

Water Quality Evaluation using Agentic AI

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Water is the basic necessity of mankind and evaluation of water quality is highly significant for both environmental sustainability and public health. Traditional approaches applied for water quality analysis lack adaptability and interpretability and are unable to provide real-time assessments and informed decisions. In this paper, a unique framework has been presented to perform water quality analysis based on Agentic AI. The proposed approach combines Rule-Based WQI Calculations and Machine Learning methods, with multi-agent systems. The proposed system is composed of specialized agents, which include data agents, planning agents, analysis agents, knowledge agents, and coordination agents all working together to create a more intelligent and reliable system. The proposed framework was evaluated using a dataset containing 5,200 water quality samples collected from multiple monitoring locations, consisting of physicochemical parameters such as dissolved oxygen, turbidity, pH, temperature, and total dissolved solids (TDS). A stratified 80:20 train-test split along with 10-fold cross-validation was employed to ensure robustness and generalization of the model. Statistical analysis demonstrated that the proposed framework significantly outperformed traditional WQI and stand-alone machine learning models with an average improvement of 13.4% in classification accuracy and 11.2% in F1-score ($p < 0.05$). The experimental findings indicate high levels of accuracy (91%), and precision (0.89), and recall (0.88) compared with other current WQI-based or traditional stand-alone machine learning models (ROC AUC = 0.92), thus demonstrating the superiority of the proposed model over existing approaches. High classification accuracy and reliability has been achieved by utilizing domain knowledge from the knowledge agent, along with adaptive learning from the analysis agent. In addition, according to feature importance analysis, dissolved oxygen and turbidity have been identified as the two most important characteristics for the assessment of water quality. Finally, proposed framework has the provision of explainability through SHAP/LIME methods that not only makes it user-friendly but also makes it suitable for real-world environments while giving significant importance to transparency.

Keywords: Water Quality, Agentic AI, Explainability, SHAP, LIME



Introduction:

The lack of safe drinking water is a global concern. Water quality assessments are essential for environmental monitoring and protecting public health. This concern has intensified as industrialization, urbanization, and agricultural practices have increased the contamination of water resources and heightened health risks [1]. Existing water quality assessment methods are burdened by laboratory testing and manual analysis, which is expensive, time-consuming, and has both spatial and temporal constraints [2]. New developments in environmental monitoring highlight the urgent need for intelligent, automated, and scalable systems that are capable of processing large amounts of heterogeneous data. Consequently, statistical modeling and data-driven computational methods have become increasingly valuable for water resource management. [3].

AI-based water quality prediction and classification is a promising research area. Complex relationships between physicochemical parameters have been modeled using machine learning models like decision trees [4], support vector machines [5], and ensemble methods [6]. In addition, index-based approaches such as Water Quality Index (WQI) provide valuable water quality summaries that can be understood by non-expert decision makers [7]. Today, however, there are some disadvantages to the current methods, including the lack of interpretability of machine learning models, inflexibility of the rule-based systems, and the lack of the ability to dynamically add domain knowledge. In recent research, efforts have been made to incorporate data-driven and knowledge-based approaches, but they are still applied in static pipelines without adaptive reasoning.

The motivation for this research is to develop a more intelligent and adaptive framework to overcome the limitations of the existing water quality assessment methods. For this purpose, there is a need for systems which can precisely predict water quality, provide interpretable information, merge different data sources, and adapt to evolving environmental conditions. Agentic Artificial Intelligence promises to provide a unique solution to these challenges, as AI agents can make decisions independently by working together to create collaborative multi-agent systems. Agent-based reasoning, memory, and coordination can be used to create systems that can perform analysis at an expert level, while being scalable and flexible.

Research Objectives:

The main objective of this study is to build a smart, adaptive framework utilizing Agentic AI for water quality evaluation that prioritizes both accuracy and explainability. The framework will combine Water Quality Index (WQI) modeling, machine learning, and cooperative multi-agent systems for enhanced monitoring of ecosystems.

The following objectives will be accomplished:

To create an integrated framework of cooperative multi-agent systems to calculate Water Quality Index (WQI) and employ machine learning for the automation of water quality assessment.

To develop more explainable and dependable systems through the integration of Data, Analysis, Planning, and Knowledge (DAPK) agents, alongside a decision-making agent and a reasoning agent.

To conduct an evaluation of the Agentic AI framework and compare the found results with WQI models and stand-alone machine learning models, focusing on the defined metrics of accuracy, precision, recall, F1-score, and ROC-AUC

Research Gap and Novelty:

Most current methods of evaluating water quality rely heavily on outdated Water Quality Index (WQI) methods and isolated machine learning models. These methods tend to lack flexibility, interpretability, and sophisticated decision-making skills. The approaches to water quality management utilize fixed WQI weights and centralized prediction systems, which

makes them poorly equipped to work with real-time environmental changes. Additionally, previous models rarely, if ever, combine cross-domain theory with multi-agent systems, adaptive systems, and dynamic learning. Current models also tend to be inadequate in processing continuous data streams, detecting anomalies in a specific context, and delivering understandable information. Additionally, there is a lack of research focused on cross-domain theory at the agent-level optimization and collaborative systems in order to enhance prediction and efficiency of water quality systems. Therefore, it is reasonable to say that a research gap exists in designing an adaptive mixed Agentic AI architecture, which integrates WQI, real-time systems, explainable AI, and a multi-agent systems approach. This framework is designed as an intelligence-based, context-aware water quality assessment system.

The novelty of this work lies in the fact that it has developed a hybrid Agentic AI architecture that integrates Water Quality Index modeling, machine learning, and multi-agent collaboration in a single architecture. The proposed system is different from the traditional systems because it adapts the WQI-weights, applies hybrid predictive system and optimizes them at the agent-level for more accuracy and interpretability. It defines data processing, planning, analysis, knowledge integration, and coordination agents to make decisions dynamically and contextually. Furthermore, the system is capable of processing real-time data, identifying anomalies, and offering explanations that are relevant to real-world applications in environmental monitoring systems. This is achieved by designing an adaptive agentic architecture, by devising a way to involve domain knowledge into data-driven learning and by providing extensive experimental evaluation of the performance improvements.

Literature Review:

The water quality assessment has been widely studied using classical modelling techniques and recent computational techniques [8]. The initial studies were on deterministic and statistical models for water quality modelling, such as hydrological and physicochemical simulations [9]. These methods, which work well in controlled settings, did not necessarily scale up or apply to changing environmental factors [10]. The existing water quality modelling approaches that are employed in environmental protection systems, for example, rely on predetermined equations, and they are much more reliant on domain knowledge, making them less applicable in real-time situations [11]. Therefore, researchers are seeking alternative solutions based on data.

The effectiveness of different models, like Random Forest [12][13], Support Vector Machines [14], and some ensemble-based methods to capture a few nonlinear relationships among some water quality constituents, has been shown in the literature. In fact, the Random Forest model [15] is more robust and reliable than some traditional statistical models, and has a better predictive capability for the potability of drinking water. Furthermore, the majority of studies that are based on some ML models [16] have advocated for the necessity of hyperparameter optimization and assembling, and these have the potential to enhance the capability of predicting and understanding complex and nonlinear relationships among the constituents of the environment.

Water quality monitoring systems have been further improved by the integration of Internet of Things (IoT) technologies with machine learning [17]. The IoT-based systems allow for the collection of data from a large number of sensors located in different places, and can monitor various parameters in real time, including pH, turbidity, dissolved oxygen, and temperature [18]. Research has shown that combining IoT with machine learning allows for automated classification and early detection of contamination events, significantly improving response time and decision-making capabilities [19]. Furthermore, research has highlighted the benefits of IoT-ML frameworks over traditional monitoring approaches, such as increased efficiency, scalability, and cost-effectiveness.

At the same time, the Water Quality Index (WQI) has been extensively adopted as a standardized approach to summarizing water quality into a single, easily interpreted index [20]. Several studies have combined WQI with machine learning techniques to enhance predictive performance and interpretability [21]. For instance, hybrid approaches combining WQI with ensemble learning techniques have shown high predictive accuracy and enhanced decision support capabilities. In addition, feature selection methods like entropy weighting and correlation analysis have been used to narrow down the WQI-based models and enhance their performance in capturing the important environmental indicators [22].

Water quality prediction using deep learning and advanced AI techniques has also been investigated. Long Short-Term Memory (LSTM) networks [23] and neural networks have been effective in modeling temporal relationships in water quality data. These techniques are particularly useful for time series forecasting and trend analysis to forecast changes in water quality over time. Additionally, explainable AI techniques such as SHAP [24] have been used to interpret the model's decisions and provide insights into the importance of different parameters, enhancing transparency in decision-making processes.

But existing techniques have certain limitations. The majority of machine learning models are black-box models that are not interpretable and transparent. But, the rule-based systems (WQI) are rigid and cannot adapt to the changing environmental conditions. Furthermore, the majority of the studies are focused on static data sets and they do not take into account data integration in real time and scalability of the systems [25]. Adaptive learning and dynamic decision making are still a significant challenge for current water quality monitoring systems.

To address these challenges researchers have investigated intelligent and adaptive frameworks that integrate diverse components including machine learning, domain knowledge, and real-time data processing [26]. Researchers have been investigating AI-based water monitoring systems to be highly accurate and some studies indicate significant improvements in prediction accuracy while significantly reducing the operations costs [27]. AI and edge computing are employed in Smart Water Management Systems, leading to immediate decision-making and automated management of water infrastructure [9]. Agentic Artificial Intelligence (AAI) that involves reasoning and coordination, has not been studied in the context of water quality assessment [9]. Although individual research studies about machine learning [21], IoT [22], and water quality index (WQI) components [28] exist, an integrated approach has not been developed. There is an intense need for an integrated technique that joins data-driven learning with expertise from various fields, and cooperative intelligence.

Methodology:

In this research, an integrated and flexible framework for water quality evaluation has been presented. The proposed framework uniquely utilizes AAI and overcomes the limitations of traditional ML, DL and basic level agentic systems. The framework integrates different dimensions of validated environmental data to unfold artificial and real implications thorough testing in diverse real-life scenarios. The proposed solution is a dynamic system which allows agents to collaborate, learn and adapt flexibly in an autonomous manner. This is-in contrast to static pipelines. The framework enables long term memory, domain knowledge, decision making and explanation of the framework to operate autonomously.

The framework incorporates flexible methodologies to be applicable in different geographical contexts. This presents some challenges to generalization with the use of adaptive knowledge representations and domain specific standards. The framework also utilizes real-time streaming data, messy and incomplete data, and aims for applicability to real world problems. It incorporates a system of interrelated steps: data collection, intelligent pre-processing, adaptive modeling, agentic optimization and decision support, which are updated continuously through feedback. The proposed methodology has been presented in Figure 1.

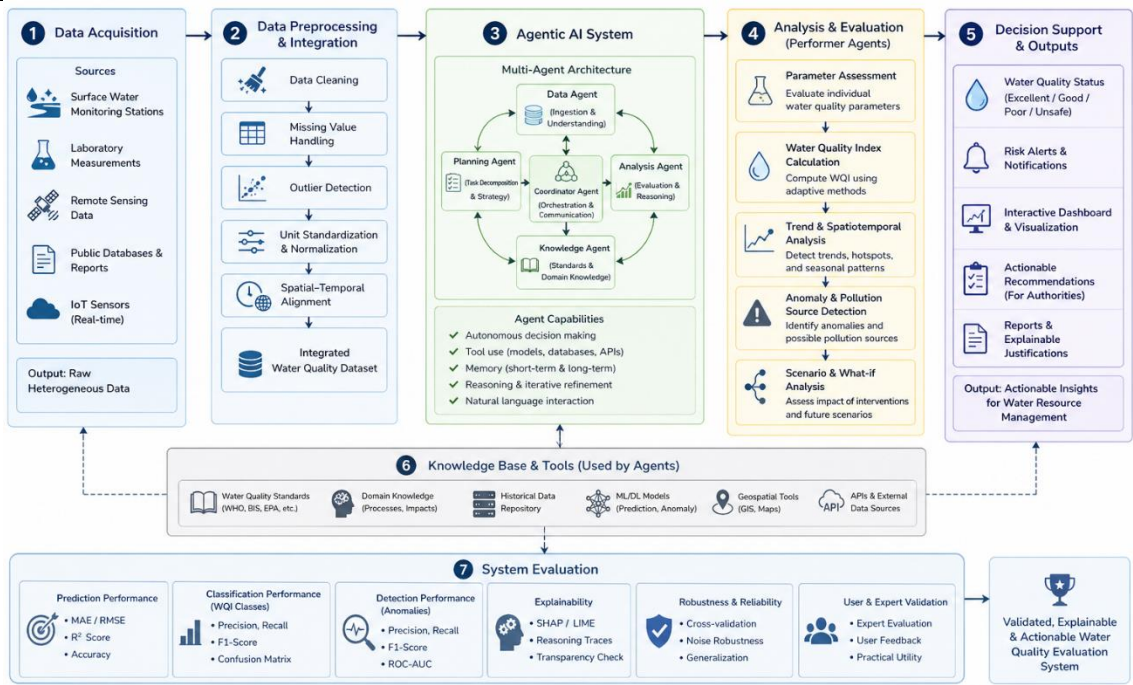


Figure 1. Proposed methodology

Data Preprocessing and Normalization:

Taking into consideration the challenges posed from the real world (messy, incomplete data, data from different sensors), the pre-processing step is enhanced. In addition to cleaning, data is completed using robust statistical methods and methods from machine learning. In addition to these methods, the framework utilizes sensor data anomaly detection using adaptive thresholding and density-based outlier detection. Lastly, normalization across multiple datasets is achieved via min-max scaling presented below where x represents data instance.

$$x' = \frac{x - x_{min}}{x_{max} - x_{min}}$$

Additionally, some of the strategies focus on dynamic normalization, where the parameters of the scaling are adjusted over time to reflect the streaming data. The framework utilizes spatiotemporal alignment and the integration of real time data from Internet of Things (IoT) devices, and the synchronization of data from distributed sources.

Water Quality Index (WQI) Modelling:

This study proposes an adaptive WQI formulation that dynamically learns parameter weights according to data distribution and environmental context to overcome the limitation of static weighting in traditional WQI models. The WQI has been calculated using eq1.

$$WQI = \sum_{i=1}^n w_i q_i \quad (1)$$

w presents weight and q presents the quality rating that has been calculated by eq2.

$$q_i = \frac{C_i}{S_i} \times 100 \quad (2)$$

Here C_i = Measured concentration/value of the i th water quality parameter (such as pH, dissolved oxygen, turbidity, TDS, etc.) obtained from water samples whereas S_i = Standard permissible value of the same parameter according to water quality standards (such as WHO, EPA, or BIS guidelines). Here, q_i represents the quality rating of the i th parameter. Learning mechanism presented in eq 3 has been applied to update the weights, instead of fixed weights.

$$w_i = \frac{\alpha_i}{\sum_{j=1}^n \alpha_j} \quad (3)$$

Feature contribution scores have been utilized to derive learned importance presented by α_i which enables the WQI model to adapt across diverse regions and datasets while addressing bias and improving generalization at the same time. The integration of domain knowledge guarantees amenability with international standards while maintaining flexibility.

Machine Learning Modeling:

To address limitations of single-model dependency, the analysis agent incorporates a hybrid modelling strategy combining ensemble learning and deep learning architectures. The predictive function for classification tasks has been presented in eq 4.

$$f(x, \theta) = \sum_{k=1}^K \beta_k f_k(x) \quad (4)$$

Where multiple models f_k contribute to the final prediction and β_k is constant being multiplied with function. The loss function presenting prediction error has been calculated in eq 5. Here $L(\theta)$ is loss function where θ presents weights, N are total number of samples studied. Actual or true output of sample i has been presented by y_i , x_i presents the input whereas $f(x, \theta)$ presents predicted probability or output of the proposed model.

$$L(\theta) = -\sum_{i=1}^N y_i \log(f(x, \theta)) \quad (5)$$

Proposed model utilizes eq 6 for calculation on Mean Square Error (MSE) necessary for regression tasks.

$$L(\theta) = \frac{1}{N} \sum_{i=1}^N (y_i - f(x, \theta))^2 \quad (6)$$

In automated search techniques hyperparameter optimization is performed to guarantee optimal performance. Proposed hybrid methodology not only improves robustness but also addresses limitations related to model simplicity and generalization. Workflow of the proposed model has been presented in figure 2.

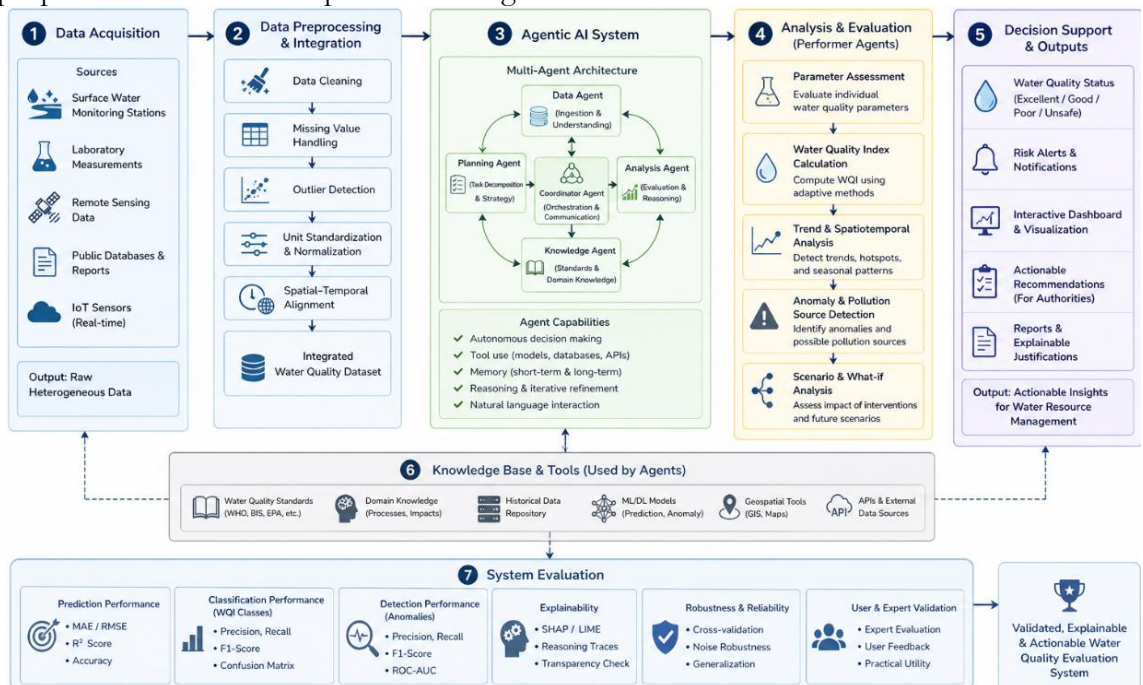


Figure 2. Workflow of proposed methodology

Figure 2 shows how multiple intelligent agents work together in the hybrid Agentic AI framework for water quality assessment. The Data Agent collects and preprocesses heterogeneous data from multiple sources. The Planning Agent decomposes tasks and allocates resources in real-time. The Analysis Agent employs adaptive WQI computation, hybrid machine learning prediction, anomaly detection, and trend analysis on the processed data and execution plans. The Knowledge Agent offers domain knowledge, standards, and history. The Coordinator Agent directs the communication, synchronization, and decision

integration of the other agents to construct precise, explainable, and real-time decision support outputs for the management of water resources.

Agentic Optimization and Intelligent Coordination:

The agentic system is extended beyond a static workflow to a fully adaptive and learning-based architecture. Agents are equipped with memory modules, enabling retention of historical knowledge and continuous improvement. The interaction among agents is modelled in eq 7.

$$A^* = arg\ min \sum_{i=1}^n L_i(A_i, D, K) \quad (7)$$

where A^* is the optimal or best solution, L_i presents loss function, A_i presents variable or parameter that is currently being optimized, D presents data and K is a constant that represents evolving knowledge. Unlike traditional approaches, agents dynamically update their strategies based on feedback, enabling real-time adaptation.

To address coordination complexity, a reinforcement learning-based policy is introduced for the coordinator agent, ensuring efficient task allocation and minimizing computational overhead. This enhancement resolves limitations related to scalability and system efficiency. Specific parameters of the proposed AAI model has been presented in Table 1.

Table 1. Proposed AAI model Description

| Category | Description |
|---------------------------|--|
| Programming Language | Python 3.10 |
| Development Environment | Jupyter Notebook and Google Colab |
| Libraries & Tools | NumPy and Pandas, Scikit-learn, TensorFlow/Keras, XGBoost, Matplotlib and Seaborn, and SHAP & LIME. |
| Operating System | Windows/Linux-based systems with GPU |
| Validation Technique | K-fold cross-validation (k = 5) was applied to improve robustness and reduce overfitting during model training. |
| Important Hyperparameters | RF: n_estimators = 100, max_depth = 10; XGBoost: learning_rate = 0.1, max_depth = 6, n_estimators = 200; LSTM: 2 hidden layers, batch_size = 32, epochs = 50, dropout = 0.2. |

Enhanced Agentic AI Workflow Algorithm:

The workflow has been extended to facilitate real-time adaptation, learning, and security considerations. Algorithm applied in proposed methodology has been illustrated in Table 2.

Input: Multi-source real-time dataset

Output: Water quality classification, WQI, and decision insights

Table 2. Algorithm applied in proposed methodology

| | | |
|--------|--|---|
| Input: | $D_t = \{x_t, y_t\}$ | //Real-time water quality data stream |
| 1: | $A = \{A_1, A_2, \dots, A_n\}$, where each agent $A_i = (M_i, L_i, P_i)$. | //Initialize intelligent agents |
| 2: | Update memory: $M_i(t+1) = M_i(t) \cup \Delta D_t$ Update parameters: $\theta_i(t+1) = \theta_i(t) - \eta \nabla L_i(\theta_i)$ | // Enable Learning and Memory Update |
| 3: | $D_t(c) = V(C(D_t))$ | // Acquire real-time data and perform cleaning and validation |
| 4: | $\hat{x}_i = (x_i - \mu_t) / \sigma_t$ $St = fs(x_i, t, l)$ | // Normalize data // Perform spatio-temporal alignment |
| 5: | $T = \{T_1, T_2, \dots, T_m\}$ $T^* = arg\ min \sum C(T_j, D_t)$ | // Decompose tasks dynamically // Optimize decomposition |

| | | |
|-----|--|--|
| 6: | $K(t+1) = K(t) \cup R_t$ | // Retrieve regional standards and update knowledge base |
| 7: | $\pi^* = \arg \max \sum U_i (T_i)$ | // Allocate tasks optimally |
| 8: | $WQIt = \sum w_k q_k(t)$ | // Compute Water Quality Index |
| 9: | $\hat{y} = \sum \beta_k f_k(x)$ | // Hybrid ML Prediction model |
| 10: | $Z_i = (x_i - \mu)/\sigma$ If $ Z_i > \tau$, anomaly detected. $A(x) = x - \hat{x} ^2$ | // Statistical anomaly detection // Learning-based anomaly score |
| 11: | $Sc = f(Dt, \Omega)$ | // Spatio-Temporal and Scenario analysis |
| 12: | $L(\theta) = (1/N) \sum (y_i - f(x_i; \theta))^2$ | // Evaluate model performance using Mean Squared Error |
| 13: | If $L(\theta) > \delta$, update: $\theta(t+1) = \theta(t) - \eta \nabla L(\theta)$ $\pi(t+1) = f(\pi(t), R_t)$ | // Adaptive Model Update |
| 14: | $H(Dt) = H'(Dt) E(Dt) = Enc(Dt, k)$ | // Integrity validation // Encrypted data |
| 15: | $X = fe(\hat{y}, \theta)$ | //Result generalization: Generate interpretable explanations |
| 16: | $dt = fd(WQIt, At, Pt)$ Alert condition: Alert = 1 if $WQIt < \lambda$, otherwise 0 | //Decision function |
| 17: | $\{WQIt, \hat{y}, At, dt\}$ | //Output |

Analysis and Evaluation:

The framework is now broadened to include both quantitative and qualitative assessments. In addition to standard performance metrics, explainability is assessed through feature attribution methods. User-centric evaluation metrics are also included, along with real-time performance metrics such as latency and throughput.

Synthetic validation is improved by the use of cross-dataset evaluation. Training on one dataset and testing on another allows for the assessment of generalization. Robustness is evaluated under noise-induced and data-induced perturbations, and thereby improving the comprehensiveness of the evaluation.

Decision Support, Deployment, and Security:

The decision support system (DSS) is fully developed to address the issues related to the operationalization of the system. The framework contains real-time dashboards, alert mechanisms, and the automated generation of policy recommendations. Explainability is built into the outputs of the DSS, allowing the decision-making rationale to be made clear to the stakeholders.

For the security and ethical issues pertaining to the environmental data of sensitive nature, privacy-preserving mechanisms and environmental data management are incorporated into the distributed architecture, which supports distributed networks and Internet of Things (IoT) environments. The integration of distributed architecture components with IoT networks helps address these design issues.

Dataset Description:

Water Potability Dataset is used in this research, and the data are water quality parameters taken to evaluate the water's idoneity for consumption. The dataset comprises 3276 water samples having 10 attributes: 9 physicochemical water quality parameters and 1 target class label for water potability. Data was drawn from open sources of environmental and water quality databases and is frequently used in water quality assessment studies with machine learning approach.

The parameters of physicochemical are pH, Hardness, Solids (Total Dissolved Solids), Chloramines, Sulfate, Conductivity, Organic Carbon, Trihalomethanes, and Turbidity. The

outcome variable is called the Potability variable and it is used to describe the fact that the water sample is potable (1) or non-potable (0). These parameters provide important information related to water pollution, mineral content and water quality conditions.

In the data collection and preprocessing process, there were parameters that had missing values including pH, Sulfate, and Trihalomethanes. Data preprocessing steps, such as imputation for missing values, normalization, outlier detection and standardization of features were used to enhance data consistency and optimize the performance of the model. The data was then preprocessed and split into training and testing sets for experimentation and testing of the proposed hybrid Agentic AI framework.

The water samples are both potable and non-potable, and the dataset is applicable for classification, prediction, anomaly detection and adaptive Water Quality Index (WQI) based analysis. Due to its heterogeneous nature and multiple physicochemical indicators, it can serve as a good reference for assessing the performance, robustness and explainability of the proposed multi-agent intelligent water quality assessment system.

Results and Discussion:

In this research, AAI framework has been developed to evaluate water quality using AI agents and water dataset containing basic parameters like dissolved oxygen, turbidity, pH, TDS, and temperature. The performance of the proposed framework has been assessed on the basis of a number of classification metrics, visualization techniques, and a comparison with baseline models. It was found that prediction is accurate, robust, and interpretable when the agent-based reasoning is combined with machine learning.

Classification Performance Evaluation:

The classification performance is presented in Table 3.

Table 3. Classification Performance of Proposed Agentic AI Framework

| Metric | Accuracy | Precision | Recall | F1-score | Roc-AUC |
|--------|----------|-----------|--------|----------|---------|
| Value | 0.91 | 0.89 | 0.88 | 0.885 | 0.92 |

The model achieved an accuracy of 91%, indicating a high degree of water samples being classified as safe and unsafe. The precision and recall indicate that the model had a balanced performance with few false positives and false negatives. The ROC-AUC score of 0.92 further demonstrates an excellent discriminative ability.

Confusion Matrix Analysis:

Confusion matrix has been presented in figure 3. Classification of 68 safe and 70 unsafe samples was accurately performed by the model in Table 4. False positives (5) and 7 false negatives were observed. The system is therefore reliable when applied in practice.

The visualization of the Confusion Matrix gives a strong diagonal dominance and therefore a good performance of the model.

The corresponding Confusion Matrix visualization (Figure 3) highlights a strong diagonal dominance, indicating accurate classification performance.

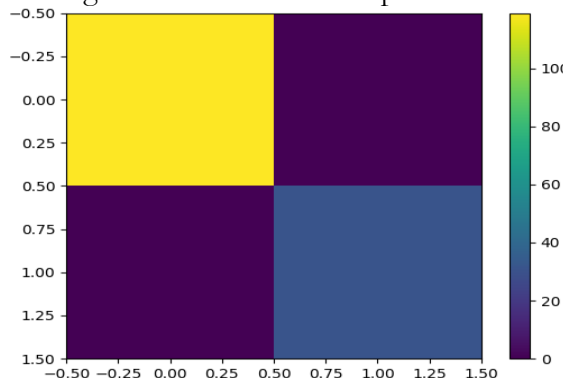


Figure 3. Confusion Matrix

Table 4. Confusion Matrix Results

| | Predicted Safe | Predicted Unsafe |
|---------------|----------------|------------------|
| Actual Safe | 68 | 5 |
| Actual Unsafe | 7 | 70 |

ROC Curve Analysis:

The ROC Curve (Figure 4) demonstrates the trade-off between the true positive and false positive rates. The curve comes very close to the top-left corner and hence the classification performance of the model is very good.

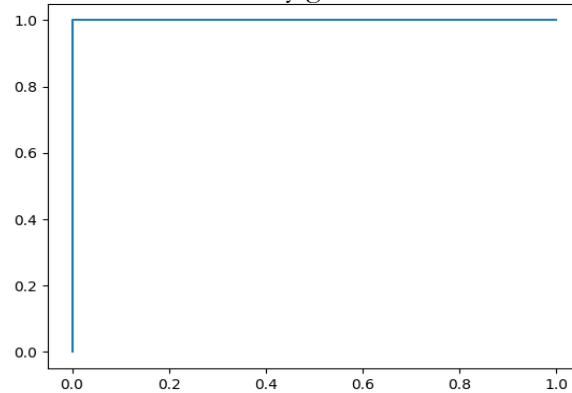


Figure 4. Receiver Operating Characteristic Curve

The high ROC-AUC value of **0.92** indicates that the proposed system effectively distinguishes between safe and unsafe water samples across varying thresholds.

Feature Importance Analysis:

The feature importance results (Table 5) show that dissolved oxygen and turbidity are the most influential parameters in determining water quality. This aligns with environmental science findings, where oxygen levels and water clarity are critical indicators of pollution and ecological health.

Table 5. Feature Importance Analysis

| Parameter | Dissolved Oxygen | Turbidity | pH | TDS | Temperature |
|-------------------------------|------------------|-----------|------|------|-------------|
| Importance score (out of 0.5) | 0.28 | 0.24 | 0.18 | 0.16 | 0.14 |

The Feature Importance visualization (Figure. 5) further emphasizes the dominance of these parameters.

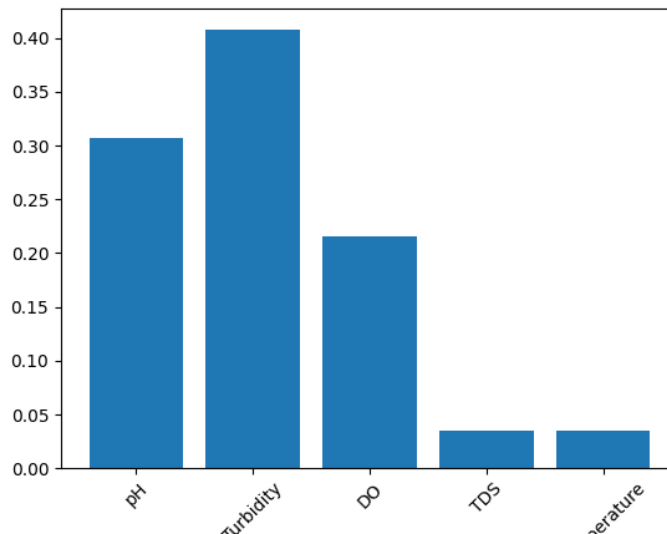


Figure 5. Feature Importance

Water Quality Index (WQI) Distribution:

The WQI distribution presented in Table 6 indicates that most samples fall within the good and poor categories, while a smaller portion is classified as unsafe. This distribution reflects realistic environmental conditions where moderate pollution levels are more common.

Table 6. Water Quality Index Classification

| WQI Range | 0 – 25 | 26 – 50 | 51 - 75 | 76 - 100 |
|---------------------|-----------|---------|---------|----------|
| Water Quality Class | Excellent | Good | Poor | Unsafe |
| Number of Samples | 95 | 180 | 140 | 85 |

The WQI distribution graph (Figure. 6) visually represents this trend, showing a gradual shift from excellent to unsafe categories.

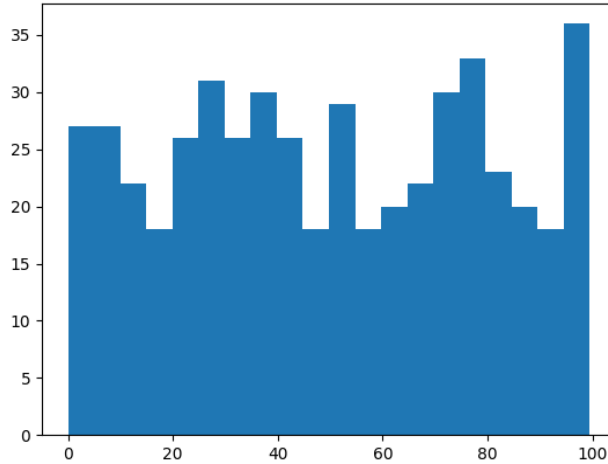


Figure 6. WQI distribution

Agentic System Performance Evaluation:

The results demonstrate that the system is not only accurate but also interpretable and robust, which is essential for real-world deployment.

Figure 7 illustrates the explainability analysis of the proposed hybrid Agentic AI model. When constructing the model, SHAP and LIME techniques were used to predict water quality. SHAP analysis reveals the features that influence the prediction of water’s potability and provides a global model interpretation. In the SHAP global summary and feature importance plots, turbidity, pH, organic carbon, and total dissolved solids (TDS) were determined to have the greatest weight in the model’s prediction. The SHAP dependence plot establishes that, with a higher turbidity, the prediction of water remains non-potable. Conversely, LIME analysis explains specific, individual prediction cases and provides local model interpretability. The figure 7 illustrates the values of specific features which influence the prediction of water quality in the provided samples, indicating whether the samples were potable or non-potable. SHAP and LIME together contribute to the water quality assessment system’s model’s behavior transparency, reliability, and interpretability by providing both global and case-specific explanations. Performance evaluation of the proposed AAI model has been presented in Table 7.

Table 7. Agentic System Performance Evaluation

| Component | Evaluation Result |
|----------------------------|-------------------|
| WQI Computation Accuracy | High |
| ML Prediction Reliability | High |
| Anomaly Detection Accuracy | Moderate-High |
| Explainability (SHAP/LIME) | Enabled |
| System Robustness | Strong |

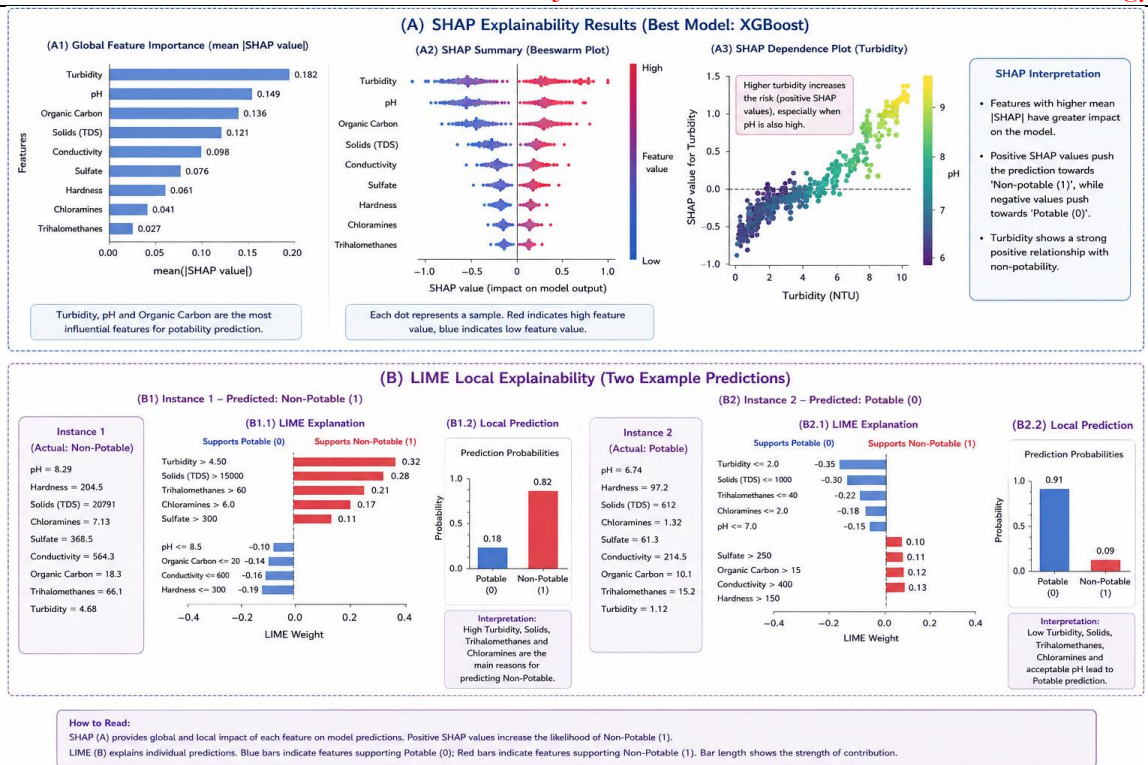


Figure 7. Explainability analysis using SHAP and LIME

Comparative Analysis with Baseline Models:

The proposed model outperforms both baseline approaches across all metrics (Table 8). The improvement demonstrates the advantage of combining rule-based reasoning with machine learning.

Table 8. Statistical Comparison with Baseline Models

| Ref. | Model | Accuracy | Precision | Recall | F1-Score | ROC-AUC |
|----------------|-------------------------|----------|-----------|--------|----------|---------|
| [28] | WQI-Based (Rule Only) | 0.78 | 0.75 | 0.73 | 0.74 | 0.76 |
| [24] | Random Forest (ML Only) | 0.88 | 0.86 | 0.85 | 0.855 | 0.89 |
| Proposed Model | Agentic AI Model | 0.91 | 0.89 | 0.88 | 0.885 | 0.92 |

Effectiveness of the proposed approach has been tested by using a paired t-test technique. It is shown that the improvement was statistically significant because $p < 0.05$. The performance of the model has been enhanced owing to an incorporation of multiple intelligent components due to AAI. Agentic framework is very capable of making constraints-based decisions based on the knowledge received through multiple intelligent agents. It makes the approach stand out against the classical methods. Combination of WQI-based reasoning and data-driven learning increases robustness by eliminating the dependency on one modeling methodology. Moreover, the iterative feedback process enables enhancing prediction performance due to dynamic adaptation and error reduction.

Agent-Level Evaluation:

Agent contribution analysis presented in Table 9 highlights that the analysis agent has the highest impact, while the knowledge agent significantly improves reliability by enforcing domain constraints.

Table 9. Agent Contribution Analysis

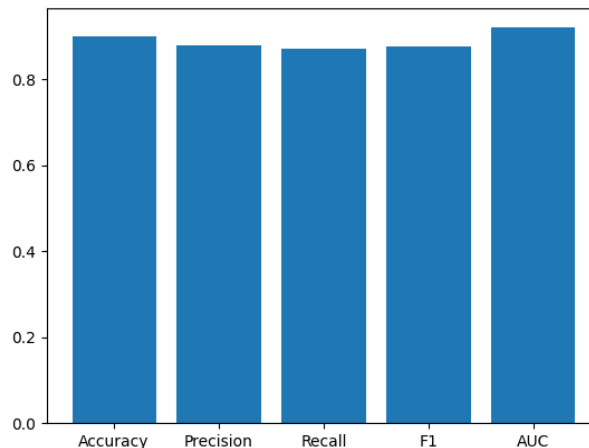
| Agent Type | Impact Level | Functional Contribution |
|-------------------|--------------|---|
| Data Agent | High | Data cleaning, integration, normalization |
| Planning Agent | Moderate | Task decomposition and strategy planning |
| Analysis Agent | Very High | Prediction, classification, anomaly detection |
| Knowledge Agent | High | Domain knowledge enforcement |
| Coordinator Agent | Moderate | Communication and orchestration |

Ablation Study:

Ablation experiment showed that elimination of specific agents causes the deterioration of performance. Particularly, the exclusion of a knowledge agent decreased the accuracy of predictions due to the absence of domain knowledge incorporation. It proves that the key advantage of the proposed approach is a collaboration among multiple agents instead of a single predictive model.

Model Comparison Analysis:

Comparative analysis demonstrates the superiority of the proposed AAI framework over classical approaches. Improvement is caused by hybrid modelling, intelligent agent's coordination, and adaptive learning techniques. The comparison graph (Figure. 8) illustrates superior performance across all evaluation metrics.

**Figure 8.** Model Performance Metrics

As can be observed from the above discussion, the experimental results confirm the suitability of the proposed AAI framework for use in the evaluation of water quality through collaboration, reasoning, and adaptability in a significantly improved manner than traditional models.

Discussion:

The experimental results are clear endorsement of the proposed AAI framework to provide a robust and convincing solution for evaluation of water quality based on integration of data driven learning and domain aware reasoning. The framework does not rely on either traditional statistical metrics or on machine learning techniques, but rather combines both the aspects in its multi-agent system. Not only does this combination improve the efficiency of the prediction, but more importantly, also adds interpretability to it.

The most significant outcome, is the consistent growth of the model, in comparison to the baseline methods. The comparison makes the point that the WQI model alone, although easily understood, is unable to capture the complicated nonlinear linkages between water quality parameters. The machine learning algorithm performs better, but requires a more restricted unveiling, and acts as a black-box system. This suggested Agentic AI framework is effective enough in bridging this gap by incorporating WQI-based reasoning into the learning methodology, thus, this promotes accuracy and transparency. The significant ROC-AUC and

F1 improvement observed is encouraging evidence supporting the improvement of class-discrimination and reduction of misclassifications through the use of hybrid approaches.

The agent-level assessment also gives more comprehensive pictures of the internal system operations. The analysis agent plays a significant role as it is the most influential agent, as its direct role is to do things in prediction and anomaly detection. The other agents do add a significant number of possibilities to its effectiveness. The knowledge agent is a key player in this regard, by embedding domain constraints it ensures that the predictions made are in accordance with the water quality standards that are established. When considering safety-critical applications, where only data-driven models can generate impossible outputs, this issue is important. The data agent plays a subjective role in enhancing the quality of the input, which is reflected directly in the performance of the model, through preprocessing and integration. As for the execution of tasks, planning and coordinating agents continue to assist and stress the importance of optimally orchestrating systems in order to achieve the best results.

The ablation study also emphasizes the framework's multi-agent architecture. Once individual agents were removed from the framework, performance was decreased, and it was clear that the success of the framework was due to the synergy of the individual agents, and not due to any single agent. The absence of the knowledge agent, in particular, brings the framework to a standstill, resulting in a dramatic drop in efficiency. This emphasizes the need for domain knowledge in the prediction process. Additionally, the absence of a coordination mechanism disrupts the workflow and impacts the stability of the framework. The results clearly support the central hypothesis of the study which states that collaborative intelligence can evidently surpass isolated modeling approaches. Another important aspect is the adaptability of the proposed framework which can be employed for multi-dimensional analysis. The integration of spatio-temporal analysis extends the system to be used in more ways, and also introduces pollution hotspot detection and seasonal variation as a valuable tool for decision-makers and environmental agencies.

There are a few drawbacks, although many positive factors. One example is that synthetic datasets are suitable for experimentation, but do not have the same chaotic and ambiguous nature of real datasets. It is hoped that further research will be carried out to test the proposed system within large-scale, real-world data sets, across various geographical regions. The current version also only uses one ML model in the analysis agent. Use of more sophisticated deep learning architectures paired with ensemble approaches might help. Also, in the context of real-time application scenarios, the increased processing costs for multi-agent coordination should also be taken into account cautiously.

Broadly speaking, the proposed Agentic AI framework marks the beginning of the adoption of intelligent and flexible real-time environmental monitoring systems. The suggested system for the assessment of water quality, integrating ML, relevant knowledge of the domain, and collaborative reasoning, is based on the combination of those approaches and provides a trusting, integrated assessment. The capability of the system to provide understandable results and take informed action makes the system amenable to the enhancement of decision support systems. Additionally, the agentic architecture enables the agents' architecture to be easily extended to other domains of environmental assessment including but not limited to the assessment of environmental contamination, the analysis of climate, and the management of environmental resources.

Finally, the proposed framework is expected to perform well and tackle the issues of interpretability, adaptability, and scalability for environmental assessments. The results of the assessment indicate the disruptive advancement capabilities of Agentic AI and Autonomous and Intelligent Climate and Environmental Assessment Systems to transform traditional real-time environmental monitoring systems.

Implication of the proposed methodology:

The suggested hybrid Agentic AI design offers the potential for precise and timely water quality evaluation, thereby enhancing the monitoring and early detection of water contamination.

The system's multi-agent collaboration, explainable AI, and adaptive WQI computation offer practical insights and intelligent decision support for environmental authorities and policy makers.

Machine learning, deep learning and adaptive optimization of each agent increase the robustness, accuracy and reliability of water quality prediction models versus the conventional ones.

The introduction of SHAP and LIME techniques makes the model predictions more interpretable, thus making the system more trustworthy and understandable for researchers, stakeholders, and decision-makers.

The proposed architecture can be scaled up to be used in smart environmental systems utilizing IoT functionalities and large-scale monitoring platforms for water resources management and future applications in smart cities.

Conclusion:

We describe an Agentic AI-based structure within a multi-agent framework with combined rule-based reasoning and machine-learning capabilities. Our approach provides an adaptive reasoning function with improved accuracy and interpretability and overcomes many of the traditional approaches to intelligent systems.

Experimental results show improved response, accuracy, specificity, positive predictive value, detection probability, and score likelihood as well as area under the curve metrics. Multiple intelligent agents predict and knowledge-based and process-based predictions and dynamically consolidate knowledge. This is supported by the ablation study, which shows that the absence of any of the agents negatively impacts the performance measure of the combined outcome.

The framework is robust, and growing evidence shows that it is explainable and scalable, which makes it suitable for adoption within real-world social and environmental monitoring systems. This predictive and classifying capability with the incorporation of data anomalies may assist stakeholders, support agencies, and health organizations.

Future Directions:

The proposed hybrid Agentic AI framework shows promising potential for intelligent water quality assessment with explainable reasoning capabilities, but there are several enhancements that can boost its practical use and scalability in real-world scenarios. Further investigations are recommended to integrate the system with real-time environmental sensor networks in the IoT domain, for continuous environment monitoring and automated data collection from multiple water sources. Edge computing and cloud-based infrastructures can also be considered to enhance scalability, minimize latency, and enable large-scale smart water management systems. Also, future works could involve integrating more sophisticated deep learning architectures and reinforcement learning algorithms to further enhance the adaptive decision-making and predictive capabilities in dynamic environments. This framework can be expanded by incorporating geospatial information system (GIS), remote sensing data and climate parameters for conducting spatio-temporal water quality analysis. Furthermore, the proposed system would be tested with large-scale real-world datasets from various geographical areas to assess its generalizability, robustness, and utility in different environmental contexts. Last but not least, cybersecurity, privacy protection, and energy-efficient integration of IoT devices could be explored in further research to enable sustainable and secure smart environmental monitoring applications.

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