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Water Quality Monitoring and Assessment Using Machine Learning: A Review of Formulation, Modeling Approaches, and Explainable Artificial Intelligence

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Abstract

Water pollution poses significant risks to human health and environmental sustainability, highlighting the need for accurate water quality assessment and prediction. This review examines the application of machine learning (ML) in Water Quality Index (WQI) assessments, focusing on WQI formulation, predictive modelling approaches, and explainable artificial intelligence (XAI) techniques. A structured literature review is conducted using major scientific databases, including ScienceDirect, Springer, and other relevant sources, following a systematic study selection process. The review analyzes commonly used water quality parameters and highlights how the deterministic structure of WQI influences machine learning modelling, often leading to high predictive performance that reflects predefined formulations rather than independent pattern learning. A comprehensive comparison of single, hybrid, and ensemble ML models is presented, showing that hybrid approaches generally provide improved robustness and accuracy in complex water quality scenarios. In addition, the role of XAI methods in enhancing model interpretability and supporting transparent decision-making is discussed. Key challenges, including limited generalization, model complexity, and interpretability constraints, are identified, and future research directions are proposed to develop more reliable and practical AI-based water quality monitoring systems. Overall, this review provides insights into the integration of machine learning and WQI, emphasizing the importance of balancing predictive accuracy with interpretability for sustainable water resource management.

Keywords: hybrid machine learning; Water Quality Index (WQI); artificial intelligence; XAI; ensemble learning methods; water quality prediction

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1. Introduction

Water pollution is a serious global challenge that threatens the sustainability of freshwater resources [1–3]. Earth's hydrosphere contains approximately 1386 million cubic kilometers of water, of which 97.5% is saline and only 2.5% is freshwater [3]. A large portion of freshwater is stored in ice and snow, while the remaining fraction consists of groundwater and surface water resources [3].

This pollution originates from natural causes, human activities, industrial waste and untreated urban wastewater [2]. This issue has become a major concern as water pollution

has severely affected public health, economic development, and aquatic ecosystems. The contaminated water becomes unsuitable for human consumption, thereby reducing the availability of safe freshwater supplies [1,2].

Water pollutants can be broadly classified into chemical and biological categories [4]. Chemical pollutants include inorganic contaminants, organic compounds, and heavy metals. Inorganic contaminants such as nitrates, phosphates, halogens, and heavy metals commonly originate from agricultural runoff, municipal sewage, and industrial discharges [4].

Thus, increasing severity of water pollution shows a definite downward trend in water quality worldwide, showing the critical need for appropriate monitoring, assessment, and management measures [3]. Individuals, governments, and companies must work together to protect water resources, because water quality is critical to ecological stability and human well-being [2], emphasizing the urgent need for effective monitoring, assessment, and management strategies.

Water quality can be measured using Water Quality Index (WQI) where it becomes a widely used tool for summarizing complex water quality data into a single, interpretable value. Accurate evaluation and prediction of WQI are essential for understanding the dynamic behavior of water bodies and necessary for supporting sustainable freshwater resource management.

In recent years, artificial intelligence (AI) techniques have gained significant attention due to their ability to model complex and nonlinear relationships in water quality datasets with relatively low operational cost. This review primarily focuses on surface water quality assessment, including rivers, lakes, and reservoirs, where WQI is commonly applied.

1.1. Previous Review Studies

Several review studies have investigated the application of artificial intelligence (AI) and machine learning (ML) techniques for Water Quality Index (WQI) prediction and classification. These studies consistently report that models such as Random Forest, Support Vector Machines, Artificial Neural Networks, and Long Short-Term Memory (LSTM) networks can achieve high predictive accuracy in WQI assessment [5]. However, their performance is often influenced by factors such as data quality, regional variability, and the selected WQI formulation method [5].

In addition to WQI-focused studies, some research has explored the application of ML techniques for predicting individual water quality parameters [6]. Empirical studies have also applied multiple ML models, including Random Forest, Neural Networks, and Support Vector Machines [6]. WQI classification and prediction often incorporate preprocessing techniques such as feature selection to improve model performance [7].

Furthermore, regional reviews, particularly those focusing on surface water systems, have compared statistical and machine learning approaches using performance metrics such as RMSE, R^2, and classification accuracy [7,8]. These studies highlight the importance of feature selection, data preprocessing, and model evaluation techniques in improving prediction reliability.

Despite these advancements, existing review studies primarily emphasize model performance comparison, with limited discussion on model design strategies, hybrid and ensemble learning approaches, and the integration of explainable artificial intelligence (XAI) techniques. In addition, challenges such as data imbalance, cross-regional generalization, and real-world deployment remain insufficiently addressed.

Therefore, this review aims to provide a more comprehensive analysis by examining WQI formulation methods, machine learning models, and explainable AI techniques within the context of surface water quality assessment. Table 1 presents a comparison of previous review studies and the scope of this work.

Table 1. Comparison of previous review studies with our study.

Previous Review Studies	WQI Formulation and Implications	Application of Single Models	Application of Hybrid Models	Classification of Water Quality	Explainable AI	Challenges and Future Works
[5]	✗	✓	✓	✓	✗	✓
[6]	✗	✓	✗	✗	✗	✓
[7]	✓	✓	✗	✓	✗	✓
[8]	✗	✓	✓	✓	✗	✓
[9]	✓	✓	✗	✓	✗	✓
Our study	✓	✓	✓	✓	✓	✓

1.2. Scope and Aim of the Review

The aim of this review is to examine recent developments in machine learning approaches for water quality assessment, with a particular focus on the Water Quality Index (WQI) for surface water. The review covers key aspects of WQI formulation and evaluates the performance of various machine learning models, including single-model, hybrid, and ensemble approaches.

In addition, this review discusses the role of explainable artificial intelligence (XAI) in improving model transparency, interpretability, and decision-making in water quality management. Key challenges such as data imbalance, model generalization, and practical implementation are also highlighted, along with potential future research directions.

To provide a comprehensive overview, several comparative tables are included, summarizing WQI frameworks, machine learning models, and XAI techniques used in recent studies.

1.3. Review Methods

This review was conducted through a structured and systematic literature search to identify relevant studies on Water Quality Index (WQI) assessment using machine learning techniques. The scope of the review focuses on key areas, including WQI formulation, machine learning models for prediction and classification, and explainable artificial intelligence (XAI) methods. The selected studies were analyzed to identify current trends, challenges, and research gaps in WQI-based modeling.

The study selection process was carried out following the Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA) guidelines. Relevant articles were identified through searches on major academic publisher platforms, including Springer, Elsevier (ScienceDirect), and MDPI. Additional articles were accessed through ResearchGate when necessary to obtain full-text versions. The search was performed using combinations of keywords such as “Water Quality Index”, “WQI”, “machine learning”, “prediction”, “classification”, and “explainable artificial intelligence”. The search covered studies published between 2021 and 2026, and only peer-reviewed journal articles written in English were included.

The initial search identified approximately 420 records. After removing duplicates and performing title and abstract screening, 120 full-text articles were assessed for eligibility. Following further exclusion based on predefined relevance criteria, 71 studies were finally included in this review. The review was done based on preferred reporting items for systematic reviews and meta-analyses [10]. The overall selection process is illustrated in the PRISMA flow diagram (Figure 1).

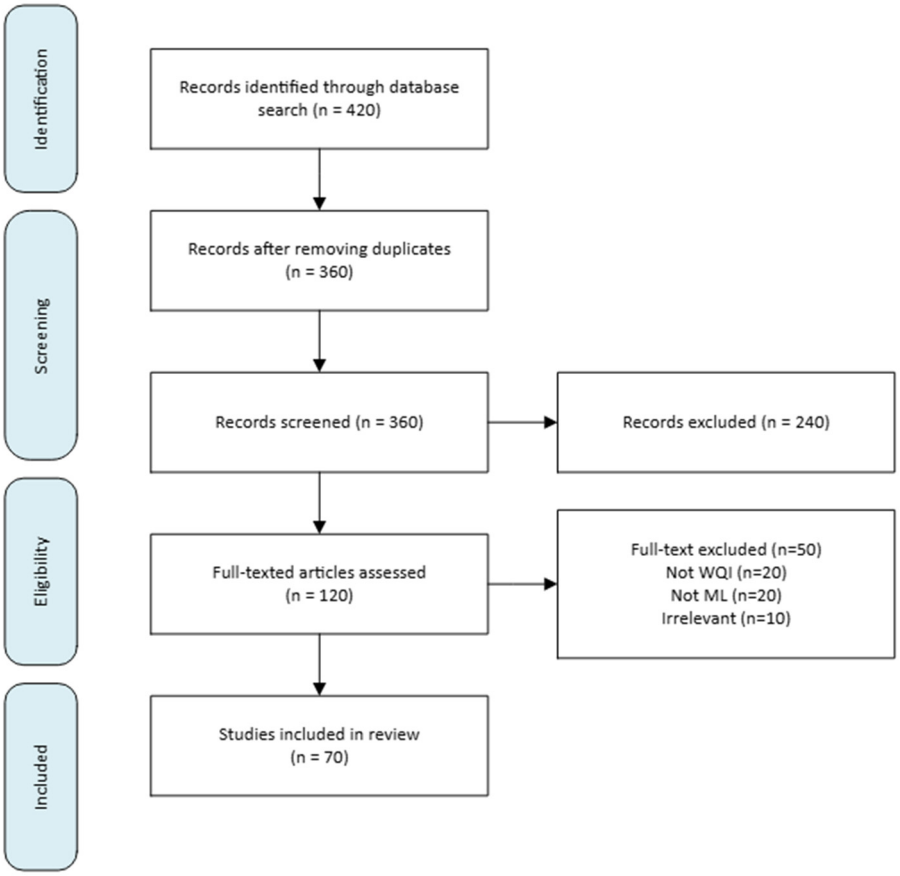

Figure 1. PRISMA Flow Diagram for Study Selection.

1.4. Structure of Review

This section outlines the overall structure of the review and the relationships between its key components. The review is organized into several interconnected parts, including water quality parameters, Water Quality Index (WQI) formulation, machine learning models, and explainable artificial intelligence (XAI) techniques. Figure 2 illustrates how these components are integrated within the context of WQI-based water quality assessment, highlighting the roles of single and ensemble models, evaluation metrics, and future research directions.

Section 1 provides an introduction and reviews previous studies on machine learning for water quality assessment. Section 2 presents the Water Quality Index (WQI) framework, water quality parameters, and the literature review methodology, including the PRISMA-based study selection process. Section 3 reviews machine learning models for WQI prediction, including single, hybrid, and ensemble approaches. Section 4 focuses on explainable artificial intelligence (XAI) techniques. Section 5 outlines key challenges and future research directions, and Section 6 concludes the review. The key contributions of this review are summarized as follows:

- A structured analysis of WQI formulation and its implications for machine learning modelling performance.
- A systematic comparison of single, hybrid, and ensemble machine learning models for WQI prediction and classification.
- A critical examination of explainable AI techniques to enhance transparency, interpretability, and decision support in WQI assessment.

- Identification of key challenges related to generalisation, model complexity, and real-world deployment, along with future research directions for robust and interpretable AI-driven water quality management.

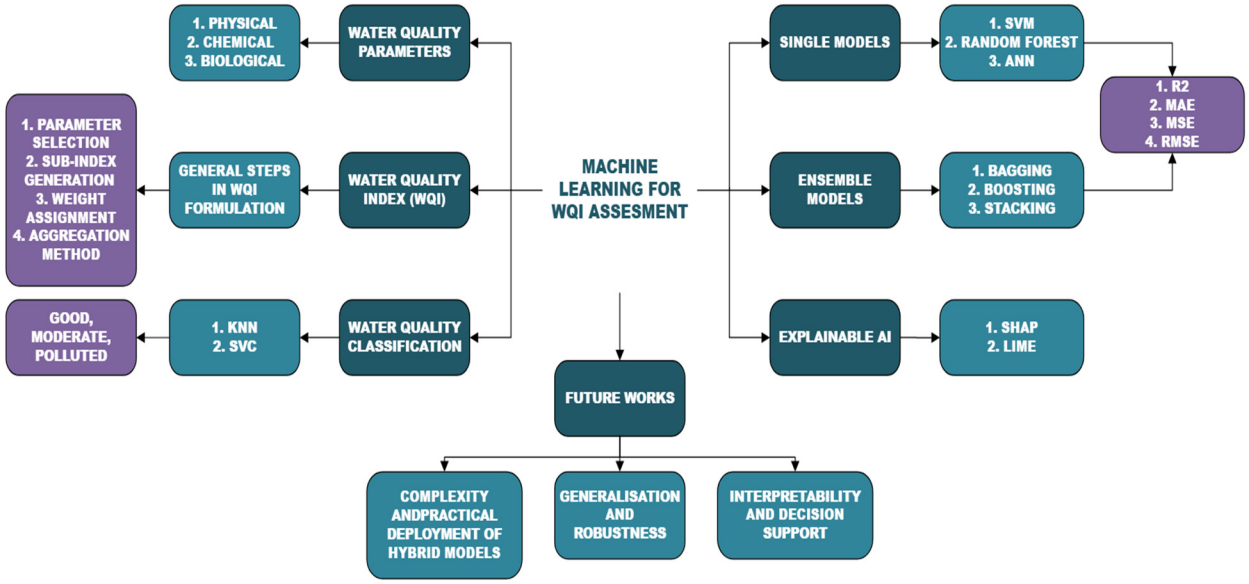

Figure 2. Overview of machine learning approaches for WQI assessment.

2. Water Quality Parameters and Water Quality Index (WQI) Formulation

Various methods are used to evaluate water quality; however, individual parameters alone cannot adequately represent the overall condition of a water resource [11]. In surface water quality assessment, multiple physicochemical and biological parameters are typically considered, including pH, electrical conductivity (EC), temperature, turbidity, total solids (TS), dissolved oxygen (DO), coliforms, biochemical oxygen demand (BOD), alkalinity, chloride (Cl^-), total phosphate (TP), and nitrate (NO_3^-) [11].

Assessing water quality using numerous parameters increases operational costs, requires extensive analysis, and is often time-consuming [11]. Therefore, a cost-effective and efficient approach is needed to simplify complex water quality data into an interpretable form.

The Water Quality Index (WQI) provides such an approach by integrating multiple parameters into a single value that reflects the overall water quality condition [11].

2.1. Water Quality Parameters

Water quality parameters are key indicators used to evaluate the condition of water in relation to human use and aquatic ecosystems [12]. These parameters are generally classified into physical, chemical, and biological categories [12–14].

Physical parameters include turbidity, temperature, colour, taste, and odour [13,15]. Turbidity represents the presence of suspended particles such as silt, clay, and organic matter, which can affect light penetration and aquatic life. Temperature influences the solubility of gases, particularly dissolved oxygen, and plays a critical role in aquatic ecosystem stability. Colour, taste, and odour are also important indicators of water quality and may reflect the presence of contaminants [15].

Chemical parameters include pH, dissolved oxygen (DO), and biochemical oxygen demand (BOD) [15–17]. The pH indicates the acidity or alkalinity of water and significantly affects chemical reactions and biological processes. Dissolved oxygen is essential for the survival of aquatic organisms and is influenced by environmental factors such as temperature and salinity. Biochemical oxygen demand reflects the amount of oxygen

required by microorganisms to decompose organic matter and is commonly used as an indicator of organic pollution [15,17].

Biological parameters refer to the presence of microorganisms such as bacteria, viruses, algae, and protozoa. These indicators are used to assess contamination levels and potential health risks. For example, coliform bacteria are widely used as indicators of fecal contamination and the possible presence of pathogenic organisms [15].

These parameters collectively provide a comprehensive understanding of water quality and form the basis for Water Quality Index (WQI) formulation.

2.2. Water Quality Index (WQI)

The Water Quality Index (WQI) is a widely used method that simplifies complex water quality data into a single numerical value, making it easier to interpret for researchers, policymakers, and the public. Since its introduction in the 1960s, WQI has been applied in water resource management, treatment evaluation, and environmental monitoring. However, the development of a universally accepted WQI remains challenging due to regional differences in environmental conditions, parameter selection, and methodological approaches [18].

The formulation of WQI generally follows a systematic process involving parameter selection, sub-index transformation, weighting, and aggregation. First, a set of relevant water quality parameters is selected to represent overall water conditions [18]. The parameters typically include physical, chemical, and biological indicators such as temperature, pH, dissolved oxygen (DO), biochemical oxygen demand (BOD), chemical oxygen demand (COD), turbidity, and total suspended solids.

Next, the measured parameter values are converted into dimensionless sub-indices using rating curves or mathematical functions, typically scaled between 0 and 100 to allow comparison across parameters with different units [12,19]. Each parameter is then assigned a weight based on its relative importance, and the weighted sub-indices are aggregated to produce the final WQI value using appropriate mathematical functions such as arithmetic or geometric means [20].

One of the earliest and most influential WQI formulations was introduced by Horton in 1965. Horton's model applies a weighted aggregation of sub-indices with additional correction factors, as shown in Equation (1) [18]:

$$QI = \frac{\sum_{i=1}^{n} W_i I_i}{\sum_{i=1}^{n} W_i} M_1 M_2 \quad (1)$$

where W_i is the sum of weight, I_i is the subindices, M_1 is the coefficients of temperature and M_2 is the coefficients of obvious pollution.

This foundational concept has influenced the development of many WQI models worldwide. For example, the National Sanitation Foundation WQI (NSFWQI) uses expert-based weighting, while the Malaysian Water Quality Index (MWQI) adapts parameter selection and weighting to reflect local environmental conditions [12,18].

Overall, WQI serves as an effective tool for summarizing water quality conditions and supporting decision-making in water resource management. It enables authorities to monitor changes over time and implement appropriate strategies to control and reduce water pollution [11].

Table 2 summarizes the key characteristics of widely used WQI models, highlighting differences in parameter selection and aggregation approaches.

Table 2. Comparison of Major Water Quality Index (WQI) Frameworks.

WQI Model	Year	Country	No. of Parameters	Key Characteristics	Limitation	Ref.
Horton Model	1965	USA	10	Considers pH, DO, chloride, conductance, alkalinity, sewage treatment, coliform density, carbon chloroform extract, temperature (multiplicative), and obvious pollution (multiplicative). Easy to compute.	Excludes toxic chemicals; subjective weighting of parameters; limited to fewer parameters.	[18,19]
National Sanitation Foundation WQI (NSFWQI)	1970	USA	Typically 9	Uses Delphi technique with over 100 experts; weights assigned to parameters; widely credible and used.	Fixed parameters may reduce flexibility; region-specific applicability; some indices outdated for modern pollutants.	[18,19]
British Columbia WQI (BCWQI)/CCME WQI	1990	Canada	Multiple	Developed by Canadian Council of Ministers of Environment; updated BCWQI known as CCMEWQI; integrates multiple parameters, including toxicity indicators.	Requires substantial data; complexity may limit use by non-experts.	[18,19]
PKWQI	2022	Pakistan	10	Seven classes from low to very good quality, region-specific	Needs validation for diverse regions; dependent on data	[21]
MWQI (DOE-WQI)	1974	Malaysia	6	Reflects Malaysian standards; simple and practical	Limited parameter coverage	[12]

Table 2 shows that WQI models have evolved from simple weighted aggregation methods, such as the Horton model, to more flexible frameworks like CCME-WQI. While early models emphasize simplicity and ease of computation, more recent models focus on adaptability and region-specific conditions. However, differences in parameter selection, weighting schemes, and aggregation methods highlight the lack of a universally accepted WQI formulation.

2.3. Implications of WQI Formulation for Machine Learning

When the Water Quality Index (WQI) is used as a target variable in machine learning models, the modeling objective shifts from predicting individual water quality parameters to approximating an aggregated index derived from those parameters. In this context, machine learning models are trained using input variables that are mathematically linked to the output through predefined sub-index equations and weighting schemes. This distinguishes WQI-based prediction from conventional environmental modeling, where the target variable represents an independently observed phenomenon.

Since WQI is deterministically computed from the same parameters commonly used as model inputs, machine learning models may primarily learn to replicate the underlying formulation rather than discover new relationships. As a result, high predictive performance may reflect the model's ability to approximate the WQI calculation rather than its capacity for generalization.

Several studies have reported exceptionally high performance under such conditions. For example, ref. [22] achieved near-perfect prediction results (MSE = 0, RMSE = 0, r = 1)

when models were trained using features derived directly from WQI formulation, while ANN models reached an accuracy of 99.96%. Similarly, ref. [23] reported R^2 values above 0.99 for Support Vector Machine and Linear Regression models using raw WQI parameters. These findings suggest that strong performance may partly arise from the deterministic nature of WQI rather than independent pattern learning.

In addition, the fixed weighting structure in WQI formulation can introduce bias into machine learning models. Parameters with higher assigned weights, tend to dominate predictions. Consequently, models may inherit this weighting bias, limiting their sensitivity to other environmentally relevant variables.

The use of region-specific WQI formulations further affects model generalization. Since parameter weights and sub-index relationships are often defined based on local environmental conditions and regulatory standards [24], models trained in one region may not perform reliably in others. This limits the scalability of WQI-based machine learning models across different geographical contexts [24].

These formulation characteristics also may influence model evaluation [9,25]. Metrics such as R^2 and RMSE may overestimate model performance when the prediction task closely resembles a known deterministic relationship [9,22,26]. Similarly, classification accuracy may be inflated when models rely on predefined WQI class boundaries rather than genuine pattern recognition [9,27,28]. Therefore, evaluation strategies should consider robustness, generalization, and interpretability in addition to standard performance metrics.

Despite these limitations, machine learning remains a valuable tool for water quality assessment. Recent studies have explored hybrid modeling approaches, alternative prediction targets, and explainable artificial intelligence (XAI) techniques to address these challenges.

Table 3 summarizes the key implications of WQI formulation on machine learning model behavior, performance, and evaluation.

Table 3. Implications of WQI formulation on machine learning.

Study	Input Features Used	Reported Performance	Key Observation	Formulation-Related Implication
[22]	WQI rating scale features (derived from sub-index formulation)	MSE = 0, RMSE = 0, r = 1 (Linear & Ridge); ANN accuracy = 99.96%	Near-perfect prediction when using formulation-derived features	Models reproduced deterministic WQI structure rather than learning independent patterns
[23]	Raw WQI parameters	R^2 = 0.992 (SVM), 0.991 (LR); RMSE < 0.30	Very high predictive accuracy using original WQI inputs	Strong performance may reflect approximation of predefined aggregation equation
[29]	Weighted WQI parameters	High influence of DO and organic pollution indicators	Dominant parameters drive prediction	ML models inherit weighting bias embedded in WQI formula
[12,22,24]	Region-specific WQI formulations	Performance varies across datasets	Dependency on national weighting schemes	Limited cross-regional generalization capability
[8,25,26]	Standard regression/classification metrics	High R^2 and classification accuracy	Metrics may overestimate real learning capability	Evaluation metrics may reflect deterministic structure rather than model robustness

Table 3 highlights that machine learning models trained on WQI data often achieve high predictive performance due to the deterministic nature of the index. Models tend to reproduce the predefined aggregation structure rather than learn independent relationships, which can lead to overestimated accuracy. In addition, the influence of parameter weighting and region-specific formulations further limits model generalization and interpretability.

3. Water Quality Index Assessment Based on Artificial Intelligence (AI)

The increasing importance of maintaining water quality has resulted in the widespread use of advanced monitoring and evaluation technology. Traditional techniques have limitations in dealing with complicated and nonlinear connections among water quality parameters.

Artificial intelligence (AI), particularly machine learning approaches, has emerged as a powerful tool for assessing water quality data. These approaches can process both historical and real-time datasets to model complicated patterns and improve WQI prediction.

In recent years, machine learning algorithms have been widely used for WQI prediction and classification, allowing for more accurate and efficient water quality assessments. The next sections discuss several machine learning approaches, such as single models, hybrid and ensemble models, and explainable artificial intelligence (XAI) techniques.

3.1. Machine Learning Models for Water Quality Assessment

Machine learning (ML) techniques have been widely applied in water quality assessment due to their ability to model complex relationships among physicochemical parameters. Among these, several single-model approaches have been extensively used for Water Quality Index (WQI) prediction.

Support Vector Machine (SVM) is commonly used for water quality prediction due to its ability to handle nonlinear relationships and high-dimensional data [29,30]. Previous studies have shown that SVM can achieve high prediction accuracy, particularly when using a reduced number of key input parameters [29,30].

Random Forest (RF) is an ensemble-based learning method that improves prediction accuracy by combining multiple decision trees [31,32]. It has been widely applied in WQI prediction, with studies demonstrating its robustness and superior performance compared to some traditional models [32].

Multiple Linear Regression (MLR) is a statistical method used to model linear relationships between water quality parameters and target variables [33–35]. While it is simple and interpretable, its limitation in capturing nonlinear relationships can reduce prediction accuracy in complex environmental systems [33,34].

Artificial Neural Networks (ANNs) are widely used in water quality prediction due to their ability to capture nonlinear patterns in environmental datasets [32,36]. Comparative studies have shown that ANN models often outperform traditional linear models in predicting key water quality indicators.

Table 4 summarizes recent studies applying machine learning models for WQI prediction across different regions and datasets.

Table 4. Recent ML studies in WQI prediction.

Year	Location	Model	Size of Data	Input Parameters	Ref.
2025	Mranti Lake (Selangor), Klang River (Selangor), Semenyih River (Selangor), Labu River (Negeri Sembilan), Malacca River (Melaka), Muar River (Johor)	Hybrid Decision Tree Regression (DTR), Autoregressive Integrated Moving Average (ARIMA) and Random Forest (RF)	-	Dissolved Oxygen (DO), Ammoniacal Nitrogen (AN), Chemical Oxygen Demand (COD), Biochemical Oxygen Demand (BOD), pH and Total Suspended Solid (TSS)	[37]

Table 4. *Cont.*

Year	Location	Model	Size of Data	Input Parameters	Ref.
2025	Mranti Lake (Selangor), Klang River (Selangor), Semenyih River (Selangor), Labu River (Negeri Sembilan), Malacca River (Melaka), Muar River (Johor)	Neuro-Adapt Fuzzy Strategist (NAFS)	-	Dissolved Oxygen (DO), Ammoniacal Nitrogen (AN), Chemical Oxygen Demand (COD), Biochemical Oxygen Demand (BOD), pH and Total Suspended Solid (TSS)	[38]
2025	Yangtze River Basin (YRB), Huai River Basin (HRB), Huangshui River Basin (HSB), China	Long Short-Term Memory (LSTM)	YRB (15 years), HRB (10 years), HSB (10 years)	Ammonia Nitrogen (AN), Biochemical Oxygen Demand (BOD), Chemical Oxygen Demand (COD), Dissolved Oxygen (DO), Total Phosphorus (TP), Hydrogen Ion Concentration (pH)	[39]
2025	Ganga river, India	Self-Attentive Long Short-Term Memory (SA-LSTM), LSTM, Convolutional Neural Networks (CNN), Artificial Neural Networks (ANN), Random Forest (RF), Gradient Boosting (GB), Extreme Gradient Boosting (XGBoost), Adaptive Neuro-Fuzzy Inference System (ANFIS), Support Vector Machines (SVM), Hybrid Models	-	Temperature, pH, COD, TP, DO	[40]
2025	Kaggle "Water Potability Dataset"	Logistic Regression, Decision Tree, Random Forest, XGBoost, Support Vector Machines (SVM), K Nearest Neighbors (KNN), AdaBoost	-	pH, Hardness, Solids (Total Dissolved Solids, TDS), Chloramines, Sulfate, Conductivity, Organic Carbon, Trihalomethanes (THMs), Turbidity	[41]
2024	Tumkur district, Karnataka state, India	Regression Tree, MLR, SVR, ANN	-	total hardness, pH, alkalinity, turbidity, chloride, dissolved solids, and conductivity	[23]
2024	Mirpurkhas, Sindh, Pakistan	Random Forest, Gradient Boosting, SVM, XGBoost, KNN, Decision Trees	2 months	TDS, Sodium, Calcium, Magnesium, Potassium, Well Depth, Nitrate (NO_3^-), etc.	[42]
2023	Langat River, Malaysia	Support Vector Regression (SVR)	19 years	DO, BOD, CO, pH, SS, AN	[30]
2022	Various rivers, India	DT, Multiple Layer Regression (MLR), RIDGE, LASSO, SVR, RF, Extra Tree Regression, ANN	11 years	DO, pH, CO, BOD, NO_3, FC	[22]
2022	Klang, Langat River, Malaysia	RF, AdaBoost, SVR DT and multilayer perception (MLP)	-	conductivity (COND, salinity (SAL), turbidity (TUR), dissolved solids (DS), nitrate (NO_3), chloride (Cl), phosphate (PO_4), arsenic (As), chromium (Cr), zinc (Zn), calcium (Ca), iron (Fe), potassium (K), magnesium (Mg), sodium (Na), *E. coli*, and total coliform	[43]
2022	Bhavani river, Kerala	RF, SVR, MLP, MLR	4 years	temperature, pH, conductivity, BOD, COD, Nitrate-N, fluoride, potassium, TC, FDS, chloride, sodium, TDS, hardness and sulphate	[44]
2022	Lattakia City Lake, Syria	MLR, Ridge	1 year	pH, Nitrate (NO_2), Nitrate (NO_3), Phosphate (PO_4), turbidity, EC	[35]
2022	Jinjiang River Basin, China	ANN-WT-LSTM (Artificial Neural Network + Wavelet Transform + LSTM)	-	Input variables consisted of water quality indicators, such as Dissolved Oxygen (DO), CODMn, and other physicochemical indicators measured over time	[45]

Table 4 shows various machine learning models that have been applied for WQI prediction, with ANN, SVM, and Random Forest are among the most frequently used approaches. These models are preferred due to their ability to handle nonlinear relationships

and complex environmental datasets. In recent years, advanced models such as LSTM and hybrid approaches have demonstrated improved performance, particularly for time series water quality data.

3.2. Hybrid and Ensemble Learning Models for Water Quality Assessment

Hybrid modelling approaches are used in water quality assessments which combine multiple machine learning algorithms to exploit the strengths of individual models and overcome their limitations. This strategy has gained increasing attention in Water Quality Index (WQI) studies, where water quality datasets often consist of complex nonlinear relationships, noise, and imbalanced class distributions [45]. These characteristics can reduce the effectiveness of single-model approaches, particularly when minority water quality classes are underrepresented but environmentally critical. Hybrid and ensemble models provide a structured means of addressing these challenges by improving prediction robustness and reliability.

The primary advantages of hybrid and ensemble models is enhanced predictive performance. This can be achieved by combining outputs from multiple learners; ensemble approaches frequently achieve higher accuracy and stability compared to individual models [46–51]. In water quality applications, this improvement is important for capturing nonlinear interactions among physicochemical parameters and reducing sensitivity to noise in monitoring data.

Hybrid and ensemble models also demonstrate improved resistance to overfitting and underfitting. Bagging-based methods, such as Random Forest, reduce model variance by aggregating predictions from multiple learners trained on different data subsets [48]. Conversely, boosting-based techniques iteratively focus on correcting errors made by previous models, thereby reducing bias and improving generalisation performance [45,48]. These characteristics are particularly beneficial for WQI prediction, where monitoring data may be heterogeneous and temporally variable.

Furthermore, hybrid models offer flexibility in handling complex datasets by integrating complementary modelling paradigms. For example, combining linear and nonlinear models enables the capture of both simple trends and intricate patterns within water quality data. This adaptability makes hybrid approaches well suited for real-world WQI prediction tasks, where datasets are often imbalanced and influenced by multiple interacting factors. As a result, hybrid and ensemble learning strategies have become an important direction for advancing data-driven water quality monitoring and prediction [45,48].

Ensemble learning has been widely used by various researchers due to its better predictive performance through multiple models. Table 5 summarizes recent studies applying hybrid and ensemble learning models for WQI prediction across different datasets and environmental conditions.

Table 5 summarizes recent applications of hybrid and ensemble learning approaches in water quality prediction. These models consistently demonstrate improved performance compared to single-model approaches, particularly in handling complex, nonlinear, and imbalanced datasets.

In water quality studies, hybrid models commonly combine deep learning architectures, such as Long Short-Term Memory (LSTM), with machine learning algorithms like XGBoost, Support Vector Machines, and Random Forest. These combinations are effective for time-series data, where temporal patterns play a significant role in water quality dynamics. In addition, optimization-based hybrid models further enhance prediction accuracy and model convergence.

Overall, the literature indicates that hybrid and ensemble approaches provide a more robust and flexible modelling framework for WQI prediction. By integrating complemen-

tary modelling techniques, these models are better suited for real-world water quality monitoring and decision-making applications.

Table 5. Recent Hybrid and Ensemble Learning Models for Water Quality Assessment.

Hybrid Model	Hybrid Strategy	Dataset	Findings	Ref.
Hybrid LSTM, XGBoost, and K-Means clustering	Combination of LSTM, XGBoost and K-Means Clustering	water quality dataset from Niger Delta	XGBoost best: R^2 = 0.95, MAE = 8.21, RMSE = 10.12; LSTM less accurate due to static data	[52]
A hybrid model combining LSTM Seq2Seq with multiple ML models (XGB, ADR, SVR, RF, and k-NN),	The LSTM Seq2Seq output is fed into machine learning models for a second prediction step, helping make the model more stable and reduce errors over longer-term predictions	Real-time univariate water quality data	The hybrid model improves accuracy, especially for mid-to-long-term predictions (up to 48 h), outperforming standalone LSTM Seq2Seq. However, delays still occur in longer-term forecasts, which future work aims to address	[53]
Stacked ensemble deep learning (SE-DL)	stacking	Water quality parameters	SE-DL achieved an impressive average accuracy of 95.69%, along with precision, recall, and F1 scores of 94.96%, 92.92%, and 93.88%, respectively	[45]
Four new hybrid models: COA-LSTM-XGBoost (CLX), COA-LSTM-LSSVM (CLL), SCOA-LSTM-LSSVM (SLL), SCOA-LSTM-XGBoost (SLG) combining optimization algorithms (COA, SCOA), LSTM, and machine learning models (XGBoost, LSSVM)	Three-step process: (1) Optimization algorithms (COA, SCOA) tune the parameters of LSTM, XGBoost, LSSVM; (2) LSTM captures temporal patterns in the water quality time series; (3) XGBoost and LSSVM use these patterns to make final WQI predictions	Monthly water quality data from 2000 to 2024	The SCOA-LSTM-XGBoost model achieved the highest accuracy (WI = 0.96, EVS = 0.95, TS = 0.021). Overall, hybrid models outperformed standalone models, and optimization algorithms (SCOA, COA) significantly improved performance	[54]
Back Propagation Neural Network (BPNN) optimized by an Adaptive Evolutionary Artificial Bee Colony (AEABC) algorithm combining dynamic adaptive factors, probability selection, and gradient initialization.	Combines machine learning (BPNN) with the improved optimization algorithm (AEABC) to enhance convergence speed and prediction accuracy for Water Quality Indexes (WQIs).	Water quality data from the Luoyang River Basin	The AEABC-BPNN model converged in 14 iterations, reduced MSE by ≥25.2%, achieved MAPE < 7.58%, and 100% PICP, showing high accuracy and robustness for long-term water quality prediction	[55]
Gradient Boosting (GB)—Random Forest (RF)	Boosting, bagging	Water quality parameters	The two ensembled ML models (GB and RF) achieved good performance for WQI prediction with R^2 values of approximately 0.85 for GB and 0.86 for RF on validation datasets	[56]
MLA-Mamba	Combines advanced sequence modeling (Mamba) + attention-driven spatial correlations + multi-task learning; optimized with Gradient Reparameterization Optimization (GRPO)	Surface water datasets	The MLA-Mamba model consistently outperforms classical statistical, machine learning, and other deep learning baselines across MSE, MAE, RMSE metrics; achieves up to 10–20% relative improvement	[57]
ANN-Wavelet Transform (WT)-Long Short-Term Memory (LSTM)	combining the outputs of the ANN and LSTM models, with the Wavelet Transform	Water quality parameters	Proposed hybrid model significantly improves prediction accuracy compared to traditional models, demonstrating the effectiveness of ANN-WT-LSTM	[58]
Ensemble 6 ML algorithms, which include DT, Logistic Regression (LR), RF, Support Vector Machine (SVM), AdaBoost, and XGBoost (XGB)	combining the predictions of multiple base classifiers through a hard majority voting mechanism	Water quality parameters	The research highlights that the ensemble model outperformed individual models, achieving an accuracy of 97.3%	[59]

3.3. WQI Classification and Water Quality Status Assessment

Machine learning classification models are widely applied to categorize Water Quality Index (WQI) into discrete water quality classes, such as good, moderate, or polluted,

based on physicochemical parameters. Commonly used classifiers in WQI studies include Random Forest, Support Vector Classification, and K-Nearest Neighbor models, owing to their ability to handle nonlinear decision boundaries and complex feature interactions [60–62].

Random Forest classifiers are frequently adopted due to their robustness to noise and reduced risk of overfitting, particularly when dealing with heterogeneous water quality datasets [60,63]. Support Vector Classification is effective in separating water quality classes in high-dimensional feature spaces, while K-Nearest Neighbour offers a simple, instance-based approach for class assignment [62]. These models have been successfully employed in various studies to classify water quality status using WQI values or derived classes [62].

Despite their reported high classification accuracy, WQI classification models are often influenced by predefined class boundaries and imbalanced class distributions. As a result, performance metrics such as accuracy may not fully reflect the model's ability to generalize across different water bodies or monitoring conditions. These challenges highlight the need for careful evaluation and motivate the use of more advanced modelling strategies, which are discussed in subsequent sections.

To provide a structured comparison of commonly used classification models in WQI-based water quality assessment, Table 6 summarizes their working principle, strengths, limitations, and sensitivity to class imbalance as reported in recent studies.

Table 6. Comparative Analysis of Machine Learning Classifiers for WQI-Based Water Quality Status Assessment.

Model	Working Principle	Strengths	Limitations	Sensitivity to Class Imbalance	Ref.
Random Forest (RF)	Ensemble of decision trees using bagging	Robust to noise; handles nonlinear relationships; reduced overfitting in heterogeneous datasets	Reduced interpretability; may bias toward majority class	Moderate	[60,63]
Support Vector Classification (SVC)	Optimal hyperplane separation in high-dimensional feature space	Effective in separating nonlinear classes; strong generalisation under balanced conditions	Sensitive to kernel selection and hyperparameter tuning	High	[61]
K-Nearest Neighbor (KNN)	Distance-based instance classification	Simple implementation; adaptable to nonlinear decision regions	Sensitive to noise; computationally expensive for large datasets; biased toward dominant class	High	[62]

The comparison in Table 6 indicates that while Random Forest provides strong robustness and general performance, models such as SVC and KNN are more sensitive to class imbalance and parameter selection. Overall, classifier performance in WQI prediction is highly dependent on dataset characteristics, highlighting the importance of appropriate model selection and evaluation strategies.

4. Interpretability and Explainable AI (XAI) in WQI Modelling

Although machine learning and hybrid models have demonstrated strong performance in Water Quality Index (WQI) prediction, their practical adoption in water quality management is often limited by a lack of interpretability. Many advanced models operate as black boxes, providing accurate predictions without clear explanations of how input parameters influence the output. In environmental applications, where decisions affect public health and ecosystems, understanding model behavior is essential for building trust and supporting regulatory decision-making.

As a result, explainable artificial intelligence (XAI) techniques have gained increasing attention as tools for improving transparency and accountability in ML-based WQI modelling.

4.1. Importance of Interpretability in ML-Based WQI Prediction

Despite the high predictive accuracy of machine learning models, their application in water quality management is often constrained by limited interpretability. Black-box models do not provide insight into the reasoning behind predictions, which can reduce user confidence and hinder their adoption in critical applications such as drinking water safety assessment [64,65]. In environmental monitoring, interpretability is therefore considered essential rather than optional.

Interpretability enables stakeholders to understand how specific physicochemical parameters influence WQI predictions. To address this issue, XAI techniques such as SHAP (Shapley Additive Explanations) and LIME (Local Interpretable Model-Agnostic Explanations) are widely used to provide feature-level insights into model behavior [64,66,67]. SHAP quantifies the contribution of each parameter to the model output, allowing researchers to identify key factors such as biochemical oxygen demand, dissolved oxygen, pH, and turbidity that significantly affect WQI predictions [66,67]. In contrast, LIME provides local explanations by approximating the model behavior for individual predictions, enabling case-specific analysis in operational scenarios [64].

Beyond improving transparency, interpretability is crucial for regulatory compliance, risk assessment, and informed decision-making. Water authorities require an understanding of model predictions to evaluate them against safety standards and environmental regulations [65–67]. Feature-level explanations help identify pollution sources, detect anomalies, and support targeted mitigation strategies. By translating complex model outputs into human-readable insights, XAI enhances model reliability and supports the deployment of machine learning in real-world water quality monitoring systems.

4.2. Explainable AI Techniques Applied in WQI Studies

Explainable artificial intelligence (XAI) techniques are increasingly used in Water Quality Index (WQI) studies to improve transparency and understanding of machine learning model predictions, particularly when complex classifiers and ensemble models are employed [65,67]. Most existing WQI-related studies rely on a small number of practical, model-agnostic explanation methods that can be applied across different machine learning algorithms without modifying the underlying model structure [65].

Among these techniques, SHapley Additive exPlanations (SHAP) is the most widely adopted approach in WQI modelling due to its ability to explain both overall model behavior and individual predictions [64,66,67]. Several studies use global SHAP analysis to identify dominant water quality parameters influencing WQI predictions or classifications, such as biochemical oxygen demand, dissolved oxygen, turbidity, chemical oxygen demand, pH, and nutrient concentrations [64,66,67]. In addition, local SHAP explanations, commonly visualized using force plots or waterfall plots, are applied to clarify why a specific water sample receives a high or low WQI value, enabling case-based interpretation and validation of model outputs [66,67].

Second technique is Local Interpretable Model-agnostic Explanations (LIME), primarily employed to interpret individual predictions in WQI and water quality classification tasks [64,66]. By approximating complex models locally around a given data instance, LIME highlights which physicochemical parameters contribute most to a particular classification, such as identifying factors responsible for categorising water as potable or polluted [64].

Some studies also apply LIME before and after data preprocessing to examine how feature transformations influence model decision boundaries and prediction behaviour [66].

Overall, the reviewed literature indicates that XAI techniques in WQI studies are mainly used to complement predictive accuracy by providing interpretable insights into model decisions rather than replacing existing machine learning models [65,67]. The combined use of SHAP for global and local explanations and LIME for instance-level analysis helps bridge the gap between complex data-driven predictions and domain understanding, thereby enhancing the reliability and practical applicability of AI-based WQI assessment systems [64,67]. Table 7 presents a comparison of commonly used XAI techniques in WQI studies, highlighting their strengths, limitations, and applications in interpreting machine learning models.

Table 7. Comparison of Explainable AI (XAI) Techniques in WQI Studies.

XAI Method	Type	Strengths	Limitations	Applications in WQI	Ref.
SHAP	Global + Local	Provides consistent and theoretically grounded feature attribution; supports both global and local interpretation; effective visualization tools	Computationally expensive; may require expertise to interpret	Identifies globally important parameters such as DO, turbidity, pH; explains contribution of features to predictions and class probabilities	[64,66]
LIME	Local	Provides interpretable explanations for individual predictions; model-agnostic and easy to apply; useful for analyzing feature influence before and after preprocessing	Explanations are local and may not generalize globally; sensitive to sampling and approximation	Explains why specific water samples are classified (potable vs. polluted)	[64,66]

Table 7 shows that SHAP and LIME are the most used XAI techniques in WQI studies, each serving complementary roles in model interpretation. SHAP provides both global and local explanations, making it suitable for identifying key water quality parameters influencing model predictions, while LIME focuses on local explanations for individual cases. Although both methods improve model transparency, SHAP is computationally more intensive, whereas LIME may lack global consistency. Together, these techniques enhance the interpretability and reliability of machine learning models in water quality assessment.

5. Challenges and Future Works

Despite the rapid growth of artificial intelligence (AI) in surface water quality evaluation, significant problems remain, limiting its real-world application and long-term reliability. The main disadvantages include limited generalization capability, lack of interpretability, high model complexity, and challenges in real-world application. Addressing these problems is critical for transforming AI-based models from experimental tools to dependable and scalable decision-support systems. This section summarizes the primary constraints observed in prior studies and proposes future research topics for establishing robust and interpretable AI-driven water quality control systems.

5.1. Generalisation and Real-World Robustness

One of the primary challenges in AI-based water quality modelling is limited generalization across different environmental conditions. Many models are trained using data from specific regions, which restricts their applicability to other geographical locations [68]. As a result, models may perform well locally but fail when applied to datasets with different climatic or hydrological characteristics.

Single machine learning models are particularly vulnerable to poor generalization due to sensitivity to model structure and parameter selection [68]. Ensemble approaches, such as stacking and Bayesian model averaging, have been proposed to improve robustness by combining multiple models. However, these methods introduce a trade-off between prediction stability and computational complexity, and they do not always outperform the best individual model [68].

Future work should focus on developing models that are validated across diverse datasets and geographical regions, as well as incorporating domain knowledge to improve robustness under varying environmental conditions.

5.2. Interpretability and Decision Support

The lack of interpretability remains a significant barrier to the adoption of AI models in water quality management. Although advanced models achieve high predictive accuracy, their black-box nature limits trust, regulatory acceptance, and decision-making transparency [69,70].

Recent studies have explored the use of explainable artificial intelligence (XAI) techniques, such as SHAP, to provide both global and local explanations of model predictions [70]. In addition, hybrid models such as the Neuro-Adaptive Fuzzy Strategist (NAFS) demonstrate that it is possible to achieve a balance between predictive performance and interpretability [38].

Future research should focus on integrating interpretable modelling techniques with high-performance models, as well as developing user-friendly explanation tools that support policymakers and water management authorities.

5.3. Complexity and Practical Deployment of Hybrid Models

Model complexity and computational requirements present major challenges for real-world deployment. Advanced ensemble and deep learning models often require extensive computational resources, large datasets, and careful hyperparameter tuning, which limits their practical implementation in operational settings [69,70].

While these models provide high predictive accuracy, simpler models such as NAFS have demonstrated competitive performance with lower computational cost, making them more suitable for real-time applications [38].

Future work should aim to develop computationally efficient models that maintain high accuracy while reducing complexity, enabling real-time deployment in resource-constrained environments.

6. Conclusions

This review provides a comprehensive analysis of water quality monitoring and prediction approaches, with a particular focus on Water Quality Index (WQI) formulation, machine learning models, and explainable artificial intelligence (XAI). The study highlights that the deterministic structure of WQI significantly influences machine learning modelling, often leading to high predictive performance that reflects the underlying formulation rather than true data-driven learning.

The findings show that while single-model approaches are widely applied, hybrid and ensemble models generally offer improved robustness and predictive accuracy in complex water quality scenarios. However, the increased complexity of these models introduces challenges in interpretability, which is critical for real-world deployment. In this context, XAI techniques play a vital role in enhancing transparency, building trust, and supporting decision-making in water quality management.

Overall, the integration of accurate predictive modelling with interpretable AI techniques is essential for developing reliable and practical WQI-based monitoring systems. Future research should focus on improving model generalization, reducing computational complexity, and strengthening interpretability to ensure the effective adoption of AI in real-world water resource management.

Supplementary Materials: The following supporting information can be downloaded at: https://www.mdpi.com/article/10.3390/environments13050267/s1, Table S1: PRISMA 2020 Checklist.

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