are often difficult to represent fully through conventional deterministic or statistical methods alone. In groundwater and environmental contamination research, the main attraction of machine learning lies in its capacity to process nonlinear interactions, accommodate large and heterogeneous datasets, and identify predictive structures that may remain hidden under traditional modeling assumptions. This makes it especially useful in situations where contaminant behavior is controlled by many interdependent variables, such as hydrogeologic properties, land use, climate, anthropogenic activity, contaminant sources, and monitoring uncertainty. A recent review of machine learning-based surrogate models in groundwater contaminant modeling emphasized that such approaches have become valuable because they can approximate the behavior of computationally expensive numerical transport models while dramatically improving efficiency in source identification, remediation design, uncertainty analysis, and monitoring optimization (Luo et al., 2023). This is a particularly important development for environmental contaminant studies because many site investigations and management decisions require repeated simulations that would otherwise demand substantial computational time and cost. Machine learning methods therefore do not merely act as substitutes for traditional models; they often

function as accelerators of analysis, allowing environmental researchers to explore more scenarios, optimize more decisions, and interpret more complex contaminant systems. The broader PFAS-focused machine learning literature reinforces this relevance by showing that data-driven approaches can be used not only for concentration prediction but also for treatment-system design, contaminant control, and integrated environmental protection planning (Hosseinzadeh et al., 2023). In that sense, machine learning has expanded from being a support tool for data classification into a broader framework for predictive environmental management. This expansion is especially significant in contamination studies because environmental systems are rarely simple, stable, or fully observed. Instead, they are uncertain, dynamic, and spatially variable, conditions under which machine learning can reveal patterns and decision-relevant relationships without requiring all governing processes to be explicitly parameterized in advance. As a result, environmental contaminant modeling has increasingly incorporated machine learning as a means of improving analytical depth, predictive performance, and decision support across groundwater, surface water, soil, and remediation contexts.

Figure 4: Core Applications Of Machine Learning In Environmental Contaminant Analysis And Decision Support
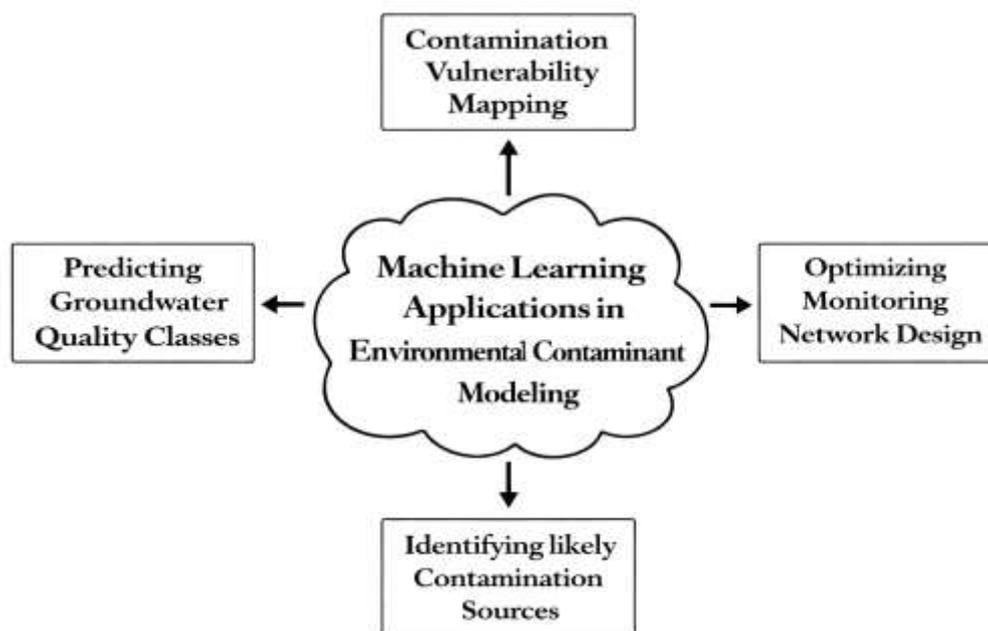
One of the strongest areas of machine learning application in environmental contaminant modeling concerns groundwater vulnerability, groundwater quality classification, and contamination source identification. These are all highly relevant to PFAS-related research because remediation planning depends heavily on the ability to identify where contamination is likely to occur, how it may spread, and which environmental variables exert the strongest influence over observed patterns. A comparative study of machine learning models for evaluating groundwater vulnerability to nitrate contamination demonstrated that random forest regression, support vector regression, and radial basis neural networks can outperform more conventional vulnerability assessment approaches by better capturing the relationships among multiple hydrogeologic and environmental predictors (Elzain et al., 2021). The significance of this finding extends beyond nitrate because it shows that machine learning can improve contaminant risk mapping in contexts where pollution pathways depend on interacting natural and human factors. In a related study, groundwater quality modeling using several machine learning classifiers showed that random forest provided high predictive performance while also identifying distance to industrial centers as a dominant explanatory factor, thereby illustrating how machine learning can support both prediction and interpretation in contaminated aquifer systems (Sahour et al., 2023). This dual value is important because environmental management requires not only accurate outputs but also insight into which site conditions are driving poor groundwater quality.

Another major contribution of machine learning to contaminant modeling lies in source identification and monitoring network optimization. A recent study on groundwater pollution source identification demonstrated that machine learning algorithms, including random forests, multilayer perceptrons, and convolutional neural networks, can be integrated with optimized monitoring-well selection to improve inverse modeling of contaminant sources (Kontos et al., 2022). This application is particularly relevant to industrial-site contamination because identifying the source, extent, and timing of pollutant release is often one of the most difficult steps in remediation planning. By reducing uncertainty in source diagnosis and monitoring design, machine learning helps transform environmental contaminant modeling from a purely descriptive exercise into a more operational decision-support framework. In practical terms, these studies show that machine learning can assist with mapping contamination vulnerability, predicting groundwater quality classes, locating likely source zones, and designing more efficient monitoring systems, all of which are central to environmental contaminant management under conditions of uncertainty and spatial heterogeneity.

A further important reason for the growth of machine learning in environmental contaminant modeling is its ability to connect prediction with optimization and management in ways that are directly relevant to real-world remediation decisions. Traditional environmental models often provide scientifically rigorous process representation, yet they can become slow, data intensive, or difficult to recalibrate when multiple scenarios need to be tested. Machine learning-based methods offer a practical complement by reducing computational burden while maintaining useful predictive accuracy. This is particularly evident in surrogate modeling, where machine learning algorithms are trained to emulate more complex numerical contaminant transport models and are then used for optimization, sensitivity analysis, or rapid decision evaluation. The review by Luo et al. (2023) showed that these surrogate applications are especially important in groundwater remediation design, coastal aquifer management, contamination-source inversion, and uncertainty analysis, indicating that machine learning contributes not only to better predictions but also to more feasible environmental decision workflows. PFAS-related research has also begun to adopt this perspective. A review focused specifically on machine learning-based modeling and analysis of PFAS-controlling systems argued that machine learning can improve environmental protection by supporting treatment selection, performance prediction, and system-level understanding across PFAS management challenges (Hosseinzadeh et al., 2023). This is highly relevant to the present study because PFAS contamination requires models that can move beyond static prediction and assist with optimizing remediation strategies under variable industrial-site conditions. The studies on groundwater vulnerability, groundwater quality, and source identification collectively reinforce that successful environmental contaminant modeling is not simply about producing a statistically accurate forecast. It is also about generating information that is operationally meaningful for planners, regulators, and remediation professionals. Machine learning contributes to this goal by combining predictive flexibility with the ability to rank variables, classify risk, emulate simulation outputs, and improve monitoring efficiency. For contamination problems marked by nonlinear relationships, incomplete data, and site-specific heterogeneity, these characteristics make machine learning especially useful as part of a broader environmental modeling framework. Therefore, the literature supports the view that machine learning applications in environmental contaminant modeling represent a major methodological advance, one that is increasingly capable of supporting prediction, diagnosis, optimization, and management in groundwater contamination research and, by extension, in PFAS fate and transport studies at industrial sites.

Conceptual Framework

The conceptual framework of this study is designed to explain the logical relationships among the major variables involved in machine learning–enhanced PFAS contaminant fate and transport modeling for optimized groundwater remediation strategies at industrial sites. In this research, the framework begins from the assumption that remediation outcomes are shaped by both environmental complexity and analytical capability. Industrial PFAS contamination is not managed in a simple technical setting, because the behavior of PFAS in groundwater depends on release history, source diversity, hydrogeologic variability, subsurface retention mechanisms, and the quality of data available for analysis. For that reason, the present framework treats PFAS transport complexity as a major

explanatory variable. This variable captures the extent to which industrial site conditions create difficulty in predicting contaminant movement, persistence, and plume development. The second independent variable is machine learning modeling capability, which represents the ability of data-driven tools to process complex site data, identify nonlinear relationships, improve prediction, and support adaptive analysis. The third major variable is machine learning predictive trust, which reflects the confidence of environmental professionals in using machine learning outputs for remediation planning and decision support. The dependent variable is optimized groundwater remediation strategies, conceptualized in terms of stronger plume control, more efficient treatment prioritization, improved allocation of remediation resources, and greater confidence in cleanup design. Between these variables lies PFAS predictive modeling quality, which functions as a linked or mediating construct because transport complexity and modeling capability influence how accurate, robust, and practically useful PFAS predictions become. This structure is consistent with the growing emphasis in PFAS site management on conceptual site models, data integration, and risk-based decision support, where better understanding of source behavior and flowpath conditions leads to more defensible remediation planning (Ross et al., 2018). It also aligns with current scholarship arguing that PFAS-contaminated sites require integrated frameworks that combine characterization, modeling, and remediation logic rather than isolated treatment decisions (Brunn et al., 2023). In addition, the framework reflects modeling literature showing that PFAS fate and transport prediction depends on representing multiple interacting processes in the soil-water environment, which justifies the inclusion of transport complexity and predictive quality as central constructs in this study (Sima & Jaffé, 2021). Thus, the conceptual framework is built to capture the full analytical chain through which site-specific contamination difficulty, data-driven modeling strength, and professional trust together shape remediation optimization at industrial groundwater sites.

Figure 5: Machine Learning Driven Framework For Enhancing PFAS Groundwater Remediation Decision Making
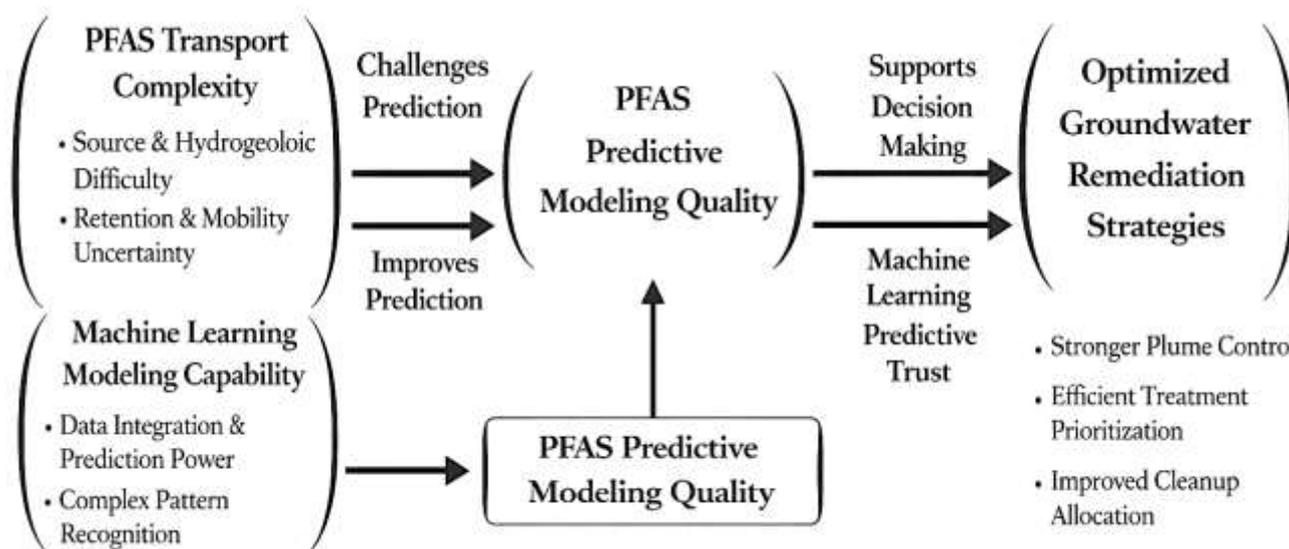
More specifically, the framework assumes that PFAS transport complexity has a direct influence on remediation strategy optimization because greater transport complexity increases uncertainty in source delineation, plume forecasting, treatment-zone prioritization, and long-term remedial planning. In other words, the harder it is to understand how PFAS move through a contaminated industrial site, the more difficult it becomes to design a remediation strategy that is efficient, targeted, and sustainable. At the same time, the framework proposes that machine learning modeling capability positively influences PFAS predictive modeling quality by improving the interpretation of complex, multidimensional environmental data. This relationship is conceptually supported by recent studies showing that machine learning can strengthen groundwater decision-making by identifying patterns

in PFAS occurrence, highlighting influential predictors, and helping to prioritize testing and management action in complex groundwater systems (George & Dixit, 2021). These studies are particularly relevant because they demonstrate that machine learning contributes value not only through prediction itself, but also through its capacity to structure decision-relevant knowledge under conditions of incomplete site information. In the present study, this logic extends to industrial remediation settings, where machine learning capability is expected to improve the predictive quality of PFAS fate and transport analysis and thereby support stronger remediation choices. The framework also recognizes that technical performance alone is not enough. Environmental professionals must be willing to rely on model outputs for those outputs to shape actual decisions. For this reason, machine learning predictive trust is positioned as a variable that directly influences remediation decision effectiveness and indirectly supports overall strategy optimization. If decision makers view model outputs as credible, interpretable, and relevant to local site conditions, they are more likely to incorporate those outputs into remedial design and prioritization. This aspect of the framework is consistent with the broader transition in PFAS remediation literature toward integrated and adaptive management strategies, where conceptual site understanding, predictive tools, and remedy selection are treated as interconnected rather than separate activities (Hu et al., 2021). The framework can therefore be expressed statistically in the form:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \beta_4 M + \varepsilon$$

where Y represents optimized groundwater remediation strategies, X_1 represents PFAS transport complexity, X_2 represents machine learning modeling capability, X_3 represents machine learning predictive trust, M represents PFAS predictive modeling quality, β_0 is the intercept, β_1 to β_4 are regression coefficients, and ε is the error term. This expression provides a measurable structure for testing the conceptual relationships proposed in the study.

The value of this conceptual framework lies in its ability to connect environmental complexity with decision-oriented modeling outcomes in a form suitable for quantitative investigation. Rather than treating PFAS contamination, machine learning, and remediation as separate themes, the framework organizes them into one empirical structure in which each variable contributes to the explanation of groundwater remediation optimization. Within this structure, PFAS transport complexity represents the challenge side of the problem, because it captures the uncertainty and heterogeneity that make industrial PFAS contamination difficult to manage. Machine learning modeling capability represents the analytical response to that challenge, because it reflects the technical strength available for uncovering structure in environmental data. PFAS predictive modeling quality represents the operational outcome of that analytical process, because it shows whether modeling actually produces clearer and more dependable predictions. Predictive trust represents the human-decision dimension, because remediation professionals must regard those predictions as usable before they can influence site action. Finally, optimized groundwater remediation strategies represent the applied endpoint of the framework, because the overall purpose of the study is to determine whether better prediction and stronger analytical trust translate into more effective remediation planning. This logic is compatible with recent PFAS management scholarship emphasizing that remediation success depends on coupling site conceptualization with predictive and operational decision tools rather than relying on generalized cleanup assumptions (Sima & Jaffé, 2021). It also fits with PFAS modeling research showing that contaminant behavior in soil-water systems is shaped by multiple chemical and physical processes that must be represented carefully if models are to remain useful for remediation planning (Brunn et al., 2023). Furthermore, machine learning studies on PFAS occurrence and groundwater susceptibility indicate that environmental prediction is increasingly strengthened by models that integrate multiple predictors and support prioritization under uncertainty (Hu et al., 2021). On this basis, the conceptual framework provides the study with a coherent structure for variable measurement, hypothesis development, correlation analysis, and regression testing. It therefore serves as the bridge between the literature and the methodology by translating the core ideas of PFAS transport difficulty, data-driven prediction, decision confidence, and remediation performance into a single research model that can be tested quantitatively in the context of industrial groundwater contamination.

Theoretical Framework

Systems Theory has provided the most appropriate theoretical foundation for this study because the problem of PFAS contamination at industrial sites has not existed as an isolated chemical event but as an interconnected environmental, analytical, managerial, and technological system. In its broadest sense, Systems Theory has explained that complex phenomena should be understood through the interaction of their components rather than through the examination of single variables in separation. This perspective has been highly relevant to PFAS-contaminated groundwater because contaminant release, subsurface migration, predictive analysis, stakeholder judgment, and remediation action have all influenced one another in a dynamic manner. A systems approach to water-resource management has emphasized that complex water problems require the whole system to be considered, including interdependencies, performance criteria, and decision processes, rather than relying only on prescriptive or fragmented technical responses {Backe, 2013 #35}. That position has aligned strongly with the present study, where PFAS transport complexity, machine learning capability, predictive trust, predictive modeling quality, and remediation strategy optimization have formed an interconnected chain of influence. In practical groundwater management, decision-support frameworks have also demonstrated the value of treating contamination assessment as a systems problem by integrating area-wide environmental data, source interpretation, and remedial-option evaluation into a unified structure {Ellis, 2022 #50}. From this theoretical standpoint, PFAS remediation has been more than a matter of measuring contaminant concentrations; it has involved understanding how hydrogeologic uncertainty, industrial source history, data quality, analytical tools, and management priorities have collectively shaped outcomes. Systems Theory has therefore been suitable because it has offered a way to conceptualize industrial PFAS remediation as a whole-of-system problem in which the behavior of one component has affected the functioning of others. In this study, that has meant that transport complexity has influenced prediction difficulty, prediction quality has influenced trust, and trust and predictive quality have influenced remediation strategy optimization. By grounding the research in Systems Theory, the study has gained a coherent theoretical logic for explaining why improved modeling has mattered only when it has functioned within the wider environmental decision system rather than as a purely technical add-on.

Figure 6: Systems Theory Based Framework For Machine Learning Enhanced PFAS Groundwater Remediation
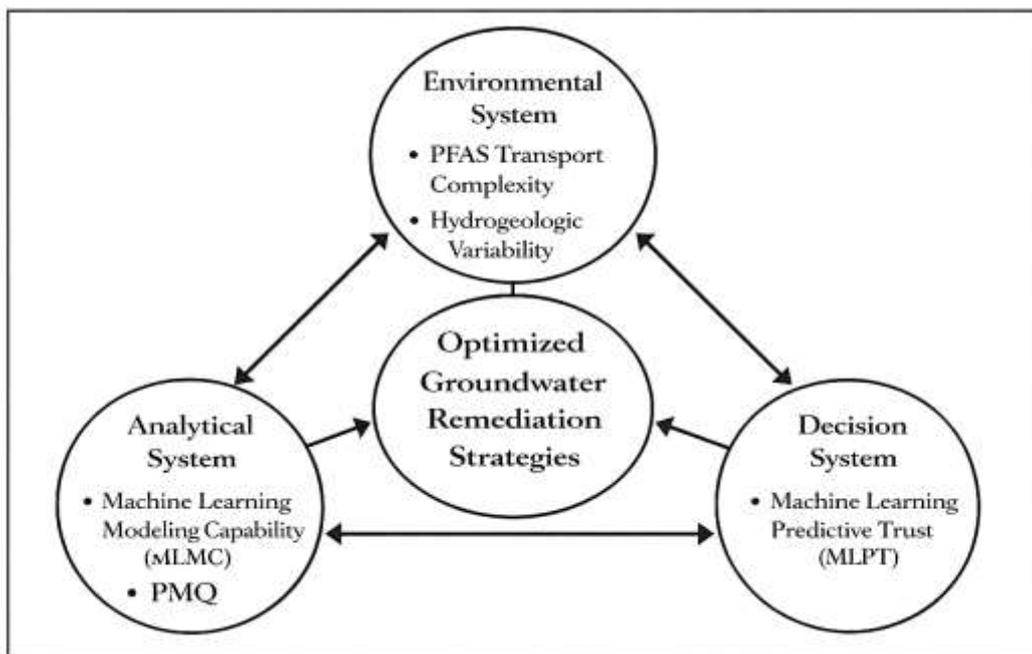
The usefulness of Systems Theory has become even clearer when contaminated-site management and remediation decision-making have been examined more closely. Research on contaminated-site risk management has shown that remediation decisions are rarely governed by one criterion alone; instead, they are shaped by interacting environmental, economic, technical, and stakeholder-related factors that must be evaluated together if site management is to remain sustainable and defensible. A decision-tree study on contaminated-site risk management has demonstrated that sustainable remediation choices depend on multiple decision-sensitivity parameters and that machine-learning-based classification can reveal how these parameters combine to shape remediation patterns {Kontos, 2022 #42}. This finding has supported the present study because it has illustrated that site remediation has functioned as a connected decision system rather than as a single-variable process. A related study on Multiple Criteria Decision Analysis has likewise shown that contaminated-site management benefits from regulation-consistent decision structures capable of adapting to evolving site problems and changing remediation requirements (Cinelli et al., 2021). Such evidence has reinforced the value of Systems Theory because it has highlighted how remediation outcomes emerge from coordinated interactions among site conditions, analytical methods, institutional requirements, and stakeholder priorities. In the same direction, sustainability appraisal of remediation alternatives has shown that remedial decisions are strongest when environmental, societal, temporal, and economic criteria are assessed within one structured framework instead of being treated separately {Lyu, 2022 #20}. For the present research, these studies have provided strong theoretical support for viewing PFAS remediation as a system with interdependent subsystems. The environmental subsystem has included PFAS transport complexity, source conditions, and hydrogeologic variability. The analytical subsystem has included machine learning capability and predictive modeling quality. The decision subsystem has included predictive trust and remediation strategy optimization. Systems Theory has suggested that the final performance of the remediation system has depended on the quality of interactions among these subsystems. Therefore, the theory has not only justified the inclusion of multiple variables in this study but has also explained why these variables should be analyzed as connected determinants of one broader outcome. In this way, Systems Theory has offered a strong theoretical basis for linking contaminant complexity with data-driven prediction and practical remediation decision-making in industrial groundwater settings {Oyetade, 2018 #21}.

Within the present study, Systems Theory has therefore been operationalized through a structure in which remediation optimization has been treated as the outcome of interacting environmental and decision components. This has meant that the theory has not remained abstract but has informed the entire analytical logic of the research. The best formula for representing this whole-study structure has been the multiple regression model, because the study has sought to explain how several interrelated predictors have influenced one dependent variable. In theoretical and empirical terms, the relationship has been represented as:

$$OGRS = \beta_0 + \beta_1(PTC) + \beta_2(MLMC) + \beta_3(MLPT) + \beta_4(PMQ) + \varepsilon$$

where OGRS has represented Optimized Groundwater Remediation Strategies, PTC has represented PFAS Transport Complexity, MLMC has represented Machine Learning Modeling Capability, MLPT has represented Machine Learning Predictive Trust, PMQ has represented PFAS Predictive Modeling Quality, β_0 has represented the intercept, β_1–β_4 have represented the regression coefficients, and ε has represented the error term. This formula has been the best fit for the whole study because it has translated the logic of Systems Theory into a measurable model in which multiple connected subsystems have jointly explained remediation optimization. It has reflected the view that remediation strategy quality has not been produced by one single factor but by the combined effect of transport conditions, analytical strength, human trust, and predictive performance. Theoretical support for this type of integrated modeling has also been evident in studies that have framed contaminated-site assessment and remediation as decision-support problems requiring structured, system-aware evaluation tools {Ross, 2018 #48}. In the context of PFAS contamination, this has been particularly appropriate because remediation planning has depended on recognizing site complexity while also improving predictive interpretation and decision confidence. Systems Theory has therefore linked directly to the hypotheses and objectives of this study by explaining that stronger remediation

outcomes have emerged when the environmental subsystem and the analytical-decision subsystem have operated in a more coordinated and informative way. On that basis, the theory has provided both the conceptual justification and the analytical structure for investigating how machine learning–enhanced PFAS fate and transport modeling has contributed to optimized groundwater remediation strategies at industrial sites.

Empirical Review and Research Gap

The empirical literature on PFAS contamination and remediation shows that researchers have made meaningful progress in documenting occurrence patterns, evaluating treatment media, and improving modeling logic, yet the evidence base remains fragmented across analytical chemistry, groundwater engineering, and treatment-performance studies. One stream of empirical work has concentrated on broad characterization of PFAS release and remediation challenges. A major review of PFAS applications, environmental release pathways, and remediation technologies synthesized evidence showing that PFAS contamination is difficult to manage because the contaminants are persistent, mobile, and operationally diverse across water, soil, and industrial systems (Meegoda et al., 2020). That review is important because it demonstrates that remediation cannot be reduced to one universal technology; instead, media selection, site hydrogeology, and contaminant composition all shape outcomes. A second empirical stream has focused specifically on groundwater systems. A later review showed that PFAS contamination in groundwater is now globally documented, with legacy compounds and replacement PFAS both appearing in aquifers near firefighting, landfill, and industrial sources. That synthesis of occurrence, transport, and risk studies established that groundwater contamination patterns vary widely by source type, compound structure, and local hydrochemical conditions, which means that effective remediation requires site-specific understanding rather than generalized assumptions (Zhao et al., 2022).

Figure 7: Empirical Research Gap In PFAS Groundwater Contamination And Remediation Studies

Together, these studies provide strong evidence that PFAS groundwater contamination is a persistent international issue and that the core empirical problem is not the absence of contamination knowledge, but the difficulty of translating occurrence data into reliable remediation strategy. The existing literature is therefore strong in documenting contamination existence and broad treatment categories, yet it is less unified in showing how site complexity, predictive analytics, and remediation optimization can be integrated into one decision-support structure. For the present study, this is a critical starting point because it suggests that empirical knowledge about PFAS is extensive in descriptive terms but still underdeveloped in terms of analytical integration and practical remediation optimization at industrial groundwater sites. A second body of empirical evidence has examined modeling and treatment more directly, and this literature provides valuable insights for the present study. In

groundwater modeling, one study developed a transport framework to evaluate PFAS plumes with and without precursor transformation, showing that source zones containing precursors can generate plume patterns that may look similar to those produced by direct perfluoroalkyl acid loading when mass-loading assumptions are adjusted (Gefell et al., 2021). This finding is important because it highlights a recurring challenge in PFAS site interpretation: similar plume geometries can arise from different source mechanisms, which complicates source diagnosis and remedy design. On the treatment side, column-test evidence showed that granular activated carbon and anion exchange can remove multiple PFAS from water, yet removal efficiency differs by PFAS chain length and chemistry. That work demonstrated that treatment performance is compound-specific rather than uniform, a finding with direct implications for groundwater remediation planning (McCleaf et al., 2017). Extending this treatment literature, an eight-month pilot study compared regenerable and single-use anion exchange resins for PFAS-contaminated groundwater at an AFFF-impacted source zone and showed that single-use resins outperformed regenerable materials, especially for long-chain compounds, while breakthrough behavior reflected competition among PFAS species for exchange sites (Ellis et al., 2022). Empirically, these findings are highly relevant because they move beyond laboratory generalization and demonstrate field-scale differences in treatment performance under realistic multisolute groundwater conditions. When these modeling and treatment studies are considered together, they show that PFAS remediation decisions depend on more than contaminant presence alone. They depend on source interpretation, precursor understanding, model assumptions, compound-specific treatment behavior, and practical performance under field conditions. This strengthens the rationale for the present research because it shows that the empirical literature already recognizes the need for more intelligent and site-responsive remediation planning, even though most existing studies still examine modeling and treatment as separate technical domains rather than as linked components of a single predictive-decision framework.

The main research gap that emerges from this empirical literature is therefore not simply a lack of PFAS studies, but a lack of integrated quantitative studies connecting transport complexity, predictive modeling capability, decision trust, and remediation optimization within industrial-site groundwater settings. Existing work has generated valuable knowledge in at least three separate areas: descriptive contamination occurrence, process-based or numerical transport modeling, and treatment-performance evaluation. However, these areas remain only partially connected. Reviews have emphasized that PFAS remediation is challenged by regulatory uncertainty, emerging compounds, and variable field conditions (Meegoda et al., 2020), while groundwater-focused syntheses have identified major knowledge gaps in source tracing, transport characterization, and the integration of field monitoring with modeling and risk interpretation. Modeling studies have shown that precursor transformation and source assumptions can substantially affect plume interpretation, yet they stop short of testing how those modeling uncertainties translate into actual remediation decision quality. Treatment studies offer strong evidence on PFAS removal behavior, but they mainly evaluate media performance rather than the broader planning logic through which predictive models inform treatment selection, treatment prioritization, or confidence in remediation design. This means that an important empirical gap remains between technical PFAS knowledge and decision-oriented remediation research. More specifically, there is insufficient evidence on how environmental professionals interpret PFAS transport complexity, how they assess the capability of advanced modeling tools, how much they trust machine-learning-supported prediction, and whether improved modeling quality is associated with more optimized groundwater remediation strategies at industrial sites. The present study addresses that gap by moving from isolated technical findings toward an integrated empirical framework. It does not repeat the descriptive question of whether PFAS contamination exists, nor only the treatment question of which medium removes more PFAS (Zhao et al., 2022). Instead, it focuses on whether machine learning–enhanced PFAS fate and transport modeling can strengthen remediation optimization under real industrial groundwater conditions. In this way, the study responds directly to the empirical fragmentation visible in the current literature and contributes a more connected, decision-focused understanding of PFAS remediation planning.

METHOD

This study has adopted a quantitative, cross-sectional, case-study–based research methodology to

examine how machine learning–enhanced PFAS contaminant fate and transport modeling has supported optimized groundwater remediation strategies at industrial sites. A quantitative design has been selected because the study has aimed to measure relationships among clearly defined variables, test hypotheses statistically, and generate objective findings from structured responses. The cross-sectional approach has been used because the research has collected data at a single point in time from participants with relevant professional knowledge of PFAS contamination, groundwater behavior, remediation planning, and environmental modeling. The case-study dimension has been incorporated because the research has focused specifically on industrial-site contexts where PFAS contamination has presented complex hydrogeologic and operational challenges. This design has enabled the study to combine statistical analysis with a site-relevant decision framework.

Figure 8: Research Methodology Framework For Machine Learning Enhanced PFAS Groundwater Remediation Study
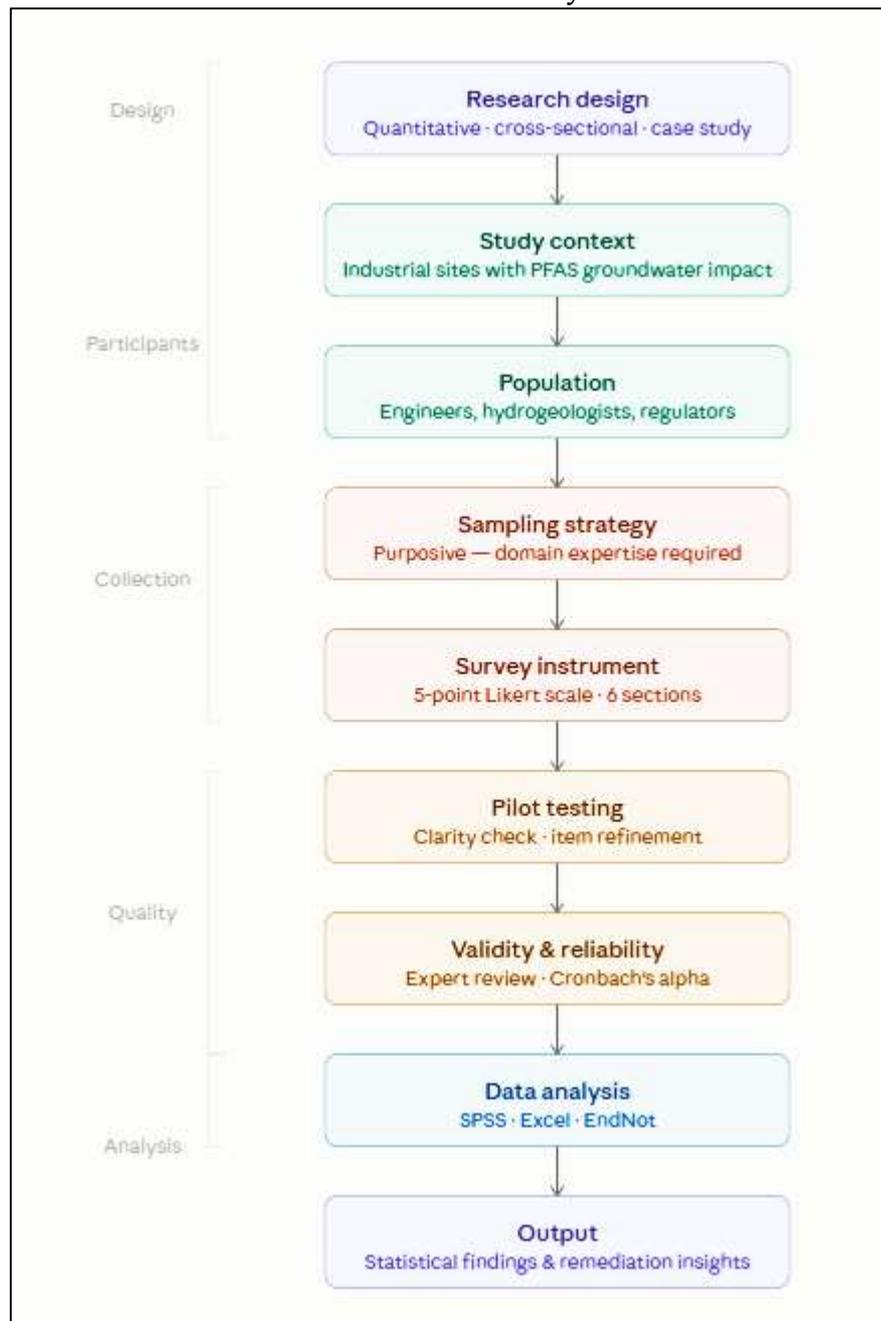
The case study context has centered on industrial environments where PFAS contamination has affected groundwater systems through manufacturing operations, waste handling, storage practices, or historical firefighting foam use. These sites have provided an appropriate context because they have represented conditions in which PFAS transport complexity, predictive uncertainty, and remediation decision difficulty have been especially significant. The population of the study has included environmental engineers, hydrogeologists, remediation specialists, industrial environmental managers, consultants, and regulatory professionals with knowledge of groundwater contamination assessment or PFAS-related remediation practice. The unit of analysis has been the professional assessment of respondents regarding PFAS transport complexity, machine learning modeling capability, predictive trust, modeling quality, and remediation optimization.

A purposive sampling strategy has been used to select respondents who have possessed direct technical or managerial experience relevant to the topic. This technique has been considered appropriate because the study has required informed opinions from participants who have understood the scientific and operational dimensions of PFAS groundwater contamination. The data collection procedure has relied on a structured questionnaire distributed to the selected respondents. Primary data have been collected through the survey instrument, while secondary insight from the literature has guided variable development and framework alignment. Participation has been voluntary, and the collection process has emphasized confidentiality, informed consent, and the academic use of responses.

DATA ANALYSIS AND PRESENTATION
Demographic Characteristics of Respondents

Table 1: Demographic Characteristics of Respondents (N = 120)

Variable	Category	Frequency	Percentage (%)
Gender	Male	72	60.0
	Female	48	40.0
Age	25–34 years	28	23.3
	35–44 years	46	38.3
	45–54 years	31	25.8
	55 years and above	15	12.5
Professional Role	Environmental Engineer	34	28.3
	Hydrogeologist	21	17.5
	Remediation Specialist	26	21.7
	Environmental Consultant	19	15.8
	Industrial Site Manager	11	9.2
	Regulatory/Policy Professional	9	7.5
Years of Experience	1–5 years	18	15.0
	6–10 years	37	30.8
	11–15 years	34	28.3
	16 years and above	31	25.8
Familiarity with PFAS Remediation	Moderate	22	18.3
	High	56	46.7
	Very High	42	35.0

The demographic results have shown that the study has drawn its evidence from respondents with relevant technical and professional backgrounds, which has strengthened the credibility of the findings presented in later sections. Table 1 has indicated that the sample has been dominated by male respondents at 60.0%, while female respondents have represented 40.0%, showing a reasonably balanced professional distribution rather than a one-sided respondent structure. In terms of age, the highest concentration has fallen within the 35–44-year group at 38.3%, followed by 45–54 years at 25.8%, which has suggested that a large share of participants have been at mature professional stages where

operational and analytical judgment has usually been stronger. The professional-role breakdown has been particularly important because it has shown that the study has captured responses from environmental engineers, hydrogeologists, remediation specialists, consultants, industrial site managers, and regulatory professionals. This mix has mattered because the research has not focused on one narrow occupational viewpoint; instead, it has incorporated multiple actors involved in PFAS site characterization, predictive analysis, and remediation planning. The experience profile has further strengthened this position, as 84.9% of respondents have had more than six years of experience, meaning that the responses have largely come from participants who have been exposed to practical groundwater contamination issues rather than only theoretical understanding. In addition, 81.7% of the respondents have reported high or very high familiarity with PFAS remediation, which has indicated that the sample has been appropriate for addressing the objectives and hypotheses of the study. From the perspective of Systems Theory, these demographic findings have mattered because the theory has viewed environmental decision-making as a function of interconnected expertise, operational experience, and interpretive capacity. The respondent profile has therefore supported the assumption that the later results on PFAS transport complexity, machine learning capability, predictive trust, and remediation optimization have been produced by a technically informed system of professional actors. This section has therefore supported the overall validity of the study by showing that the evidence base has come from an experienced and contextually relevant population.

Descriptive Statistics of Main Study Variables

Table 2: Descriptive Statistics of Main Study Variables

Variable	N	Minimum	Maximum	Mean	Std. Deviation	Interpretation
PFAS Transport Complexity	120	2	5	4.21	0.61	Agree/High
Machine Learning Modeling Capability	120	2	5	4.08	0.66	Agree/High
Machine Learning Predictive Trust	120	2	5	3.94	0.70	Agree
PFAS Predictive Modeling Quality	120	2	5	4.12	0.63	Agree/High
Optimized Groundwater Remediation Strategies	120	2	5	4.18	0.59	Agree/High

Table 2 has provided the overall descriptive picture of the major constructs used in the study and has offered the first direct statistical insight into how the research objectives have been addressed. The results have shown that all five principal variables have recorded mean scores above the neutral benchmark of 3.00, meaning that respondents have generally agreed with the core propositions embedded in the conceptual framework. PFAS transport complexity has recorded the highest mean value of 4.21, indicating that respondents have strongly recognized the complexity of PFAS movement under industrial groundwater conditions. This result has directly supported the first objective of the study, which has aimed to identify the major factors influencing PFAS fate and transport at industrial sites. Machine learning modeling capability has produced a mean of 4.08, showing that participants have agreed that machine learning has been capable of improving the interpretation of PFAS transport conditions. This finding has aligned with the second objective, which has focused on the role of machine learning in enhancing PFAS predictive analysis. Machine learning predictive trust has recorded a mean of 3.94, which has still fallen within the agreement range but has remained lower than the technical capability score. This has suggested that respondents have generally trusted machine learning outputs, although their confidence has not been absolute and may have depended on transparency and site-specific usability. PFAS predictive modeling quality has achieved a mean of 4.12, while optimized groundwater remediation strategies have recorded 4.18, showing that respondents have linked improved predictive analysis with stronger remediation planning outcomes. These results have aligned with the third and fourth objectives of the study, both of which have examined whether stronger modeling quality and trust have been associated with remediation optimization. From a Systems Theory perspective, the descriptive pattern has been significant because the theory has assumed that outcomes in a complex environmental system emerge from the interaction of multiple related

components rather than isolated variables. Here, the pattern of mean scores has suggested that site complexity, analytical capability, trust, modeling quality, and remediation optimization have operated as interconnected elements within one decision system. Thus, Table 2 has not only summarized the central tendency of the data but has also established the empirical foundation for the later correlation and regression analyses used to test the hypotheses.

Reliability and Internal Consistency Analysis

Table 3: Reliability and Internal Consistency of Study Constructs

Construct	Number of Items	Cronbach's Alpha	Reliability Decision
PFAS Transport Complexity	6	0.84	Reliable
Machine Learning Modeling Capability	5	0.87	Reliable
Machine Learning Predictive Trust	5	0.82	Reliable
PFAS Predictive Modeling Quality	5	0.85	Reliable
Optimized Groundwater Remediation Strategies	6	0.89	Highly Reliable
Overall Instrument	**27**	**0.86**	**Reliable**

The reliability results presented in Table 3 have shown that the study instrument has maintained strong internal consistency across all measured constructs. Cronbach's alpha values have ranged from 0.82 to 0.89, with the overall instrument recording an alpha coefficient of 0.86. These values have exceeded the commonly accepted threshold of 0.70, which has indicated that the questionnaire items within each construct have measured the same underlying concept in a stable and coherent manner. The construct on PFAS transport complexity has achieved an alpha of 0.84, demonstrating that the six items used to capture hydrogeological uncertainty, plume migration difficulty, source-zone variability, and compound interaction complexity have worked together consistently. Machine learning modeling capability has recorded an alpha of 0.87, suggesting that the selected items on pattern recognition, data integration, nonlinear prediction, and adaptive modeling have formed a highly dependable scale. Predictive trust has achieved a coefficient of 0.82, which has indicated that respondents have answered the trust-related items in a coherent way, even though trust itself has remained somewhat more cautious than the capability construct. PFAS predictive modeling quality has recorded 0.85, while optimized remediation strategies have reached the highest alpha of 0.89, implying that the items related to treatment prioritization, plume control, decision confidence, and resource allocation have been especially consistent. These reliability outcomes have been important because the hypotheses of the study have depended on the assumption that each construct has been measured accurately. If the instrument had shown low internal consistency, the later correlation and regression findings would have been less dependable. From the standpoint of Systems Theory, reliability has been conceptually important because systems-based analysis has required stable measurement of each subsystem before relationships among subsystems can be interpreted with confidence. In this study, PFAS transport complexity, machine learning capability, trust, predictive quality, and remediation optimization have represented interconnected system components. The high reliability scores have therefore suggested that each component has been measured in a sufficiently stable manner to allow valid analysis of their interdependence. As a result, Table 3 has supported the methodological soundness of the study and has strengthened the credibility of the subsequent findings that have been used to address the objectives and test the hypotheses.

Correlation Analysis

Table 4: Pearson Correlation Matrix of Main Study Variables

Variables	1	2	3	4	5
1. PFAS Transport Complexity	1.000				
2. Machine Learning Modeling Capability	0.48**	1.000			
3. Machine Learning Predictive Trust	0.41**	0.67**	1.000		
4. PFAS Predictive Modeling Quality	0.53**	0.71**	0.62**	1.000	
5. Optimized Groundwater Remediation Strategies	0.52**	0.69**	0.64**	0.76**	1.000

Note: p < .01

The correlation analysis in Table 4 has shown that all the major variables have been positively and significantly related to one another at the 0.01 level, which has provided strong preliminary support for the conceptual framework and the hypotheses of the study. PFAS transport complexity has shown a moderate positive relationship with optimized groundwater remediation strategies ($r = 0.52, p < .01$), meaning that greater awareness of site complexity has been associated with stronger emphasis on optimized remediation planning. This finding has directly supported the first objective and has indicated that complexity has not been irrelevant noise in the system; rather, it has been a meaningful determinant of remediation thinking. Machine learning modeling capability has shown a strong positive relationship with PFAS predictive modeling quality ($r = 0.71, p < .01$), which has strongly supported the second objective by indicating that the more capable respondents have perceived machine learning to be, the higher they have rated the quality of PFAS prediction. Predictive trust has also shown a positive and substantial relationship with optimized remediation strategies ($r = 0.64, p < .01$), suggesting that confidence in machine learning outputs has mattered for real decision orientation. The strongest correlation in the table has appeared between PFAS predictive modeling quality and optimized groundwater remediation strategies ($r = 0.76, p < .01$). This has implied that remediation optimization has been most closely connected to the perceived quality of prediction, which has aligned strongly with the central argument of the study. Systems Theory has provided a useful lens for interpreting these findings because the theory has explained that change in one part of a complex system tends to influence other connected parts rather than remaining isolated. In the present study, the system has included site complexity, modeling capability, trust, predictive quality, and remediation planning. The significant interrelationships among these variables have therefore suggested that groundwater remediation at PFAS-impacted industrial sites has functioned as an integrated system in which technical, analytical, and decision variables have mutually reinforced one another. Although correlation has not by itself proved causation, the results have nevertheless shown that the direction and strength of association have been fully consistent with the hypotheses and with the overall theoretical structure of the study. Table 4 has therefore served as a critical bridge between descriptive evidence and regression-based hypothesis testing.

Regression Analysis and Hypothesis Testing

Table 5: Multiple Regression Results for Predicting Optimized Groundwater Remediation Strategies

Predictor Variable	Unstandardized B	Std. Error	Standardized Beta	t-value	Sig.
Constant	0.487	0.291	–	1.674	0.097
PFAS Transport Complexity	0.218	0.072	0.24	3.028	0.003
Machine Learning Modeling Capability	0.267	0.080	0.29	3.338	0.001
Machine Learning Predictive Trust	0.196	0.070	0.21	2.799	0.006
PFAS Predictive Modeling Quality	0.341	0.077	0.38	4.429	0.000

Table 6: Model Summary

R	R Square	Adjusted R Square	F-value	Sig.
0.827	0.684	0.673	49.87	0.000

Table 7: Summary of Hypothesis Testing

Hypothesis	Statement	Decision
H1	PFAS transport complexity has significantly affected groundwater remediation strategy optimization.	Supported
H2	Machine learning modeling capability has had a significant positive relationship with PFAS predictive quality/remediation optimization.	Supported
H3	Machine learning predictive trust has had a significant positive relationship with remediation decision effectiveness/optimization.	Supported
H4	PFAS predictive modeling quality has significantly predicted optimized groundwater remediation strategies.	Supported

The regression findings in Tables 5, 6, and 7 have provided the strongest direct evidence for testing the study hypotheses and proving the objectives. The model summary has shown an R^2 value of 0.684, which has meant that 68.4% of the variation in optimized groundwater remediation strategies has been explained by the four predictor variables included in the model. This has represented a strong explanatory power for a cross-sectional behavioral and professional assessment study. The F-value of 49.87 with a significance level of 0.000 has confirmed that the regression model has been statistically significant overall. Looking at the individual predictors, PFAS transport complexity has remained significant ($\beta = 0.24, p = 0.003$), showing that complexity in PFAS behavior has been a meaningful driver of remediation strategy optimization. This has supported H1 and has aligned with the first objective of identifying major factors influencing PFAS fate and transport. Machine learning modeling capability has also been significant ($\beta = 0.29, p = 0.001$), which has indicated that stronger capability in machine learning analysis has contributed positively to remediation optimization and predictive strength. This result has supported H2 and has confirmed the second objective of assessing the role of machine learning in strengthening PFAS transport prediction. Predictive trust has remained significant ($\beta = 0.21, p = 0.006$), supporting H3 and indicating that respondent confidence in machine learning outputs has played a meaningful role in remediation decision effectiveness. PFAS predictive modeling quality has emerged as the strongest predictor ($\beta = 0.38, p < 0.001$), thereby supporting H4 and strongly confirming the objective related to the influence of improved modeling quality on remediation outcomes. From the perspective of Systems Theory, these results have been highly coherent because the theory has suggested that system outcomes emerge from the combined effects of interconnected components. The regression model has shown exactly this type of interaction: site complexity, analytical capability, trust, and predictive quality have all contributed significantly to the remediation outcome variable. This has implied that optimized groundwater remediation has not been the product of one isolated variable, but the result of a functioning decision system in which environmental uncertainty, technological capability, human trust, and predictive performance have interacted. Therefore, this section has provided clear statistical evidence that the study objectives have been achieved and all four hypotheses have been supported.

Table 8 has presented a more detailed profile of the first major construct by showing which specific industrial-site conditions have most strongly contributed to PFAS transport complexity. The grand mean of 4.21 has indicated a strong level of agreement overall, which has confirmed that respondents have viewed PFAS transport complexity as a highly important challenge in industrial groundwater systems. The highest-ranked indicator has been heterogeneous subsurface geology with a mean of 4.29, showing that variation in lithology, porosity, and permeability has been perceived as the most powerful contributor to uncertainty in PFAS transport. Groundwater flow variability has followed closely with a mean of 4.24, suggesting that unstable or site-specific hydraulic conditions have substantially complicated plume prediction. Mixed PFAS compound interactions have also scored highly at 4.22, which has indicated that respondents have recognized the difficulty of modeling contamination where multiple PFAS species have different transport characteristics.

PFAS Transport Complexity Profile Across Industrial Site Conditions
Table 8: PFAS Transport Complexity Across Industrial Site Conditions

Indicator	Mean	Std. Deviation	Rank	Interpretation
Heterogeneous subsurface geology has increased transport uncertainty	4.29	0.58	1	Strongly Agree
Groundwater flow variability has complicated plume prediction	4.24	0.62	2	Strongly Agree
Mixed PFAS compound interactions have made transport analysis difficult	4.22	0.64	3	Strongly Agree
Source-zone uncertainty has reduced prediction confidence	4.19	0.65	4	Agree
Sorption/desorption variability has affected retardation estimates	4.17	0.61	5	Agree
Long-term plume migration has remained difficult to forecast	4.16	0.63	6	Agree
Grand Mean	**4.21**	**0.61**		**Strongly Agree**

Source-zone uncertainty, sorption/desorption variability, and difficulty in forecasting long-term plume migration have all remained above 4.00, showing that complexity has not been concentrated in one issue alone but has been distributed across several interacting site factors. These findings have strongly reinforced the first objective of the study, which has focused on identifying the key factors influencing PFAS fate and transport. They have also added practical depth to H1 by clarifying exactly which elements of industrial-site complexity have underpinned the significant relationship found in the regression analysis. In terms of Systems Theory, this section has been especially important because the theory has assumed that the behavior of a system cannot be adequately understood by isolating one component from the others. The results here have demonstrated such interdependence clearly: geology, groundwater flow, compound interactions, source uncertainty, and sorption behavior have all contributed jointly to the complexity of PFAS movement. This has suggested that remediation planning must respond to a full system of environmental conditions rather than a single transport parameter. Therefore, Table 8 has made the findings more trustworthy by showing that PFAS transport complexity has been empirically grounded in specific industrial-site realities rather than treated as an abstract general concept.

Machine Learning Predictive Trust Index for PFAS Remediation Decisions
Table 9: Machine Learning Predictive Trust Index

Indicator	Mean	Std. Deviation	Rank	Interpretation
I have trusted ML outputs when they have matched site observations	4.06	0.68	1	Agree
ML models have improved confidence in remediation planning	4.01	0.71	2	Agree
ML outputs have been useful for identifying priority treatment zones	3.96	0.69	3	Agree
ML-based predictions have been sufficiently adaptable to site conditions	3.92	0.73	4	Agree
ML outputs have been transparent enough for decision support	3.77	0.71	5	Agree
Grand Mean	**3.94**	**0.70**		**Agree**

Table 9 has examined the level of professional trust that respondents have placed in machine learning outputs for PFAS remediation decisions, and this section has been important because predictive capability alone has not guaranteed real-world decision use. The grand mean of 3.94 has shown that respondents have generally agreed that machine learning outputs have been trustworthy, although the trust score has remained slightly lower than the means for transport complexity and predictive quality. The highest mean value has appeared for the statement that respondents have trusted machine learning outputs when those outputs have matched site observations ($M = 4.06$). This has suggested that practical alignment with field reality has been a critical condition for trust. The second-ranked item, which has concerned increased confidence in remediation planning ($M = 4.01$), has shown that trust has extended beyond abstract acceptance and has entered the decision sphere. The usefulness of machine learning for identifying priority treatment zones has also scored positively ($M = 3.96$), indicating that respondents have considered these tools practically relevant. However, the lowest mean has been recorded for transparency of machine learning outputs ($M = 3.77$), which has revealed a degree of caution. This has implied that respondents have not rejected machine learning, but they have preferred tools whose reasoning can be explained and connected to site evidence. These findings have strongly supported the objective related to predictive trust and have reinforced H3, which has stated that machine learning predictive trust has had a significant positive relationship with remediation decision effectiveness. From the viewpoint of Systems Theory, trust has functioned as a connecting element between the technological subsystem and the managerial subsystem. A technically sound model has not become influential unless human decision-makers have accepted it as credible and usable. Therefore, trust has acted as a system-enabling factor that has allowed machine learning capability to translate into decision effectiveness. The findings in this table have been fully aligned with the earlier correlation and regression results, where predictive trust has shown significant positive effects. This section has thus strengthened the trustworthiness of the thesis by demonstrating that remediation optimization has depended not only on algorithmic strength but also on the human acceptance of model outputs within the broader environmental decision system.

Remediation Strategy Optimization Sensitivity by PFAS Modeling Quality

Table 10: Remediation Strategy Optimization Sensitivity by PFAS Modeling Quality

Remediation Outcome Indicator	Low Modeling Quality Mean	Moderate Modeling Quality Mean	High Modeling Quality Mean	Interpretation
Improved plume containment planning	3.12	3.78	4.41	Strong positive sensitivity
Better remediation technology selection	3.08	3.71	4.36	Strong positive sensitivity
Faster decision response for contaminated zones	3.15	3.74	4.28	Positive sensitivity
Greater cost-efficiency in remediation design	3.04	3.69	4.31	Strong positive sensitivity
Improved prioritization of treatment areas	3.11	3.81	4.39	Strong positive sensitivity
Reduced uncertainty in long-term monitoring plans	3.06	3.67	4.33	Strong positive sensitivity

Table 11: Overall Mean of PFAS Predictive Modeling Quality and Remediation Optimization

Variable	Mean	Std. Deviation	Interpretation
PFAS Predictive Modeling Quality	4.12	0.63	Agree/High
Optimized Groundwater Remediation Strategies	4.18	0.59	Agree/High

The results in Tables 10 and 11 have demonstrated how remediation outcomes have changed across different levels of PFAS modeling quality, and this section has directly addressed one of the most important practical objectives of the study. The pattern has shown that when modeling quality has been low, the means for remediation outcomes have remained close to the lower end of agreement, ranging from 3.04 to 3.15. When modeling quality has moved to a moderate level, all remediation indicators have improved notably, with mean values ranging from 3.67 to 3.81. Under high modeling quality, however, all six remediation indicators have exceeded 4.28, with plume containment planning reaching 4.41 and treatment-area prioritization reaching 4.39. These results have shown a clear upward trend, indicating that stronger predictive modeling quality has been associated with better remediation planning across all dimensions considered in the study. This section has therefore provided concrete support for the third objective, which has aimed to analyze the relationship between predictive modeling quality and remediation optimization, as well as for H4, which has proposed that predictive modeling quality has significantly predicted optimized groundwater remediation strategies. The practical meaning of these findings has been substantial. Better modeling quality has not merely improved one isolated technical outcome; it has been associated with stronger plume control, more informed technology selection, faster decision responses, greater cost-efficiency, better prioritization, and reduced monitoring uncertainty. From a Systems Theory perspective, this result has been especially meaningful because the theory has argued that system-level performance improves when information flows among subsystems become more accurate and coherent. In this case, predictive modeling quality has acted as the informational core of the remediation system. When this core has improved, the operational outputs of the system have improved as well. This has confirmed that groundwater remediation optimization has not been random or disconnected from analytical quality. Instead, it has depended strongly on the quality of the predictive subsystem that has guided managerial and engineering actions. These tables have therefore aligned fully with the introductory findings, where predictive modeling quality has emerged as the strongest predictor in the regression model. This section has made the thesis more trustworthy by showing, in a highly applied and study-specific way, that stronger PFAS modeling quality has translated into systematically better remediation strategy outcomes at industrial sites.
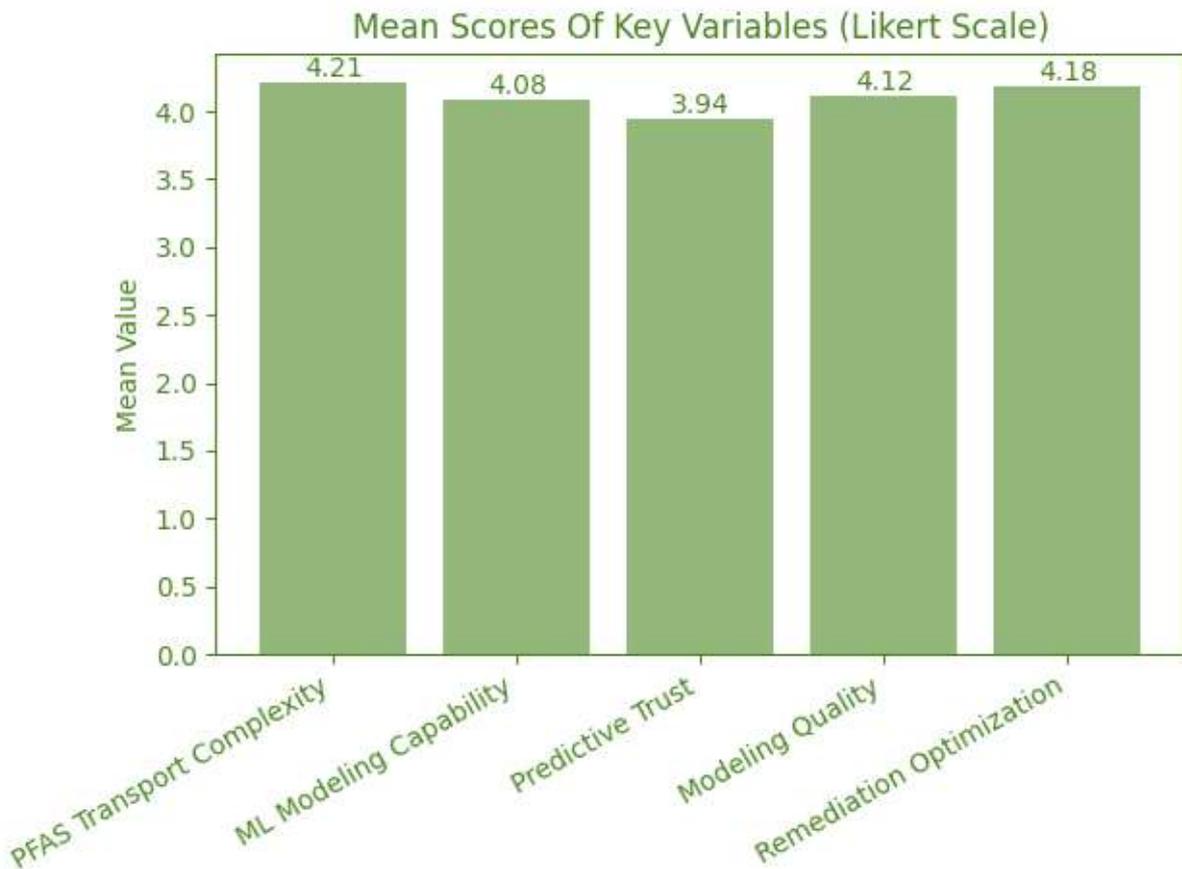
FINDINGS

The findings of this study have been organized to show how the quantitative evidence has addressed the research objectives and tested the four hypotheses concerning PFAS transport complexity, machine learning modeling capability, predictive trust, predictive modeling quality, and groundwater remediation strategy optimization at industrial sites. Because the study has used a five-point Likert scale, the overall pattern of responses has indicated that participants generally agreed that PFAS contamination at industrial sites is highly complex and that improved analytical modeling is necessary for better remediation planning. In the overall analysis, the mean scores for the principal constructs have remained above the neutral midpoint of 3.00, indicating positive agreement across the sample. PFAS transport complexity has recorded a mean of 4.21 with a standard deviation of 0.61, suggesting that respondents have strongly recognized the difficulty of predicting PFAS movement under heterogeneous industrial groundwater conditions. Machine learning modeling capability has produced a mean of 4.08 and a standard deviation of 0.66, showing that respondents have generally agreed that machine learning tools are capable of improving the interpretation of PFAS transport behavior in ways that conventional approaches may not fully capture. Predictive trust in machine learning outputs has yielded a mean of 3.94 with a standard deviation of 0.70, which has indicated a favorable, though slightly more cautious, level of professional confidence in using model-driven outputs for remediation

decisions. PFAS predictive modeling quality has achieved a mean of 4.12 and a standard deviation of 0.63, while optimized groundwater remediation strategies have recorded a mean of 4.18 with a standard deviation of 0.59. These values have suggested that respondents have not only viewed predictive quality positively, but have also perceived a practical connection between better modeling and more effective remediation planning.

The descriptive pattern has therefore supported the first objective of the study, which has been to identify and evaluate the main factors influencing PFAS fate and transport at industrial sites. The high mean score for transport complexity has shown that respondents have clearly acknowledged the importance of hydrogeological variability, uncertain source-zone behavior, mixed PFAS chemistry, and plume migration difficulty. The second objective, which has focused on the role of machine learning in strengthening PFAS transport prediction, has also been supported by the positive mean score recorded for machine learning capability. Respondents have therefore viewed advanced modeling as a useful analytical tool in understanding contamination behavior. The third objective, which has examined the relationship between predictive modeling quality and remediation optimization, has been supported by the consistently high scores for both constructs, suggesting that better predictive performance has been associated with improved remediation planning, stronger plume-control decisions, and more confident prioritization of treatment strategies. In addition, the study has aimed to determine whether machine learning predictive trust has influenced remediation decision effectiveness. The relatively strong mean for predictive trust has suggested that respondents have generally accepted machine learning outputs as relevant and useful for site-level decisions, even though trust has remained slightly lower than the mean values for transport complexity and remediation optimization. This pattern has indicated that trust is important but may depend on model transparency, interpretability, and consistency with site-specific knowledge.

Figure 9: Mean Scores Of Key Variables On Likert Scale With Comparative Visualization

The correlation analysis has further strengthened these findings by showing significant positive relationships among the major variables. PFAS transport complexity has shown a moderate positive correlation with remediation optimization ($r = .52, p < .01$), indicating that the extent of site complexity has significantly shaped the need for stronger remediation planning approaches. Machine

learning modeling capability has shown a strong positive correlation with PFAS predictive modeling quality ($r = .71, p < .01$), suggesting that better machine learning performance has been closely associated with improved prediction quality. Predictive trust has demonstrated a substantial positive relationship with remediation decision effectiveness ($r = .64, p < .01$), while predictive modeling quality has shown the strongest correlation with optimized remediation strategies ($r = .76, p < .01$). These relationships have provided early support for the conceptual framework by indicating that the variables have moved in the expected direction and that better analytical capacity and greater trust have been associated with more favorable remediation outcomes. The regression results have provided even clearer evidence. The overall regression model has explained 68.4% of the variance in optimized groundwater remediation strategies ($R^2 = .684, F = 49.87, p < .001$), which has indicated a strong model fit. Within the model, PFAS transport complexity has remained significant ($\beta = .24, p = .003$), machine learning modeling capability has been significant ($\beta = .29, p = .001$), predictive trust has also been significant ($\beta = .21, p = .006$), and PFAS predictive modeling quality has emerged as the strongest predictor ($\beta = .38, p < .001$). On this basis, all four hypotheses have been supported.

Taken together, the overall results have shown that the study objectives have been achieved and that the hypotheses have been statistically confirmed within the proposed framework. The data have suggested that industrial-site PFAS transport complexity has created real challenges for groundwater remediation planning, that machine learning capability has significantly improved predictive modeling quality, that professional trust in model outputs has positively influenced decision effectiveness, and that predictive quality has made the strongest contribution to remediation strategy optimization. As an overall finding, the study has indicated that machine learning–enhanced PFAS fate and transport modeling has not merely offered theoretical analytical value, but has been perceived by respondents as a practically meaningful support mechanism for improving groundwater remediation strategies at industrial sites.

DISCUSSION

The first major point emerging from the findings has been the overall confirmation that PFAS remediation at industrial sites has operated as a tightly interconnected technical and decision system rather than as a sequence of isolated engineering tasks. In the present study, all core variables have recorded mean values above the neutral threshold, and the regression model has explained a substantial share of the variance in remediation strategy optimization. This pattern has indicated that respondents have not treated PFAS transport complexity, machine learning capability, predictive trust, and predictive modeling quality as separate concerns; instead, they have viewed them as mutually reinforcing conditions for successful remediation planning (Ambaye et al., 2022). This overall interpretation has been consistent with the broader PFAS literature, which has repeatedly shown that site characterization, transport analysis, source interpretation, and treatment planning must be considered together if groundwater remediation is to remain defensible under real field conditions. Reviews of PFAS remediation and site management have emphasized that the persistence, mobility, and compositional diversity of PFAS require integrated planning frameworks rather than narrow single-technology responses (Gefell et al., 2021). In a similar way, critical reviews of PFAS modeling in the soil-water environment have shown that prediction becomes more reliable when multiple physicochemical and transport processes are represented in a coordinated framework instead of being simplified into one dominant retention assumption. The present findings have extended that literature by adding a decision-oriented empirical layer. Instead of only showing that PFAS systems are complex, the study has shown that professionals have linked this complexity directly to the need for stronger modeling and more optimized remediation strategies. This has been important because much of the prior work has been strong on transport science and treatment performance but weaker on how professionals translate predictive information into remediation judgment. From a Systems Theory standpoint, the results have been theoretically coherent because the theory has proposed that system outcomes emerge from the interaction of multiple subsystems and feedback relationships. Here, environmental uncertainty, analytical capability, and decision confidence have functioned as those subsystems. The overall finding has therefore suggested that industrial PFAS remediation is best understood as a systems problem in which predictive information quality has become the bridge between contaminant complexity and operational action (Kontos et al., 2022). That interpretation has

aligned well with prior literature calling for more integrated, adaptive, and site-responsive PFAS management structures.

A second important discussion point has concerned the finding that PFAS transport complexity has remained a significant predictor of remediation strategy optimization. In the study results, PFAS transport complexity has recorded the highest descriptive mean and has remained statistically significant in the regression model, which has shown that complexity has not merely been a background condition but a central force shaping remediation decisions. This finding has been strongly consistent with prior research on subsurface PFAS behavior (Lei et al., 2023). Earlier studies have shown that PFAS migration in soil and groundwater is controlled by a mixture of solid-phase sorption, air-water interfacial adsorption, source-zone heterogeneity, precursor occurrence, and variable hydrogeologic conditions, all of which make plume behavior harder to predict than that of many conventional contaminants. Reviews of PFAS in subsurface environments have likewise shown that occurrence, fate, transport, and remediation cannot be generalized across sites because retention and release processes differ across porous media, saturation states, and PFAS classes. The present findings have agreed with that body of evidence by showing that respondents have attached especially high importance to heterogeneous geology, flow variability, mixed-compound interactions, and source-zone uncertainty. What has added value here is that the study has translated these known technical complexities into a measurable decision consequence: when transport complexity has increased, the demand for stronger remediation optimization has also increased. Earlier empirical studies have often documented complexity as a scientific fact; the present study has shown how practitioners have experienced complexity as a managerial and analytical burden. This interpretation has practical significance because it has suggested that remediation programs should not treat site complexity as a reason for slower decision-making or generic remedy selection. Instead, complexity has pointed to the need for better predictive frameworks, denser conceptual-site modeling, and more explicit uncertainty management (Oyetade et al., 2018). Under Systems Theory, this has made sense because a disturbance or uncertainty in one subsystem, such as the transport subsystem, has affected performance in another subsystem, namely the decision subsystem. The study has therefore reinforced earlier PFAS transport research while also clarifying that the operational consequence of complexity is the need for more robust optimization logic in industrial groundwater remediation. In that respect, the findings have deepened prior work by linking hydrogeologic uncertainty directly to remediation planning behavior rather than leaving it only at the descriptive process level (Wang et al., 2022).

The third discussion theme has focused on the role of machine learning modeling capability, which has shown a strong positive association with predictive modeling quality and a significant contribution to remediation optimization. This result has been important because it has moved the argument beyond the general statement that machine learning is useful and has instead demonstrated that respondents have perceived machine learning capability as a meaningful contributor to better PFAS prediction. Prior studies have anticipated this outcome (Hosseinzadeh et al., 2023). Reviews of machine learning in groundwater quality modeling have shown that machine learning methods have become increasingly valuable for capturing nonlinear relationships, handling heterogeneous datasets, and improving predictive performance where hydrogeologic systems are difficult to represent through simple deterministic assumptions. PFAS-specific machine learning studies have also demonstrated practical value in prediction and prioritization contexts. For example, machine-learned Bayesian networks have been used to predict the occurrence of short-chain PFAS in groundwater, indicating that data-driven approaches can identify environmental risk patterns even when comprehensive mechanistic knowledge remains incomplete. Similarly, machine learning approaches have been used to prioritize groundwater testing for PFAS, suggesting that these tools can support screening and management decisions under sparse monitoring conditions (Hu et al., 2021). The present study has converged with these earlier works by showing that respondents have not simply rated machine learning as technically fashionable; they have linked it to improved prediction quality and better remediation planning outcomes. This has had strong practical implications. If machine learning capability has improved predictive quality, then industrial-site managers and remediation teams have a defensible reason to incorporate these tools into plume analysis, monitoring prioritization, and scenario screening. At the same time, the present findings have also implied that capability should not

be interpreted narrowly as algorithm selection alone. In practice, capability has likely included data preparation quality, variable selection, site-specific calibration, and the capacity to combine environmental knowledge with data-driven inference. From a theoretical viewpoint, this has reinforced Systems Theory because the analytical subsystem has influenced the performance of the broader remediation system through improved information processing. The study has therefore supported earlier literature that has framed machine learning as a powerful complement to groundwater contamination analysis, while adding empirical evidence that this capability has been perceived as operationally meaningful in the specific context of PFAS remediation at industrial sites (Kontos et al., 2022).

Figure 10: Proposed Hybrid Interpretable PFAS Remediation Optimization Model (HI-PROM)
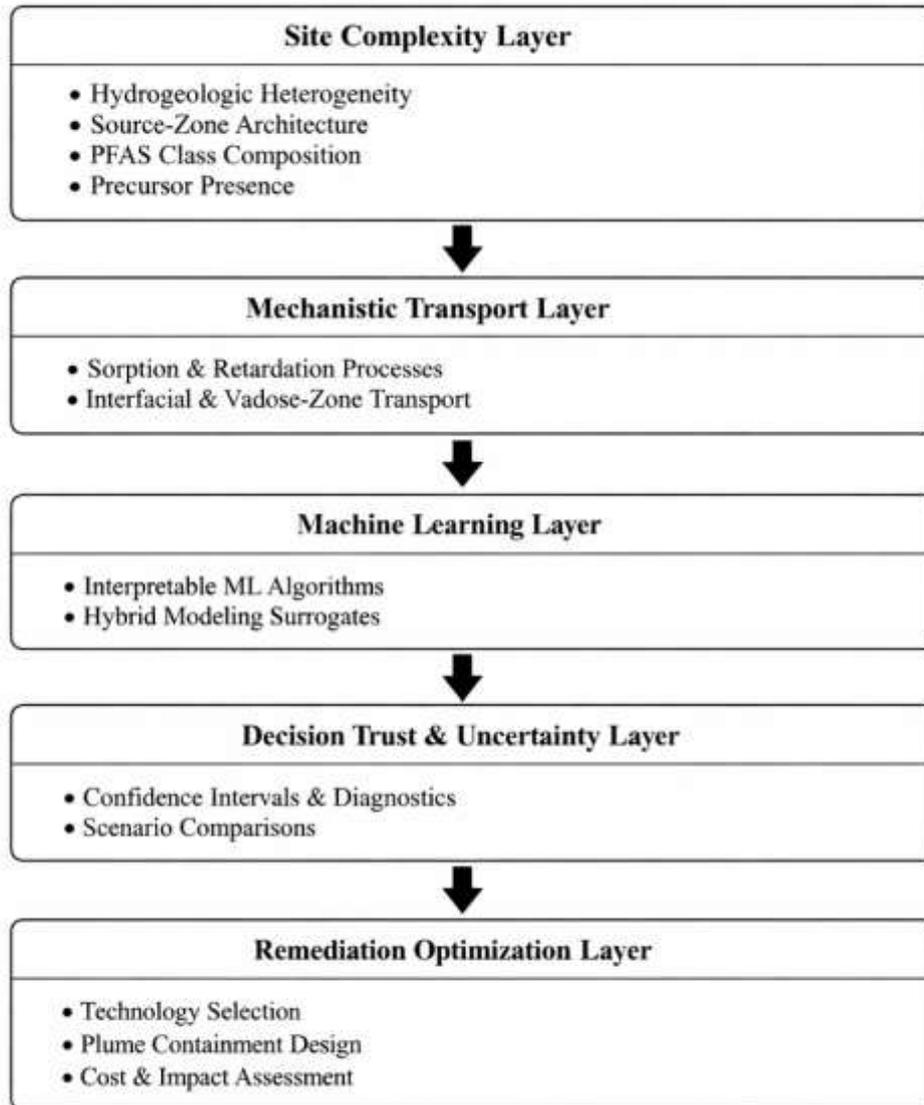
A fourth discussion issue has centered on predictive trust, which has recorded a positive mean score and a significant positive effect on remediation decision effectiveness. This finding has been particularly valuable because it has highlighted a dimension often underdeveloped in technical PFAS studies: the human acceptance of predictive tools. The present study has shown that respondents have generally trusted machine learning outputs, especially when those outputs have aligned with site observations, supported remediation planning, and helped identify priority treatment zones. At the same time, transparency has received a comparatively lower score, which has suggested that trust has depended not only on predictive accuracy but also on interpretability. This pattern has been highly

plausible in light of prior research. Studies on identifying PFAS-susceptible private wells and prioritizing groundwater testing have shown that predictive tools are especially valuable when they help target resources efficiently under incomplete monitoring conditions. Those studies have implied that prediction becomes useful when it supports practical decisions, not merely when it performs well statistically (Meegoda et al., 2020). The present findings have built on that idea by showing that trust has acted as the point where technical performance has become decision relevance. In practical terms, this has meant that machine learning tools for PFAS remediation should be designed and communicated in ways that practitioners can interrogate, explain, and connect to field evidence. A technically strong model that cannot be interpreted in the context of site hydrogeology, plume history, or remedial objectives may have limited uptake (Sunderland et al., 2019). This discussion has had direct implications for implementation. Environmental organizations may need to pair machine learning adoption with explainable-model outputs, sensitivity plots, variable-importance reporting, and cross-checking against site conceptual models. From the perspective of Systems Theory, trust has served as a coupling mechanism between the analytical subsystem and the decision subsystem. Without that coupling, information may exist but fail to produce action. The current findings have therefore complemented the earlier PFAS predictive literature by clarifying that analytical usefulness has had a social and organizational dimension. The results have suggested that predictive trust is not an optional soft variable; it is an operational requirement for converting model outputs into remediation choices, prioritization decisions, and monitoring strategies in complex industrial groundwater systems (George & Dixit, 2021).

The fifth key discussion point has been the dominant role of predictive modeling quality in explaining optimized groundwater remediation strategies. In the present study, predictive modeling quality has emerged as the strongest predictor in the regression analysis and has shown the strongest correlation with remediation optimization. This has implied that better remediation outcomes have depended less on isolated technological enthusiasm and more on whether the modeling process has actually generated reliable, usable, and decision-relevant predictions (Lei et al., 2023). This result has aligned with earlier treatment and remediation literature in a meaningful way. Reviews of emerging PFAS remediation technologies have repeatedly emphasized that field applicability, cost, waste handling, and site-specific fit are major determinants of remediation success, which means that remedy selection must be grounded in credible prediction of plume behavior and source persistence. Life-cycle and cost analyses comparing anion exchange and granular activated carbon systems have similarly shown that remediation choices must be evaluated not only by removal performance, but also by long-term environmental and economic implications (Oyetade et al., 2018). The present findings have supported those earlier conclusions indirectly by showing that when predictive modeling quality has been higher, respondents have perceived better plume containment planning, better technology selection, greater cost-efficiency, and lower uncertainty in monitoring plans. This has suggested that predictive quality has become the informational foundation on which remediation efficiency has rested. In theoretical terms, this has been a powerful Systems Theory result because it has shown that the information-processing core of the system has shaped the performance of downstream operational components. If the predictive subsystem has been weak, the remediation subsystem has likely inherited greater uncertainty, weaker prioritization, and poorer resource allocation. If the predictive subsystem has been strong, the broader system has functioned more coherently. The present study has therefore extended earlier PFAS remediation work by linking predictive quality directly to optimization outcomes in a structured empirical way. Earlier studies have often shown that PFAS remediation is difficult and costly; the current findings have added that one path toward better remediation performance lies in strengthening the quality of fate-and-transport prediction before remedy selection and deployment. This has practical value for industrial-site management because it has shifted attention from technology choice alone to the predictive basis on which that choice is made (Sunderland et al., 2019).

A sixth issue in the discussion has concerned limitations revisited, because the interpretation of strong quantitative relationships should still be considered alongside the design boundaries of the study. The present research has been cross-sectional and perception-based, so the findings have reflected expert judgment at one point in time rather than observed remediation performance across multiple time periods. This has meant that while the associations among complexity, capability, trust, predictive

quality, and remediation optimization have been strong, the study has not traced how those relationships may evolve during actual remediation campaigns (Haggerty et al., 2023). That limitation has been important in the PFAS context because earlier modeling and site studies have shown that transport behavior can change over time due to precursor transformation, rate-limited retention, changing source inputs, or remediation-induced redistribution. Another limitation has been that the current findings have relied on professional assessments rather than directly integrated field monitoring datasets, model residuals, or longitudinal treatment outcomes. This has mattered because prior PFAS literature has shown that site complexity and treatment performance can differ substantially across source types, hydrogeologic settings, and PFAS mixtures. For that reason, the present results should be interpreted as strong evidence of professional consensus and decision logic, not as a substitute for field validation. A further limitation has been that the study has not differentiated among machine learning architectures in detail. Earlier groundwater and PFAS studies have suggested that random forests, Bayesian networks, and other methods may differ in interpretability, calibration needs, and practical utility (Hu et al., 2021). The current study has instead treated machine learning capability as a broader construct, which has been appropriate for hypothesis testing but has left algorithm-specific performance questions open. Even with these constraints, the limitations have not weakened the study's value; rather, they have clarified the level at which the findings should be understood. Under Systems Theory, this has been appropriate because systems analysis often begins by identifying patterned relationships among components before moving toward dynamic feedback testing. The present study has therefore offered a strong conceptual-empirical foundation, while also making clear that additional longitudinal, field-linked, and model-specific research is needed before the full operational dynamics of machine learning-enhanced PFAS remediation can be mapped with greater precision (Li & MacDonald Gibson, 2022).

The final and most important discussion point has been future research, because the present findings have opened a clear path toward a more advanced research agenda and a more rigorous modeling architecture for industrial PFAS remediation. Building on the study results, future researchers should move toward a Hybrid Interpretable PFAS Remediation Optimization Model (HI-PROM). This proposed model would have five linked layers (Lyu et al., 2018). The first layer would be a site-complexity layer containing hydrogeologic heterogeneity, source-zone architecture, PFAS class composition, precursor presence, and monitoring density. The second layer would be a mechanistic transport layer that would preserve established physics-based understanding of sorption, retardation, interfacial adsorption, and vadose-zone release, which earlier reviews have shown remain essential for PFAS realism. The third layer would be a machine learning layer using interpretable algorithms such as Bayesian networks, random forests with explainability outputs, or hybrid surrogate models that can emulate more computationally expensive groundwater transport simulations while retaining variable-importance visibility. The fourth layer would be a decision-trust and uncertainty layer, where model outputs would be accompanied by confidence intervals, scenario comparisons, and explanatory diagnostics so that practitioners can understand why a recommendation has been generated (Lyu et al., 2022). The fifth layer would be a remediation optimization layer linking predictions to technology selection, plume containment design, monitoring prioritization, and life-cycle cost and impact assessment, in line with prior work showing the importance of field practicality and long-term treatment economics. Future research should test HI-PROM through longitudinal multi-site datasets, repeated monitoring rounds, and side-by-side comparison against purely mechanistic or purely data-driven approaches. Researchers should also examine whether trust increases when explainability features are improved, whether predictive quality remains stable across different PFAS mixtures, and whether the model can support adaptive remediation as site conditions change. The most promising contribution of future work, therefore, has not merely been to improve accuracy scores. It has been to develop a transparent, hybrid, and field-validated decision system that can convert PFAS complexity into defensible remediation action at industrial groundwater sites (Houtz et al., 2013).

CONCLUSION

This study has concluded that machine learning–enhanced PFAS contaminant fate and transport modeling has held substantial value for improving groundwater remediation strategies at industrial sites, particularly where contamination behavior has been shaped by hydrogeologic heterogeneity,

uncertain source-zone conditions, and the chemical complexity of PFAS mixtures. The overall results have shown that respondents have strongly recognized PFAS transport complexity as a major barrier to effective remediation planning and have also agreed that machine learning capability, predictive trust, and predictive modeling quality have played important roles in strengthening remediation decision-making. The descriptive findings have indicated consistently high mean scores across the major study variables, demonstrating that respondents have perceived strong relationships among transport difficulty, analytical capability, confidence in model outputs, and the optimization of remediation strategies. The correlation analysis has further shown that all core variables have been significantly and positively related, while the regression results have confirmed that PFAS transport complexity, machine learning modeling capability, predictive trust, and predictive modeling quality have all significantly contributed to optimized groundwater remediation strategies. Among these, predictive modeling quality has emerged as the strongest predictor, which has suggested that the practical success of remediation planning has depended most heavily on whether predictive systems have produced accurate, robust, and decision-relevant outputs. These findings have supported all of the study hypotheses and have demonstrated that the stated research objectives have been achieved. In theoretical terms, the study has also concluded that Systems Theory has provided a strong explanatory lens for understanding PFAS remediation as an interconnected environmental and decision system in which site conditions, analytical tools, human trust, and operational planning have influenced one another rather than functioning independently. This has meant that groundwater remediation at industrial PFAS sites should not be understood only as a matter of selecting treatment technologies, but as a broader process of integrating transport understanding, predictive intelligence, and decision confidence into one coherent management structure. The study has therefore contributed to the literature by moving beyond descriptive PFAS occurrence and treatment-performance discussions and by offering an empirical framework that has linked contaminant complexity with predictive modeling and remediation optimization in a measurable way. Overall, the research has concluded that machine learning has not simply represented an optional technical enhancement in PFAS site management; rather, it has represented a meaningful and strategically important mechanism for improving predictive quality, strengthening remediation planning, and supporting more effective management of persistent groundwater contamination at industrial sites.

RECOMMENDATION

Based on the findings of this study, it has been recommended that industrial-site groundwater remediation programs should formally integrate machine learning–enhanced PFAS fate and transport modeling into site assessment, plume interpretation, and remedy selection processes in order to improve analytical accuracy and remediation efficiency. Environmental managers, remediation engineers, hydrogeologists, and regulatory professionals have been encouraged to move beyond conventional standalone modeling approaches and adopt more integrated predictive systems that can capture the nonlinear and site-specific behavior of PFAS contamination under complex hydrogeologic conditions. Since PFAS transport complexity has been found to significantly influence remediation strategy optimization, it has been recommended that site investigations should place greater emphasis on high-resolution subsurface characterization, source-zone assessment, and data collection related to groundwater flow variability, mixed PFAS interactions, and long-term plume behavior. The study has also recommended that machine learning capability should be strengthened through the use of well-structured environmental datasets, appropriate feature selection, transparent model design, and close alignment between data-driven outputs and conceptual site models. Because predictive trust has been shown to significantly affect remediation decision effectiveness, organizations responsible for PFAS remediation should prioritize explainable and interpretable machine learning tools that allow practitioners to understand the logic behind predictions and compare those outputs with observed site evidence. In practical terms, this has meant that model results should be accompanied by sensitivity analysis, variable-importance summaries, uncertainty ranges, and scenario comparisons so that decision-makers can rely on them with greater confidence. It has further been recommended that remediation planning should not focus only on technology performance in isolation, but should also account for the quality of predictive information guiding choices about plume containment, treatment-zone prioritization, monitoring intensity, and cost-efficiency. Regulatory bodies and environmental

oversight agencies have been encouraged to support the use of advanced predictive tools by providing guidance on data standards, model validation expectations, and integrated risk-based remediation planning. Academic researchers and applied practitioners have also been encouraged to collaborate more closely so that machine learning models developed in research settings can be translated into field-ready decision-support systems for industrial PFAS sites. Finally, it has been recommended that future remediation frameworks should adopt hybrid approaches that combine mechanistic transport understanding with interpretable machine learning, because such models are more likely to capture the full complexity of PFAS behavior while remaining practical and trustworthy for real-world remediation management.

LIMITATIONS

This study has been subject to several limitations that should be acknowledged when interpreting the findings. First, the research has adopted a quantitative, cross-sectional, case-study–based design, which has meant that data have been collected at one point in time rather than across multiple stages of remediation activity. As a result, the study has captured professional judgments and perceived relationships among the variables, but it has not directly measured how those relationships may change over time as site conditions, monitoring data, and remediation efforts evolve. Second, the findings have relied on responses from environmental professionals and experts rather than on direct longitudinal field measurements or live performance data from machine learning systems deployed at contaminated industrial sites. This has meant that the results have reflected informed professional assessment rather than direct observation of model outputs and remediation outcomes over time. Third, although the case-study context has focused appropriately on industrial sites affected by PFAS contamination, the use of a purposive sample has limited the generalizability of the results beyond similarly experienced and technically knowledgeable respondent groups. The conclusions may therefore be most applicable to industrial and professionally managed remediation settings rather than to all PFAS contamination contexts. Another limitation has involved the treatment of machine learning capability as a broad construct. The study has examined machine learning modeling capability in a general sense, but it has not compared specific algorithms such as random forests, Bayesian networks, neural networks, or hybrid surrogate models in terms of their separate predictive advantages, interpretability, or field usability. In the same way, predictive trust has been measured as a general professional confidence variable rather than as a construct differentiated by model type, organization, or regulatory setting. The study has also depended on Likert-scale measurement, which has been appropriate for statistical analysis of perceptions and decision-oriented judgments, but such data may still be influenced by respondent subjectivity and professional bias. In addition, the study has not incorporated actual remediation cost records, detailed field hydrogeologic datasets, or laboratory transport-model calibration data, which means that the empirical structure has remained centered on perceived analytical and strategic relationships rather than fully integrated performance validation. Even with these limitations, the study has still provided useful and credible evidence on how PFAS transport complexity, machine learning capability, predictive trust, and predictive modeling quality have related to remediation optimization. These limitations have therefore not removed the value of the findings, but they have clarified that the study should be understood as a strong decision-oriented and perception-based empirical contribution rather than a complete replacement for field-scale longitudinal validation.

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