

An Efficient Machine Learning System for Prediction of Water Quality with Explainable AI Technique

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Abstract

Water availability and quality have been issues globally, especially in developing nations. Unchecked urbanization and industrialization contaminate natural water supplies and aquifers, potentially introducing physical, chemical, and biological contaminants. Over 80% of illnesses are caused by drinking tainted water, according to a WHO assessment. As clean water sources become more at risk, water quality protection has become of human, environmental, and economic importance worldwide. These water sources, crucial for thousands of communities that draw their water from them, have become increasingly polluted by industrial effluence, farmer's leachate and expanding urban development. The skilled factors, such as pH, turbidity, temperature and total hardness act as parameters to check water quality. AI and ML are truly game changers in water quality monitoring, given that by considering big data, they allow the early prediction of contamination levels. LIME techniques are a subset of the broader Explainable AI (XAI) techniques which aim at increasing interpretability by explaining what a model has decided. Such developments promote better management of water resources and improve the quality of water in the environment.

Keywords: Water quality, rivers, contamination, pH, turbidity, total hardness, artificial intelligence (AI), machine learning (ML), water monitoring, predictive analysis, public health

INTRODUCTION

There is a clear correlation between water quality and ecological and public health concerns. Drinking, farming, and manufacturing are just a few of the many uses for water. With the increased butchered aquatic amusement park and tourist sports in recent years, tourism had a tremendous boost. These factors have made rivers the most used water source by human civilizations throughout history. Salt or groundwater may sometimes be appropriate for solving many issues [1]. Some of the issues that may arise due to the utilization of groundwater are the sinking of land due to less recharge and pollution through the transmission of elements connected with salt water. Hence, river use has garnered interest. A new branch of engineering called river engineering has emerged from the many studies on rivers across the globe. Research on river engineering's most important topics include morphological changes, sediment movement, water purity, and pollutant transmission processes. River engineering specializes

in river hydraulics, including river morphology, sediment transport and flow structure studies.

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A subfield of AI, ML defines the ability of systems to improve and adapt through experience without a specific set of instructions. Therefore, ML methods require data analysis to determine appropriate modifications to make to themselves [2]. In water research, ML offers excellent prospects for evaluating, categorizing, and forecasting water quality WQ indicators [3]. For example, when sufficient data sets are available, ML models may accurately estimate hydrological processes and the transfer of contaminants [4]. For

example, photosensors that depend on identifying the wavelength for a certain color are readily available and may be used to detect WQ characteristics [5]. For instance, one may use calorimetry to determine phosphorus; the reaction of phosphorus with a specific reagent leads to color formation. Different dissolved water pollutants may be detected by other sensors that depend on changes in capacitance values. The results of these methods may provide a large quantity of data that can be reliably and rapidly analyzed using AI.

Forecasts about water purity employing various models, AI models are opaque and seen as black boxes from which choices are extracted without the underlying logic being disclosed. Validation frameworks for water quality management in the current generation may be made more justifiable, transparent, and explainable using systems based on Explainable AI (XAI) [6]. XAI, a white-box solution, may address uncertainty around AI's categorization and regression issues. Using a model-agnostic approach, XAI allows the interpretation of machine learning models to be handled separately.

LIME is one XAI model that explains the local surrogacy connection between a particular characteristic and relevant others. This suggests that, except the dataset's one-row value, the other independent variables may be used to associate a target attribute. For this purpose, LIME may elucidate the desired categorization of water quality for a singular row instance. The proposed work uses XAI, which utilizes locally and globally surrogates and incorporates SHAPLEY [7]. The model offers a solution that considers the importance of each item in defining the goal, the connections and interdependencies between characteristics, and using several plots to illustrate choices, including force plots, summary plots, dependency plots, and decision plots. A thorough description of the characteristics of the water quality and how they affect its classification may be provided using the framework, which is very adaptable [8].

Organization of This Paper

The paper begins with an Introduction to water quality monitoring. Section II reviews AI and ML fundamentals, while Section III covers XAI techniques like LIME for transparent assessment. Technology for water quality monitoring and management is discussed in Section IV. Section V presents the Literature Review, and Section VI concludes with Findings and Future Work on enhancing water quality monitoring and environmental management.

WATER QUALITY PREDICTION: AN OVERVIEW

Water is one of the most valuable resources essential to all life. Water pollution deteriorates the quality of the water, which affects the health of marine life and, therefore, the people who utilize it. Water quality monitoring is thus essential to ensuring the existence of marine life [9].

Rivers, lakes, and streams, among other ambient water bodies, are often graded according to established criteria. Water requirements for various purposes also exhibit standardization. For example, it is important that irrigation water is not too salty or contains compounds that might damage ecosystems when they are absorbed by plants or soil. Additionally, many industrial operations need distinct water quality characteristics. Natural water resources include some of the most inexpensive potable water sources, including surface and groundwater. Natural and anthropogenic processes alike may contaminate these resources [10].

As a result, water quality has been declining at an alarming pace due to fast industrial expansion. In addition, infrastructures have a major impact on water quality due to their lack of cleanliness and public awareness. Polluted water supplies devastate human health, ecosystems, and infrastructures. U.N. estimates put the yearly death toll from water-related illnesses at 1.5 million. An estimated 80% of health issues in underdeveloped nations stem from water contamination. The yearly toll is five million fatalities and 2.5 billion cases of diagnosed disease. More people die from this cause than from terrorist attacks, crimes, or accidents combined [11].

Some Important Physico-Chemical Parameters of Water Quality

Figure 1 shows the normal breakdown of water properties into physical, biological, and chemical groups. The physical characteristics encompass turbidity, temperature, total suspended solids (TSS), and electric conductivity (EC). Biological parameters consider the presence or absence of microorganisms in the water. Contrarily, sulfate, pH, heavy metals, and total nitrogen are chemical parameters.

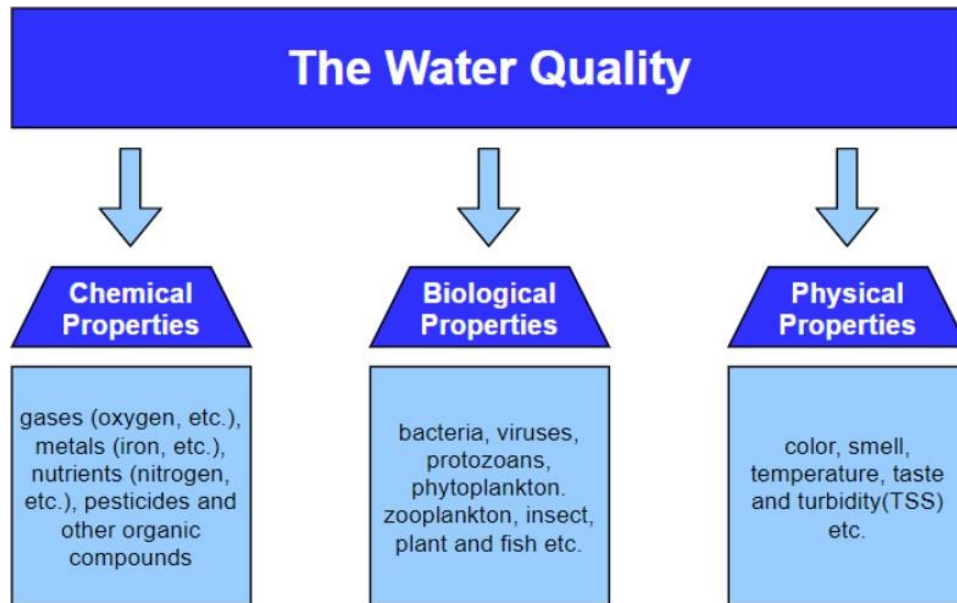


Figure 1. Water quality parameters.

A significant aesthetic metric for water quality testing includes cloudiness, color, odor, and taste; additional relevant qualitative metrics are turbidity, total suspended and dissolved solids, residual chlorine, temperature, and total dissolved solids.

- **Color:** A colorless water is safe to drink. Water has several potential sources of color, including pigments, metals (such as iron, chromium, and manganese), algae, phytoplankton, and industrial waste. At the time of sampling, make mental notes on the color and overall look of the water. As per ASTM-D1209, the commonly used Pt-Co or HU color scale may be described as follows: 0 for colorless water and 500 for very dark, contaminated water [12].
- **Odor and Taste:** For domestic and drinking needs, utilize water that is odorless and tastes well. Water with an unpleasant smell or taste could result from microorganisms, plants, aerobic or anaerobic decay, detergents, metal ions, or even industrial runoff containing ammonia, hydrogen sulfide, phenols, halogens, hydrocarbons, and other chemicals. Odor and taste tests can be done immediately to rule out these potential causes.
- **pH:** Water quality monitoring relies heavily on pH testing, with 7.0 being the ideal pH. Acidity and basicity are indicated by the potential activity of hydrogen ions, which is measured by it. Analyses are conducted using portable pH electrodes and meters. Also, you may get a rough idea of the sample's pH by looking at its color on litmus paper; red indicates an acidic medium and blue indicates a basic one [13].
- **Turbidity:** The degree to which water is impure for human consumption and prohibitively expensive to filter out is a major problem caused by colloidal and suspended particles. Pathogens are also encouraged to flourish with sewage sludge. Due to changes that might occur during shipping, agitation, and storage, turbidity analysis is vital, particularly when done on-site using a turbidity meter. The turbidity of drinking water should not exceed 1 NTU for safety reasons.
- **Total Hardness:** Water hardness has both static and dynamic components. Boiling dissolves the soluble calcium and magnesium bicarbonate salts that cause the material to become temporarily hard. Because boiling cannot dissolve soluble sulfides, chlorides, or nitrates, it causes the

substance to become permanently hard. Water that is too hard to drink, does not lather, and encourages scale buildup in pipes and boilers is unfit for human consumption. A total hardness level of 200 mg/L is within acceptable limits [14].

EXPLAINABLE AI IN WATER QUALITY PREDICTION

In the real world, systems and machines that mimic human intellect to carry out tasks are called artificial intelligence (AI). AI may teach a system to tackle specific issues by analyzing data and drawing on past experiences. The data used may help it develop itself heuristically. Some examples of AI-powered products and services include healthcare, recommendation systems, games, automated driving cars, and sophisticated online search engines.

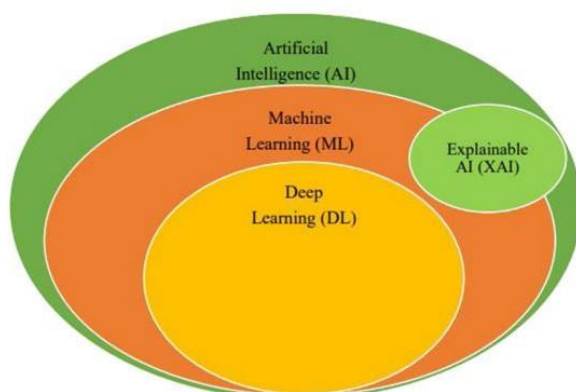


Figure 2. AI vs. ML vs. DL vs. XAI.

Figure 2 illustrates the relationship among AI, ML, DL, and Explainable AI.

Machine Learning Models in Water Quality Prediction

The term “machine learning” (ML) refers to a set of techniques that allow computers to learn from their own experiences and improve their prediction accuracy, pattern recognition, and overall performance. Create an AI-powered app with the help of Machine Learning. For this, they rely on ML methodologies.

ML has become a popular tool for discovering patterns and making predictions in massive datasets generated by various sources. Data capture, method selection, model training, and validation are necessary before implementing machine learning. The selection of an algorithm is a critical step in these procedures.

Here are the two most common types of ML,

- *Supervised Learning*: This type of learning is used when they have been given input and output and must find a mapping function for testing the data. They have used this learning mechanism in the proposed work.
- *Semi-directed Learning*: This is like supervised learning with a difference, that the dataset consists of some missing output labels.
- *Unsupervised Learning*: This type of learning mechanism is used when there is no output label. One of the examples of this learning is clustering technique. This is the technique when similar items are clustered in one group depending upon their properties and behavior irrespective of the output label.
- *Reinforcement Learning*: This learning mechanism is environment-specific learning. This is done to ensure maximum reward for a particular situation.

From the four methods shown above, they have settled on supervised learning since it is well-suited to and produces excellent results with datasets that include class labels, and our data set includes labels

for water quality. The next logical step is obtaining an algorithm compatible with parameter weights [15].

Deep Learning

Deep learning (DL) is concerned with algorithms impacted by how the human brain is structured and functions. Deep Learning (DL) uses Artificial Neural Networks (ANNs) to build a smart model and address important issues. For model training, DL uses both structured and unstructured data; this is shown by visual assistants, such as Alexa and Siri, facial recognition, and other similar technologies. Research in the medical field and the prognosis of potentially fatal illnesses both make use of DL. Deep Neural Networks (DNNs) have shown astonishing predictive capabilities as of late [16].

These days, deep learning is all the rage because of its improved solution for more datasets and its expanded range of computing capacity. An ANN is the basis of a subset of AI known as deep learning (DL) [17]. This DL method uses mathematical examples to train the input data autonomously [18]. Deep learning models include CNNs, ResNets, VGGNets, U-nets, Deep feed-forward networks, Siamese networks, and graph neural networks. Model optimization, feature extraction and recognition, and data pre-processing are the three main components of a Deep Learning model [19].

Explainable AI

In this case, the user's business choice was influenced by an AI algorithm, but neither the program's result nor its methodology is known to humans. Users have a hard time making sense of both the product and the process that led to it. This leads to the use of XAI, or Explainable Artificial Intelligence.

XAI aims to make the inner workings of models intelligible by users by outlining their techniques, procedures, and outputs. The acronym "XAI" stands for "Explainable AI", a concept developed by the DARPA. White box refers to the model's process explanation.

A common definition of XAI is a collection of procedures for describing deep learning models that account for model transparency, accuracy, and results in AI systems. To make the results produced by DL algorithms more understandable and trustworthy, XAI techniques try to provide explanations in a human-readable style. In water quality prediction, XAI approaches provide light on the inner workings of AI models (such as DL, NN, or ensemble methods) and help humans make sense of the results. Building trust, boosting model performance, and allowing stakeholders like scientists, politicians, and environmental managers to test and act on AI-driven predictions are all greatly aided by these explanations.

Local Interpretable Model-Agnostic Explanations (LIME)

The post-hoc method of explanations called Locally Interpretable Model agnostic explanations is to simulate any black-box ML model using a local, interpretable model that may provide an individual explanation for each prediction. Since LIME is not dependent on the original classifier, the authors imply that it may be used to explain any classifier, regardless of the prediction method. The fact that LIME is observation-specific and operates locally implies that it will eventually explain predictions about individual observations. The LIME method looks for nearby data points like the observed one to fit a model. Options for the local model include DT, linear models, etc., all of which are interpretable. For every observation, the following explanations are derived from LIME [20].

USE OF TECHNOLOGY IN MONITORING AND MANAGING WATER QUALITY

Real time data through mere sensors and automated systems has been upheld as pivotal to water quality monitoring and/or management. About the improvements in health conditions and protection of the environment these technologies can help in conducting accurate assessments, detection of pollutants at early stages and efficient management of water resources. Managing and monitoring water quality via the rising use of technological means. Geographic information systems and remote sensing are used

to identify the WQI, monitor land use changes, and identify the source of pollutants. Combining geographic information system (GIS) data with water quality data, can do things like analyze trends, map pollution hotspots, and make better water management choices [21]. Numerous water reservoirs, wastewater treatment stations, and industrial effluent discharges use online monitoring systems to check on water quality parameters in real time. It makes it possible to recognize pollution events promptly, apply measures instantly, make information-based decisions, and follow water quality standards. The results are authentic and accurate when water quality parameters are determined from actual and real-time sampling with modern instruments, such as sensors and probes. Such technologies include conductivity meters, spectrophotometers, fluorometers, and optics and electrochemistry techniques [22].

The general safety and especially the purity of the water sources, primarily rivers, need a constant attention to their quality. Collecting data on these characteristics becomes much easier when field sampling is done manually, and sensors are monitored in real-time [23]. The data is then processed using a machine learning method that utilizes Artificial Neural Networks to forecast and foresee any future water quality problems. There is hope that sensor and information technology-based water quality management, transmission, and monitoring may be enhanced. Professionals utilize these tools to track the water quality indicators shown in Figure 3.

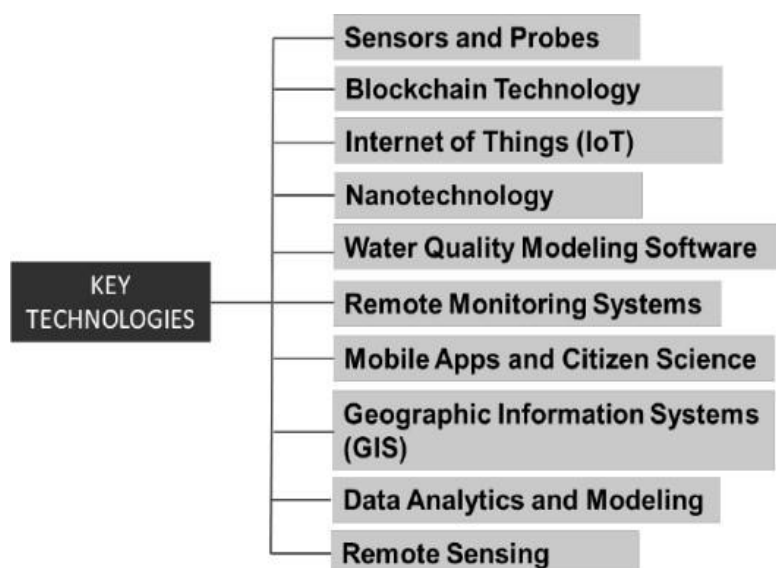


Figure 3. Several key technologies are used for monitoring and managing water quality.

Mathematical models and simulation tools are used in water quality modeling to forecast water quality dynamics, analyze the movement of pollutants, create hypothetical situations, and assess the efficacy of pollution control strategies [24]. Models, such as MIKE, WASP, and QUAL2K improve our comprehension of intricate interactions between bodies of water. By consolidating data on water quality, mobile applications and platforms make it possible for the public to report on the issue and for groups of people to work together to make decisions. Smart water management systems integrate IoT, sensors, and cloud computing to optimize resources and perform real-time monitoring. AI and ML comb through large datasets to identify trends, patterns, predictions, and optimizations in monitoring. Early warning systems round out the system [25]. Improved data accuracy, decision assistance, and cost savings are some advantages. However, there are still hurdles to overcome, such as technology limits, data security, and interoperability [26].

CHALLENGES AND FUTURE DIRECTIONS

The public's access to safe drinking water depends on monitoring and managing water quality. Several problems in this area still need fixing, which comes with the following set of difficulties.

- Data collection, gathering a mountain of data is crucial for efficient water quality management. However, manual data collection in the field is labor-intensive and takes time.
- Heterogeneity and missing data are prevalent in water quality databases, which makes analysis and drawing reliable conclusions challenging.
- It is possible that small water suppliers, public health offices in rural areas, and other organizations may lack the means to adequately check water quality by rules.
- Real-time sensor monitoring is becoming more common but only uses three parameters: water level, temperature, and conductivity. Consequently, it is limited to partially evaluating water quality and identifying possible pollutants.

Managing and monitoring water quality presents both challenges and possibilities. Incorporating cutting-edge technologies like IoT devices, AI, ML, and big data analytics into water treatment systems is something to think about for the future. Novel sensor technologies, intelligent water purification systems, nanoparticles, and environmentally friendly approaches to water recycling, wastewater treatment, and pollution prevention are additional factors to consider [27]. Technical innovation, legislative changes, community involvement, industry partnerships, capacity development, and climate resilience will all need to be part of a plan for water quality monitoring and management in. Green technology, circular economic ideas, sustainable behaviors, and CSR initiatives are all part of the solution, as are better regulatory frameworks and incorporating water quality issues into state and federal water policy [28].

LITERATURE WORK

In this study, Singh, Ramkumar and Hasija (2024) compared analysis of two machine learning algorithms. The Water quality assessment is done using XGBoosting and CatBoosting algorithms. The accuracy of XGBoosting (96%) is higher than the CatBoost algorithm with an accuracy of 94%. Further, there are many solutions to this problem like wastewater treatment and stopping the inlet of pollution into the rivers. But there can be a natural way like planting *Prosopis Juliflora* trees in the affected areas. The roots of these trees efficiently absorb heavy metals from the groundwater, improving water quality in the area [29].

Kularbphettong et al. (2023) employed carefully chosen predictive modeling approaches to semi-automate water quality classification (WQC) and water quality index (WQI) tasks, which may then be used to aid in planning, problem-solving, and decision-making. Here are the preliminary findings, which are satisfactory. The neural network model (NN) performs better than the MLR and the SVM when predicting WQI. The MAE is lower when using the NN model, and when predicting WQC using SVM and ANN models, the accuracy score is higher with SVM [30].

Manoj et al. (2023) evaluated the efficacy of several ML techniques, like LR, KNN, DT, RF, and DL models. With an accuracy of 79.6093%, Random Forests outperformed other ML algorithms, according to data. Deep learning models also showed promising results, with an accuracy of 70.9402% [31].

Murivhami Tartibu and Olayode (2023) generated WQI predictions using an ANN. They considered seven crucial water quality indicators: dissolved oxygen (DO), pH, conductivity, biochemical oxygen demand (BOD), nitrate, total coliform bacteria, and fecal coliform bacteria. The research modeled and predicted the water quality index using seven characteristics. This paper lays forth the basic idea for a water purifying system. The suggested model is clearly effective with a prediction performance of 0.98114 [32].

Hasan and Alhammadi (2021) focused on investigating the feasibility of using machine learning classifiers to track the purity of Abu Dhabi's drinking water. The water department of Abu Dhabi used five ML algorithms – LR, SVM, KNN, NB, and DT – to monitor water quality based on standard physical and chemical data. When predicting water quality levels, the findings reveal that Decision Tree

is more efficient than LR, SVM, KNN, and NB (Table 1). Outperforming LR, SVM, KNN, and NB, DT achieved an accuracy of 97.7011% [33].

Table 1. Summary of the related work on comparative study.

Reference	Methodology	Objective	Key Findings	Challenges
Singh, Ramkumar, and Hasija (2024)	XGBoosting and CatBoosting algorithms.	To assess water quality using machine learning algorithms.	XGBoosting showed higher accuracy (96%) than CatBoost (94%). Solutions include wastewater treatment and natural remediation (e.g., Prosopis Juliflora trees).	Limited to the scope of machine learning models and natural solutions.
Kularbphetong et al. (2023)	Neural Networks (NN), Multiple Linear Regression (MLR), Support Vector Machine (SVM).	To automate water quality classification and index prediction for decision-making.	Neural Network (NN) outperformed MLR and SVM in predicting Water Quality Index (WQI) with lower MAE. SVM performed better in Water Quality Classification (WQC) with higher accuracy.	Balancing model complexity with accuracy.
Manoj et al. (2023)	Deep Learning, SVM, Naive Bayes, K-Nearest Neighbors, Decision Trees, Random Forests, Logistic Regression.	Comparing various machine learning algorithms for water quality assessment.	Random Forests achieved the highest accuracy (79.6093%), while deep learning models showed promising results with 70.9402%.	Diverse model performance and data quality.
Murivhami, Tartibu, and Olayode (2023)	Artificial Neural Network (ANN).	To predict Water Quality Index (WQI) using multiple water quality parameters.	ANN model predicted WQI with an accuracy of 0.98114, using parameters like DO, pH, BOD, etc.	Parameter selection and model adaptability.
Hasan and Alhammadi (2021)	Logistic Regression, SVM, K-Nearest Neighbors, Naive Bayes, Decision Trees.	To monitor drinking water quality in Abu Dhabi.	Decision Tree outperformed all other algorithms, achieving 97.7011% accuracy.	Challenges in handling regional water quality variability.

CONCLUSIONS AND FUTURE WORK

The problems related to water quality increase with time, and therefore, there is the need to develop advanced and efficient methods of monitoring to protect health and environment. Parameters, such as pH, turbidity, temperature and total hardness were essential in determining the water quality in this study. Several advances have been made in recent years, including the use of AI and ML principles to achieve greater prediction towards contamination and realize enhanced data-driven solutions. Moreover, LIME methods have enhanced model interpretability to promote transparency in water quality prediction. Using actual-time surveillance systems, GIS, and sensor-based technologies has also enhanced pollution identification and control advancements. These innovations create the basis for more efficient and rational water management behaviors and actions.

Future work should be directed towards improving the accuracy and scalability of AI and ML water quality models and by gathering more data from different water sources. Therefore, IoT with AI can allow automatic surveillance in different parts of the globe in real time. Moreover, finding more reliable solutions between the AI-based approach and the conventional water quality assessment might be possible. Additional studies on affordable and environmentally friendly technologies will also be important for extending the technology's availability to underdeveloped and rural areas. Collaboration between policymakers, scientists, and technologists will play a key role in implementing these solutions to achieve long-term water quality management and conservation.

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