Artificial Intelligence and Explainable AI for Groundwater Quality Assessment: A Comparative Review

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Abstract: Groundwater quality assessment is critical for determining the suitability of groundwater resources, especially in areas where groundwater resources are being affected by urbanization, industrialization, and other sources of contamination. Traditional evaluation methods relying on physicochemical parameters, statistical analysis, and Water Quality Index (WQI) can be helpful but may lack the power to reflect the complex interactions in large and heterogeneous groundwater data sets. In view of this, groundwater-quality assessment and/or prediction tasks have increasingly been studied using machine learning (ML), deep learning (DL), and Explainable Artificial Intelligence (XAI) approaches. This paper compares and contrasts the AI and XAI methods used for groundwater and related water-quality assessment. A set of studies focused on the dataset characteristics, groundwater quality parameters, modelling approaches, integration of the WQI, explainability, and implementation were analysed. Both the comparison and the results suggest that ML models and DL models can offer robust prediction capabilities, and XAI techniques like SHAP, LIME, and feature-importance methods can enhance the interpretability of complex models. The review additionally pinpoints the low level of integration of predictive modelling, explainability, environmental-health assessment, and actionable decision support. Geographically diverse data sources, multi-parameter modelling, and integrated systems need to be focused on in future studies.

Keywords: Groundwater Quality, Artificial Intelligence, Machine Learning, deep learning, explainable AI, Water Quality Index, XAI, environmental assessment

Introduction

Groundwater is a vital source of water for drinking, farming needs, household supplies, and industry, especially in areas where surface-water supplies are scarce. As urbanization grows, industrial usage, agricultural activities, and improper disposal of wastes, however, can also affect groundwater quality and contaminate groundwater with chemicals like dissolved solids, nitrate, fluoride, arsenic, and other substances. Hence, it is essential to conduct a systematic groundwater quality assessment at least to assess the suitability of the water but also as a tool for environmental health monitoring and groundwater management in a sustainable manner [1].

Most traditional groundwater evaluations involve water quality index, statistical analysis, and physicochemical measurements to assess contamination and compliance with drinking-water standards [2]. While these approaches do give information on groundwater conditions, they are often more descriptive in nature and may have limited ability to include complex, non-linear relationships,

to represent future conditions or to deliver integrated decision support over large and disparate datasets. Groundwater assessment practices are also often limited to predicting just one parameter or an overall water-quality index, rather than using predictive analysis along with environmental-health interpretation.

Artificial intelligence (AI) and ML techniques have been applied in the assessment on groundwater quality, with the availability of more groundwater monitoring data, which is increasingly available. AI techniques can detect complex relationships between physicochemical parameters, aid in classification and prediction, and offer data-driven insights that can be used in conjunction with traditional statistical methods [3]. Recently, Explainable Artificial Intelligence (XAI) has been introduced that seeks to generate more interpretable model predictions by determining what factors influence the model's predictions or the model's behaviour as a whole [4]. This is important especially in environmental applications where the prediction must be comprehensible to the researchers, the environmental agencies, the policy makers, and other decision makers, and not just outputs from the black-box models as brief in Figure 1.

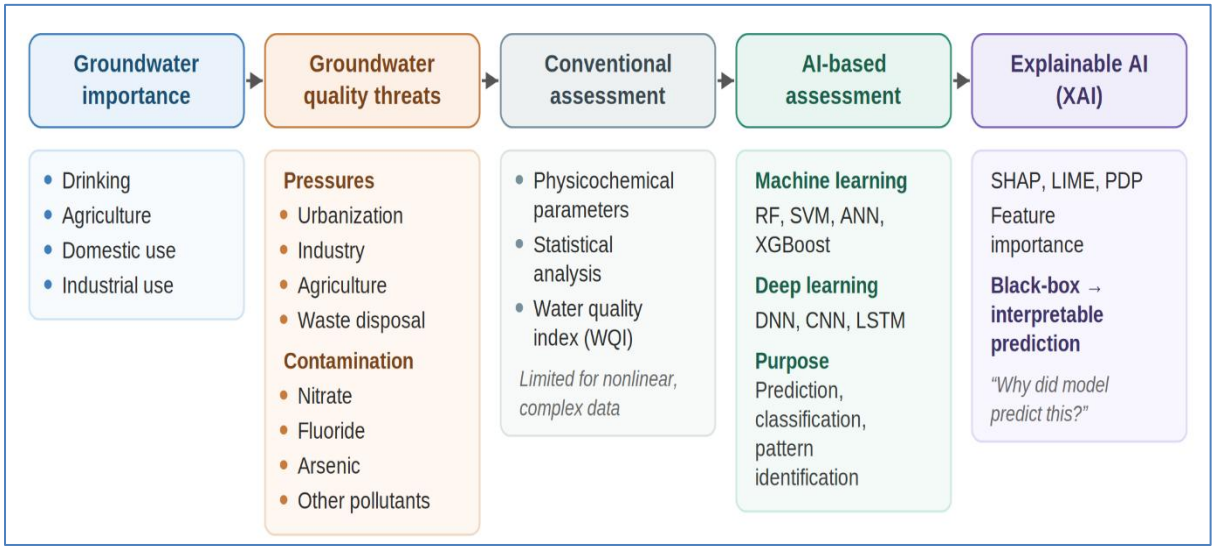


Figure 1. Overview of groundwater-quality assessment, evolution of methods towards AI and XAI, and the need for comparative evaluation

Although these progressions have been made, the available literature is spread across various methodological areas such as conventional groundwater assessment, machine learning, deep learning, and XAI. Furthermore, groundwater-quality predictive studies do not always result in a clear groundwater health assessment or decision support. The need for a more focused comparison of current approaches, both in terms of predictive capacity and interpretability and environmental-health relevance and applicability.

Hence, this paper compares and contrasts AI and XAI-based groundwater quality assessment methodologies focusing on their predictive ability, interpretability, environmental-health relevance, and decision support capability.

Related work

A systematic literature search was performed to find studies on AI, machine learning, deep learning, explainable artificial intelligence, and groundwater-quality assessment. Relevant literature was searched based on the IEEE Xplore, ScienceDirect, SpringerLink, and PubMed databases, and Elicit was employed as an auxiliary tool to discover literature.

Combinations of keywords used in the search were: "groundwater quality" AND "machine learning", "groundwater quality" AND "deep learning", "groundwater quality" AND "explainable AI", "groundwater quality" AND "SHAP", "groundwater quality" AND "Water Quality Index", and "groundwater assessment" AND "artificial intelligence". Where relevant, other groundwater prediction and assessment and AI combinations were considered. Studies were only considered for inclusion in this study when they were peer-reviewed, relevant to groundwater or related to water-quality assessment, and addressed the following methodological components: ML, DL, WQI, XAI, and AI-based prediction. Studies that were duplicated, studies not related to groundwater or water-quality assessment, and papers lacking sufficient methodological information were omitted. Recent literature was emphasized and earlier studies were included which were representative and important in terms of methodology.

For each study, the following data were extracted: publication year, geographic area, dataset characteristics, groundwater-quality parameters, methods for modeler-linguistic interface (ML/DL), integration of WQI, and the application of XAI techniques and the practical or decision-support relevance of the study. Predictive performances and major limitations were also noted, when available. The information that was extracted was further synthesized to form a comparative capability matrix and methodology table for the identification of methodology trends and differences, as well as the gaps in groundwater-quality assessment research.

Groundwater quality assessment has been steadily shifting from empirical, physicochemical analysis to data-driven AI and Explainable Artificial Intelligence (XAI) solutions. There are currently four approaches to such assessment: Conventional assessment, Machine learning, Deep learning, and Explainable AI. This taxonomy can be used as a framework to assess the similarities and differences in the understanding of groundwater quality by different methods, in identification of parameters of importance, and in environmental-health assessment.

A. Conventional Approaches

The approach mainly used for the assessment of groundwater is the conventional physicochemical analysis where parameters like pH, electrical conductivity (EC), total dissolved solids (TDS), nitrate, fluoride, arsenic, hardness, chloride and sulphate are measured to characterize groundwater. These measurements give direct data concerning the composition of water, and are frequently compared to drinking-water standards [2].

WQI methods go beyond a single-parameter analysis by using more than one physicochemical parameter to calculate an overall water-quality score or category. WQI based approaches are relatively simple and interpretable, but aggregation to a single WQI can impair the information regarding the importance of individual contaminants. Other statistical techniques such as descriptive statistics, correlation analysis, outlier analysis and distribution analysis are also commonly used to determine variability of parameters and relationships between groundwater-quality indicators [5] [17].

B. Machine Learning Approaches

The use of ML techniques to predict and classify groundwater quality has become more common recently because they are able to model the complex relationships between several environmental

variables that are nonlinear. Typical methods are Random Forest (RF), Support Vector Machine (SVM), Artificial Neural Networks (ANN) and Extreme Gradient Boosting (XGBoost). These models can be used to assist in groundwater quality classification, parameter prediction, contamination assessments, and modelling for risk assessment [5].

Complex relationships within environmental datasets can be achieved with ML methods that offer a greater flexibility than conventional statistical methods [9]. Their effectiveness relies on the quality of the datasets, feature selection, model validation and geographical representativeness, however. On top of this, there are many high performing ML models that only offer a small amount of insight as to why a specific prediction is made.

C. Deep Learning Approaches

DL is a form of machine learning that utilizes multilayer neural-network architectures that can learn complex representations from data [3]. Groundwater related information that is spatially distributed or can be expressed as image-like is suitable for Convolutional Neural Networks (CNNs) while groundwater related information that is sequential or temporal in nature is better suited for Long Short-Term Memory (LSTM) networks. CNN-LSTM models are one such hybrid architecture which can be used to fuse spatial and temporal feature learning when applicable [6].

While highly complex patterns can be modeled using DL approaches, they usually require larger datasets and more computational resources than usual ML approaches. A lack of transparency in their decision making process also makes complementary explainability techniques necessary in cases where they are applied in environmental decision support [13].

D. Explainable Artificial Intelligence

Explanatory Artificial Intelligence (XAI) is one of the key areas of AI that involves creating predictions that can be easily explained to the user. Popular methods are SHapley Additive exPlanations (SHAP), Local Interpretable Model-Agnostic Explanations (LIME), feature importance analysis, and Partial Dependence Plots (PDP) [4]. The methods can identify the influential parameters of groundwater and help to understand the contribution of each variable to the model predictions.

XAI is especially important for groundwater and environmental-health applications, where success in prediction may be insufficient for decision making. Knowing which parameters are important for a prediction can be useful for researchers and environmental authorities to understand the model results and what needs to be studied further [7] [8]. Therefore, XAI could potentially help to connect high-performance predictive models with interpretable environmental decision support.

E. Groundwater Quality and Human Health-Risk Assessment.

Groundwater-quality studies conducted in recent years have tended to be focused on deriving water-quality indices, rather than assessing possible health effects from the ingestion of contaminants. Exposure-related terms like Chronic Daily Intake (CDI), Hazard Quotient (HQ) and Hazard Index (HI) are commonly used in conventional health-risk assessment to assess the non-carcinogenic health risk from contaminants in groundwater [10]. These approaches offer a more health-oriented interpretation than WQI or EWQI alone, as they consider contaminant-specific exposure, and enable the potential risk posed by individual pollutants to be investigated.

Machine-learning models have also been investigated recently for integration with groundwater health-risk assessment. These can be used to detect non-linear relationships between the physicochemical parameters and the risk indicators, and to minimise the number of times conventional assessments need to be carried out [11]. For instance, machine-learning-based prediction models for groundwater quality and health-risk indices have been studied recently, with ensemble methods like Random Forest (RF) and XGBoost (XGB) being commonly used which can

model nonlinear interactions among multiple water-quality parameters. Explainable AI techniques, in particular SHAP, have also been applied to uncover the impact of each component on the quality or risk of the prediction.

Nevertheless, health risk assessment and prediction of groundwater using AI are still seen as independent analysis pieces. It is important to note that the model may correctly classify groundwater quality or predict a WQI/EWQI, but may not be a direct indicator of potential health impacts from exposure to individual contaminants. By contrast, traditional HQ and HI calculations allow for the estimation of health risk, but they rarely use the health-risk prediction and pattern-learning ability of AI.

The literature shows a methodological evolution from measurement and statistical evaluation → machine learning → deep learning → explainable AI. This development offers enhanced predictive capability, but also poses questions about interpretability, integrating environmental health into groundwater management, and converting AI outputs into actionable groundwater management decisions.

Comparative analysis

The studies in the review were compared in terms of a number of characteristics of the data sets, groundwater quality parameters, modelling methodologies, WQI integration, explainability, and practical applicability. The literature is as varied as summarized in Table 1 in terms of the geographical extent of the coverage, the number of datasets used, the purpose of prediction, and the combinations of methods. The intention of the comparison is thus to detect the common method trends and differences in the algorithms and not only to compare the reported performances.

Table 1. Comparative Methodological Characteristics of Reviewed Studies

Study	Location	Dataset/ Parameters	ML	DL	WQI	XAI
Raheja et al. (2022) [5]	Haryana, India	392 datasets; 12 hydrochemical parameters	✓	✓	✓	_
Alshehri & Rahman (2023) [6]	Saudi Arabia	122 sites; groundwater-quality parameters	✓	✓	✓	✓ SHAP
Clark et al. (2025) [7]	Australia	Spatiotemporal groundwater observations	✓	_	_	✓ SHAP
Angelov et al. (2021) [8]	General XAI literature	Review/benchmark literature	✓	✓	_	✓
Singha et al. (2021) [9]	Arang, Raipur district, Chhattisgarh, India	226 groundwater samples; pH, TDS, TH, Ca^{2+}, Mg^{2+}, Na^{+}, K^{+}, HCO_3^{-}, Cl^{-}, SO_4^{2-}, NO_3^{-}, F^{-}, PO_4^{3-}	✓ RF, XGBoost, ANN	✓	✓ EWQI	— Variable importance
Challagundla et al. (2025) [12]	Water potability; India-based study	3,000 samples; pH, turbidity, chlorides, dissolved solids, alkalinity, fluorides	✓	—	—	✓ SHAP, LIME
Khan et al. (2023) [13]	Groundwater-level forecasting;	109 research articles (2008–2022)	✓	✓	—	—

	global literature					
Müller et al. (2020) [14]	Butte County, California, USA	Daily groundwater-level observations + streamflow, precipitation and ambient temperature; single- and multi-well cases	✓	✓ MLP, LSTM, CNN, RNN	—	—
Hussein et al. (2020) [15]	Southern Africa; groundwater storage/availability prediction	Monthly GRACE groundwater/terrestrial water-storage maps; temporal, spatial and global features	✓ XGB, RF, LR, SVR	✓ MLP	—	— Feature importance
Aderemi et al. (2025) [16]	Global water-quality monitoring literature	60 peer-reviewed articles**,** 2011–mid-2025; groundwater, surface water and IoT monitoring	✓	✓	✓/varies by reviewed study	✓ SHAP, LIME, counterfactuals
Haggerty et al. (2023) [17]	Global groundwater-quality literature	Literature/meta-analysis covering 1994–2022**;** >300 unique input-parameter types across studies	✓	✓	✓ WQI is a major target	✓ identified as future direction
Bramm et al. (2025) [18]	Global hydrological forecasting literature	83 included studies**;** runoff, streamflow, reservoir inflow and water level	✓ XGBoost, RF, ensembles	✓ LSTM, GRU, CNN, Transformers	✓	✓ SHAP, LIME, Grad-CAM, ICE, attention

As shown in the comparison Figure 2, machine learning is the most widely adopted method across the literature, and deep learning seems to be gaining traction, especially for complex groundwater and hydrological prediction problems. Different studies showed the application of ML/DL models for prediction of WQI or EWQI, while some of other studies helped in the extension of applications of AI-based modelling to groundwater-level, storage or water quality prediction. Reported best-performing models differ from study to study, suggesting that model performance is very sensitive to the dataset, target variable, input features, and validation strategy. Hence, there is no literature that connects to the existence of a universally optimal model of AI for groundwater evaluation.

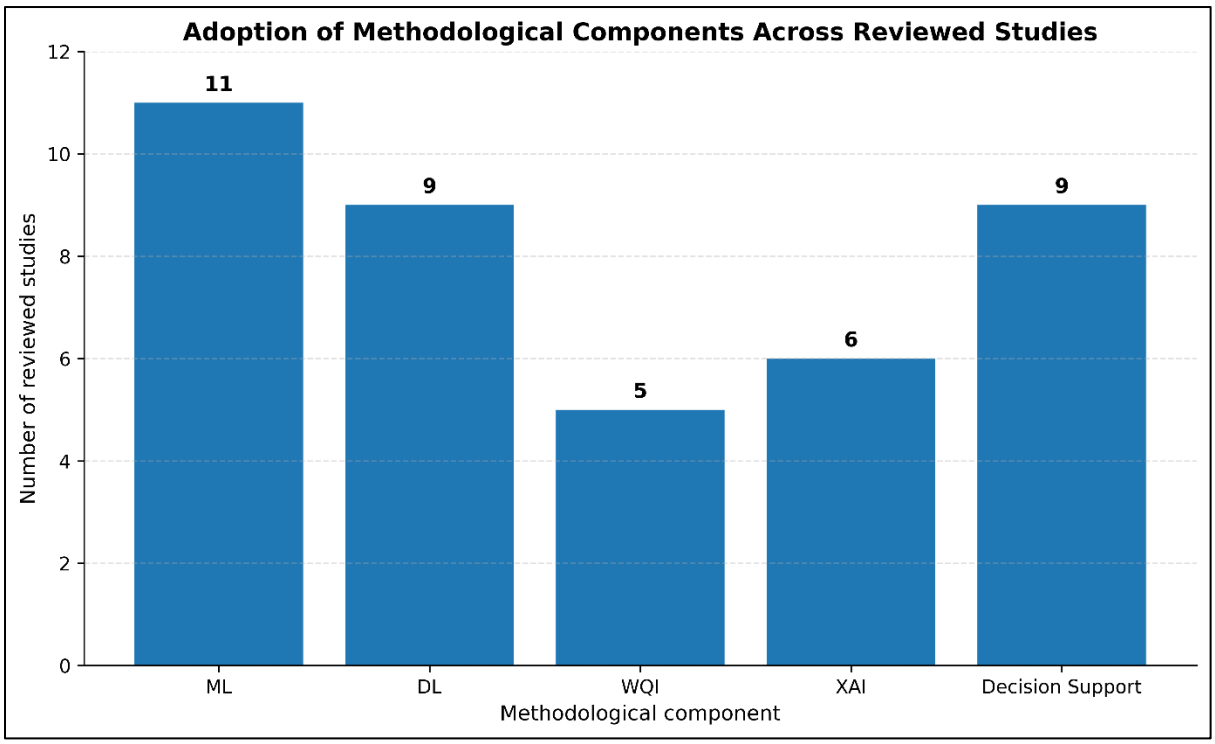


Figure 2. Comparative capability matrix of reviewed studies

Another important difference is the methodological integration, which is emphasized by the capability matrix. For groundwater quality assessment where the purpose is to capture a summary of water quality by a single indicator, WQI continues to play significant role. XAI, on the other hand, is a newer and less well-developed element. As an example, studies using SHAP, LIME, feature importance, or other methods show how much more focus is now placed on explaining model predictions, and not just the predictive performance alone. The reviewed papers as shown in Figure 3, however, vary in regard to whether they adopt explainability as a direct approach or whether they speak about it in a theoretical way or leave it as a future research direction.

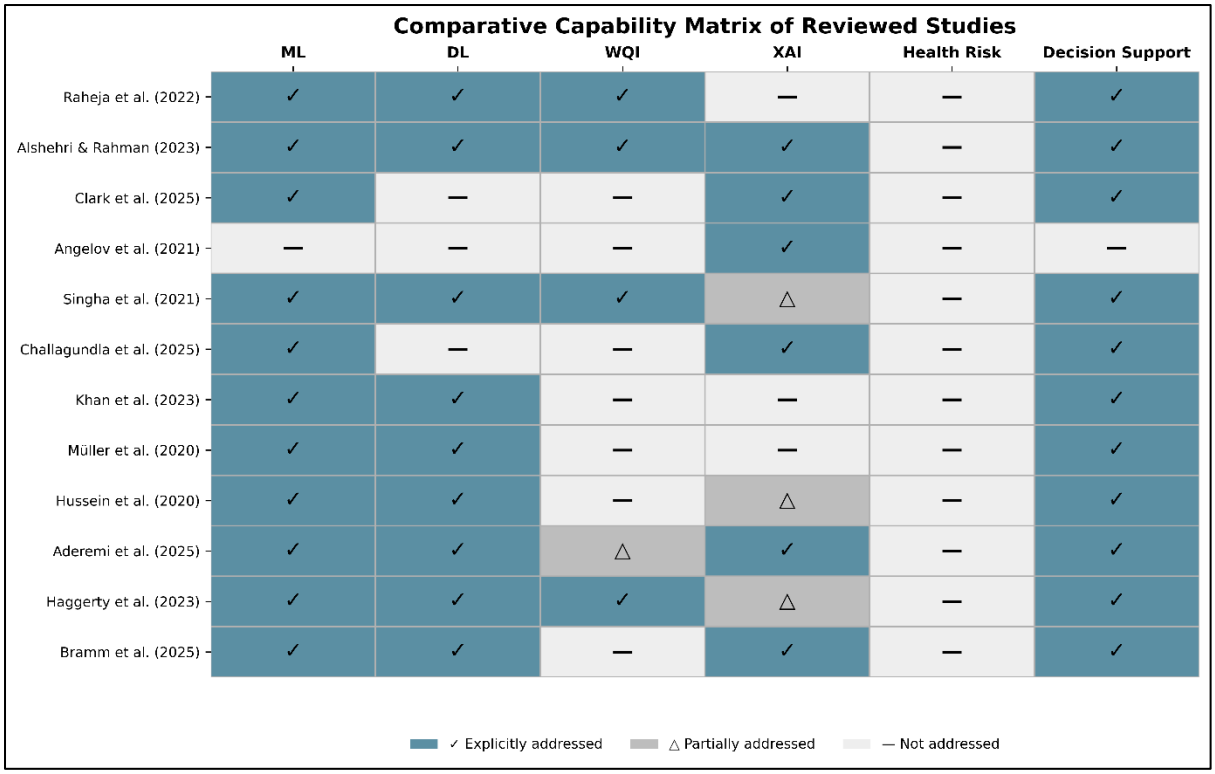


Figure 3. Adoption of methodological components across the reviewed studies

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Future research directions and gaps

The comparative analysis of the existing studies shows that AI has been progressively employed in the assessment of groundwater-quality and can reveal the complex relationships between groundwater-quality parameters by using machine-learning and deep-learning models. More recent research has also combined incorporate XAI to better explain model predictions. A review of the literature in Table 2, however, also uncovers some gaps which restrict the general applicability and usefulness of current approaches.

A. Limited integration of prediction, explainability and health assessment

Most of the studies currently conducted are based on one or more specific aspect, including prediction of groundwater quality, estimation of WQI, or interpretation of the models. Despite recent studies developing XAI techniques like SHAP and LIME, the combination of predictive modelling with a contaminant-specific environmental-health assessment is still relatively scarce [7] [19]. A groundwater-quality prediction (high or low) does not, in itself, provide an indication of the health effects that may result from exposure to any particular contaminant. Future research should thus

explore strategies to link groundwater-quality prediction to the appropriate environmental-health risk assessment.

B. Generalization in Space and Time - Limited

There are a significant number of studies on ground water that have used only small or short time series data sets. These data can yield good predictive results in the study area but may not be representative of seasonal, hydrogeological or regional variations [20]. The literature reviewed therefore suggests the need for greater numbers and a wider range of data across space (locations) and time (sources or years) [11] [15]. Model transferability between regions, seasons and various hydrogeological conditions should be assessed rather than doing random train-test splits within one data set.

C. Need for more comprehensive multi-parameter modelling (MPM)

Frequently, groundwater-quality studies have focused on a single contaminant or multiple indicators, WQI. While these methods are helpful, they can only capture a narrow range of variables if they are applied to a single set of variables that are considered to represent the multi-dimensional nature of groundwater quality [5]. Further studies may include multi-parameter modelling in which multiple physicochemical parameters and contaminant specific indicators are taken into account together. This may result in a more holistic picture of groundwater conditions, and still capture data relating to individual parameters [9].

D. Inconsistent Evaluation of Explainability

The more XAI is used, the more it doesn't give reliable or meaningful explanations. Each of these types of interpretation (SHAP, LIME, feature importance, and Partial Dependence Plots) can yield different results based on the model, data, and type of explanation [8]. Reviewed literature shows there is a need for more systematic analysis of the quality of the explanations to be used in addition to the traditional predictive metrics like R2R^2, RMSE, MAE and accuracy. Evaluation of groundwater models using XAI should include properties like explanation stability, consistency, fidelity, and plausibility for the domain of the model [14][16].

E. Translation of AI Predictions to Decision Support

However, while a few studies talk about groundwater management and decision making, the translation of model scenarios and explanations to actionable recommendations is still limited. The information generated by an AI model could be a high-risk groundwater condition or an influential parameter, but it needs to be presented in a way that can inform monitoring prioritisation, further investigations or groundwater-management decisions. Further studies are thus needed to examine possibilities for decision-support mechanisms which integrate predictive output with meaningful parameter contributions and suitable environment criteria.

F. Need for Robust and Interpretable AI Frameworks

The literature examined in this study shows that a compromise must be made between the level of prediction and the interpretability of the modeling. More sophisticated models, such as deep-learning models, can model nonlinear relationships well but can be hard to explain without other model explanation methods [3]. On the other hand, simpler models could be more transparent, but may not necessarily be as predictive as more complex models [6][16]. Future research efforts should thus aim to develop strong AI frameworks that not only deliver high accuracy at prediction but also possess interpretability, generalizability, and usability.

Table 2. Application & Research-Gap Comparison

Ref.	Decision Support	Main Contribution	Major Limitation
Raheja et al. (2022) [5]	Limited	DNN, GBM and XGBoost for WQI/EWQI prediction	No formal XAI or quantitative health-risk framework
Alshehri & Rahman (2023) [6]	✓	Water Quality Index Prediction and SHAP Interpretations for Water Management	No formal health-risk assessment, Limited training data.
Clark et al. (2025) [7]	✓	Spatiotemporal groundwater prediction with SHAP-based interpretation	Groundwater prediction (not integrated health-risk assessment)
Angelov et al. (2021) [8]	Conceptual	Provides XAI taxonomy and interpretation concepts	General XAI review; not groundwater-specific
Singha et al. (2021) [9]	✓	DL outperformed RF, XGBoost and ANN for EWQI prediction; DL R2=0.996R^2=0.996. Variable-importance analysis identified influential parameters.	There is only one monsoon dataset and authors suggest further hydrogeometeorological inputs and multi-season data.
Challagundla et al. (2025) [12]	✓	Implements ML potability classification along with SHAP + LIME to enhance transparency of model decisions. Logistic Regression got 94.5% after LDA and Gaussian NB got 97% before LDA.	The authors state that there is a need for DL, data distributed across seasons/geographies, real-time IoT deployment and increased combined explainability.
Khan et al. (2023) [13]	✓	Comprehensive comparison displays the effectiveness of the ML/DL to forecast groundwater levels; highlights the importance of model selection, temporal modelling and long-term forecasting.	Critics argue that focus is on groundwater level, rather than groundwater quality; there is a stronger focus on short-term forecasting than multi-year prediction in the literature.
Müller et al. (2020) [14]	✓	Optimized the hyperparameters of the DL model to improve prediction of groundwater flow: in general, the MLP model showed the best accuracy and prediction deviations of around ≤2 m.	There is a need to test the generalization to other watersheds, sensitivity to input variables and training data volume needs to be studied further.
Hussein et al. (2020) [15]	✓	Proved the ability of ML techniques to predict future groundwater-storage images with temporal, spatial and global features. The combination of SVR generally achieved the best results, and global features derived from GMM showed improvement in prediction.	Mainly forecasts water availability/storage instead of groundwater quality or health threat; future work includes more meteorological parameters, more robust missing value imputation and multi-parameter prediction.
Aderemi et al. (2025) [16]	✓	Provides a systematic exploration of the expanding use of XAI in water quality monitoring applications; SHAP, LIME and	Absence of uniform evaluation metrics for XAI, computational difficulties, availability of heterogeneous

		counterfactual reasoning are gaining currency for being used to explain and trust AI predictions.	data, and lack of adoption in resource-limited settings.
Haggerty et al. (2023) [17]	✓	Detailed literature review on application of ML in GWQ modelling. High focus on nitrate and WQI, strong adoption of neural networks, and growing trend towards DL and XAI.	High geographic concentration, repetitive modelling of well-studied contaminants, need for DL/XAI, new study areas, underrepresented parameters, open datasets/code and practical GWQ management applications.
Bramm et al. (2025) [18]	✓	Properly categorizes XAI for hydro forecasting and demonstrates that SHAP, LIME, Grad-CAM and attention can isolate the variables that most affect AI predictions and increase trust in predictions.	There is no single metric for interpretability, little spatial/seasonal validation, few physics-aware/causal explanations, and uncertainty-aware XAI and human-in-the-loop decision support haven't matured.

Conclusion

This paper is about a comparative review of groundwater-quality assessment using AI and XAI approaches. The literature was reviewed and clearly showed the methodological evolution from traditional physicochemical and WQI to machine learning, deep learning and explainable predictive methods.The literature was reviewed and the clear evolution of methodology was seen from the conventional physicochemical and WQI to machine learning and deep learning to explainable predictive methods were observed. The potential of ML and DL models in capturing nonlinear relationships and enhancing prediction of groundwater quality has been demonstrated, and XAI methods like SHAP, LIME, and features importance have helped reveal the factors that affect model predictions.

The comparison also shows that reported performance is highly dependent on the characteristics of the dataset, the prediction goals, geographical scope and validation methods. So, the suitability of an AI approach to environmental applications can't be judged by its accuracy. Several ongoing gaps are identified, including spatial and temporal generalisation, inconsistent XAI explanation evaluation, limited multi-parameter modelling and lack of integration of predictive modelling with EHA and actionable decision support.

In general, groundwater-quality studies in the future should strive not to focus on individual, high-accuracy prediction models, but on practical, interpretable, generalizable, and robust AI frameworks. This can help to achieve better linkages between groundwater-quality prediction, parameter-level interpretation, environmental relevance and decision support.

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