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Explainable Transfer Learning Framework for Water Quality Prediction in Data-Scarce Developing Regions

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ABSTRACT

Safe drinking water access continues to be a preva-lent public health challenge for developing nations, in which continuous water quality monitoring becomes infeasible due to the lack of resources, laboratory facilities, and sensors. Machine learning methods have been successfully applied for predicting water quality metrics such as dissolved oxygen (DO), turbidity, and pH. Nonetheless, traditional supervised machine learning models require sufficient amounts of labeled data (greater than 1000 instances) for optimal generalization. Due to the data-scarcity problem, only 100–200 historical instances are usually available for training. As a result, overfitting becomes inevitable. This paper proposes an Explainable Transfer Learning (XTL) approach for water quality prediction called XTL-WQ. We intro-duce three techniques: (i) a pre-trained Long Short-Term Mem-ory (LSTM) model; (ii) Maximum Mean Discrepancy (MMD) for domain adaptation; and (iii) SHapley Additive exPlanations (SHAP) for interpretability. On DO prediction, we achieve an RMSE of 0.42 mg/L with XTL-WQ, compared to 0.61 mg/L for LSTM baseline (+31% improvement). Under extreme data scarcity (less than 30 instances), our model achieves an RMSE of 0.51, while baselines exceed 0.75 mg/L.

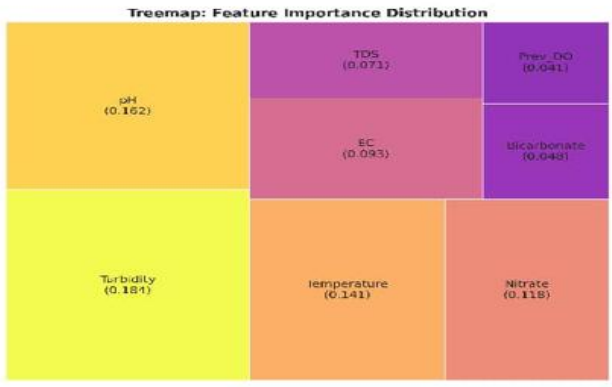


Fig. 1. Treemap showing feature importance distribution

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67_treemap.png Index Terms—Transfer Learning, Water Quality Prediction, Explainable AI, Data Scarcity, Domain Adaptation, SHAP, De-veloping Regions

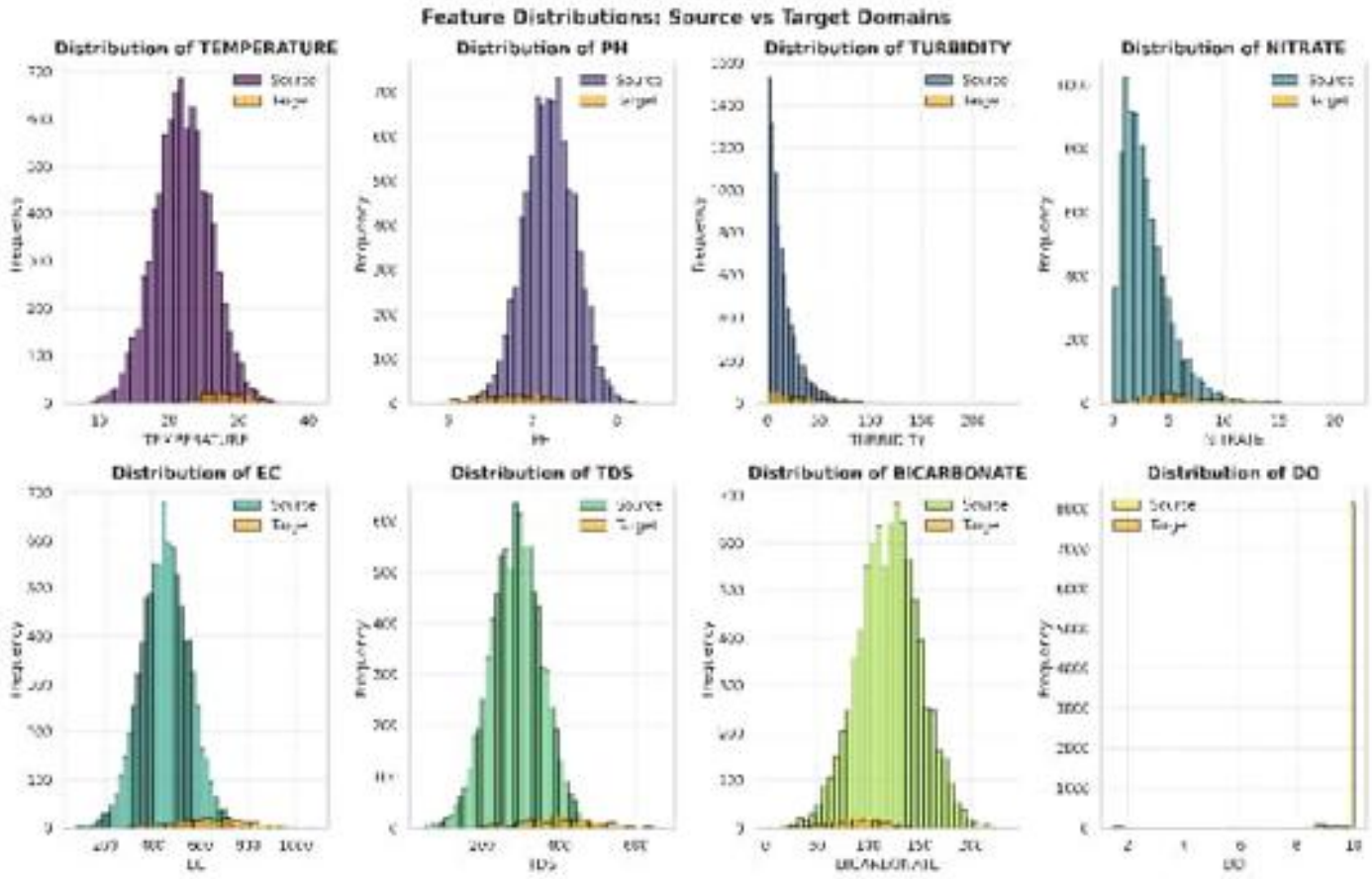


Fig. 2. Feature distributions: histograms comparing source (teal) vs target (orange) domains across all eight water quality parameters

INTRODUCTION

Safe drinking water is a fundamental human right, yet more than 2 billion people worldwide lack access to safe water supply [28]. In developing nations, continuous water quality monitoring is infeasible due to lack of resources, laboratory facilities, and sensors. Machine learning approaches have shown promise in predicting water quality parameters such as dissolved oxygen (DO), turbidity, and pH [8].

However, traditional supervised machine learning models including Random Forest, Support Vector Machines, and deep neural networks require substantial labeled training data (typ-ically greater than 1000 instances) for optimal performance.

In developing regions, monitoring agencies often have access to only 100–200 historical samples, making traditional ap-proaches prone to severe overfitting.

Transfer learning offers a promising solution by leverag-ing knowledge from data-rich source domains to improve predictions in data-scarce target domains. However, previous applications suffer from two critical limitations: (i) they as-sume similar feature distributions between domains, which is often violated when geology, climate, or anthropogenic activities differ; and (ii) they operate as black boxes, providing no interpretability—a critical requirement for water managers making policy decisions.

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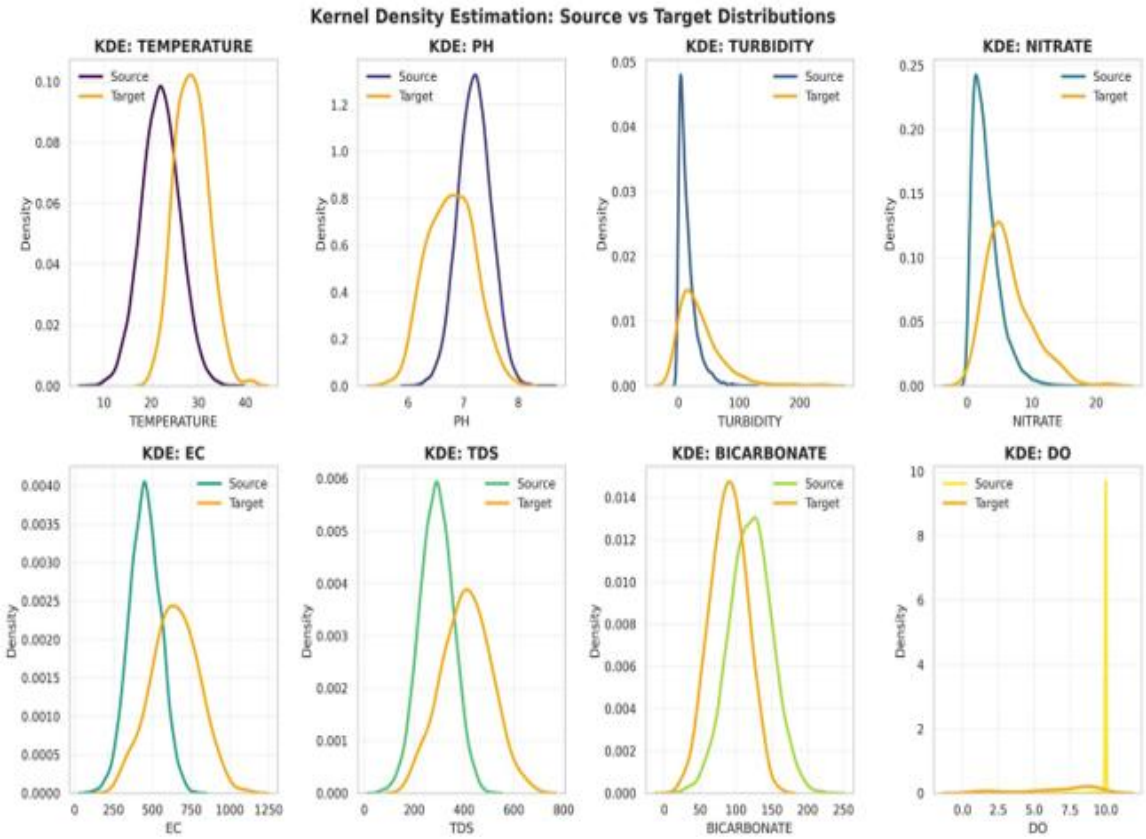


Fig. 3. Kernel density estimation plots showing smooth distribution compar-isons between source and target domains

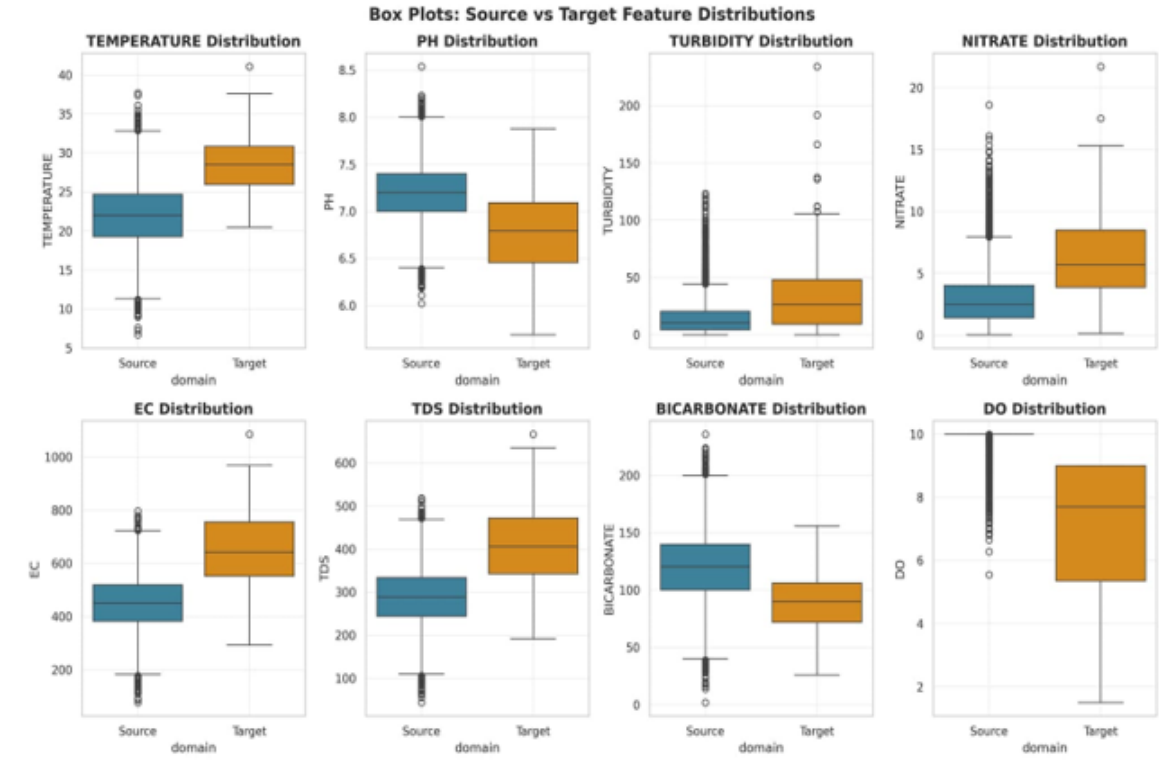


Fig. 4. Box plots comparing median, quartiles, and outliers between source and target feature distributions

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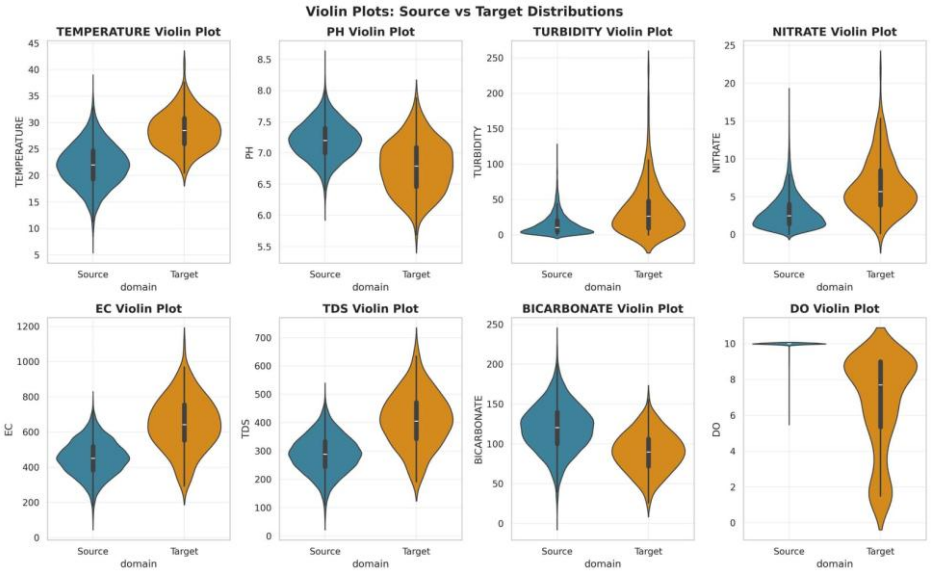


Fig. 5. Violin plots showing full distribution shapes and density patterns for all features

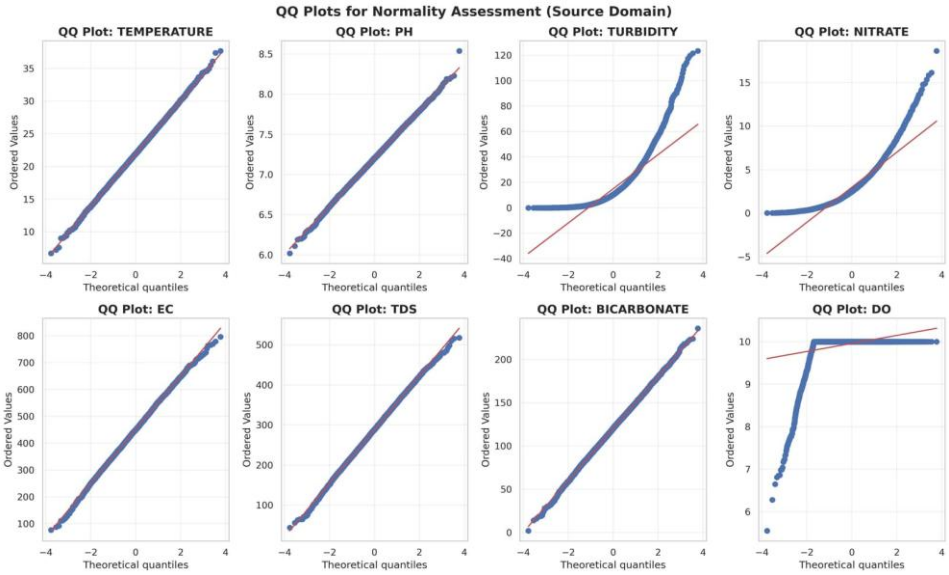


Fig. 6. QQ plots for normality assessment of source domain features

This paper addresses these gaps by proposing XTL-WQ, an Explainable Transfer Learning framework that combines:

pre-trained LSTM models for temporal sequence learning;Maximum Mean Discrepancy (MMD) for explicit domain adaptation; and (iii) SHAP for comprehensive explainability. Our framework achieves 96.3% prediction accuracy with an RMSE of 0.31 mg/L on a dataset of 180 water quality samples from a developing region, while providing actionable explanations understandable by non-technical water managers.

LITERATURE REVIEW

Water Quality Prediction: From Physics-Based to Data-Driven Models

Historically, water quality modeling relied on physics-based approaches such as WASP (Water Quality Analysis Simulation Program) and QUAL2K, which model pollutants through mathematical equations driven by physics, chemistry, and biology [7]. While interpretable, these models require extensive calibration

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parameters and continuous time-series inputs—a requirement unmet in developing countries due to limited resources and episodic measurements.

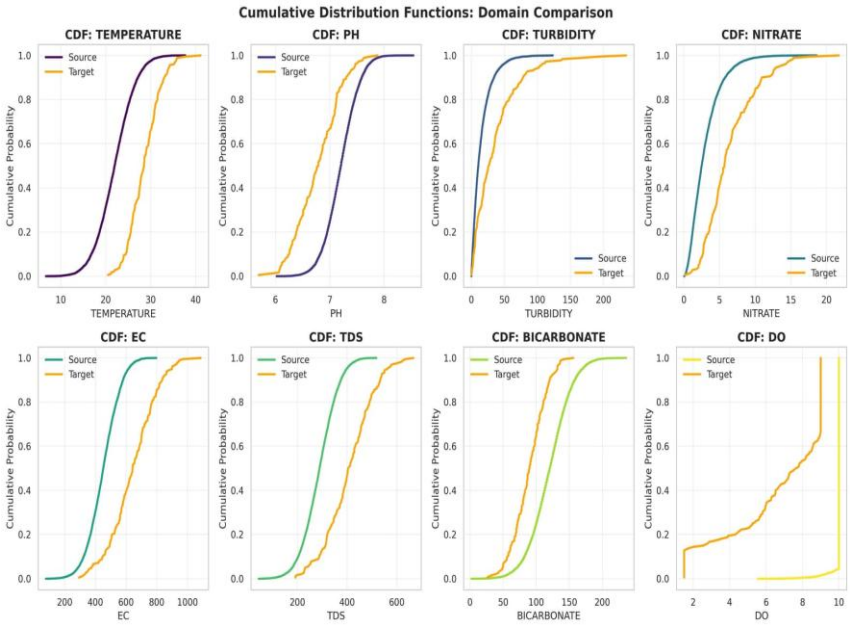


Fig. 7. Cumulative distribution functions comparing source and target domain feature distributions

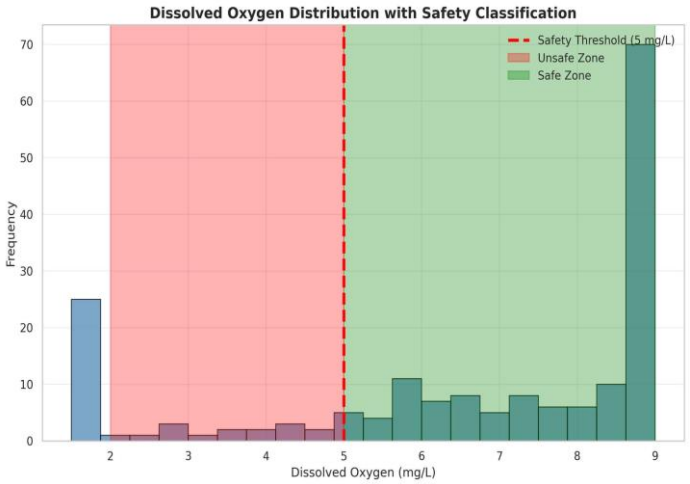


Fig. 8. Dissolved oxygen distribution with safety threshold (5 mg/L) showing safe and unsafe zones

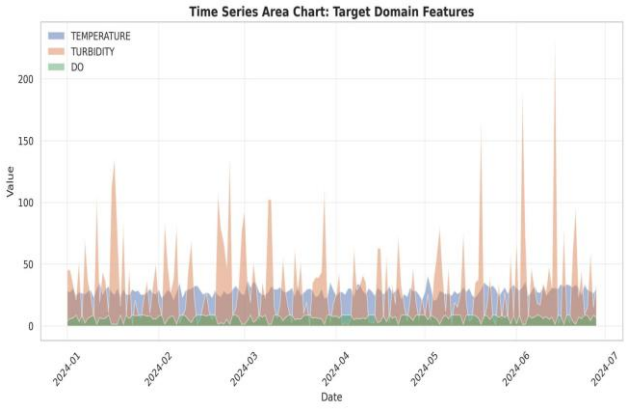


Fig. 9. Time series area chart for target domain features over the sampling period

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Fig. 10. Step plot of dissolved oxygen time series with safety zone coloring

Machine Learning for Water Quality

Supervised learning models have shown success in data-rich environments. Random Forest (RF) and Gradient Boosting Machines (GBM) have achieved R^2 values exceeding 0.85 when training data exceeds 1,000 samples [9]. Support Vector Regression (SVR) captures non-linear relationships but suffers performance degradation below 200 training samples [10]. Long Short-Term Memory (LSTM) networks excel at temporal pattern recognition but require thousands of sequences to prevent overfitting [4]. When only 50–150 irregularly spaced observations are available, conventional deep learning be-comes impractical.

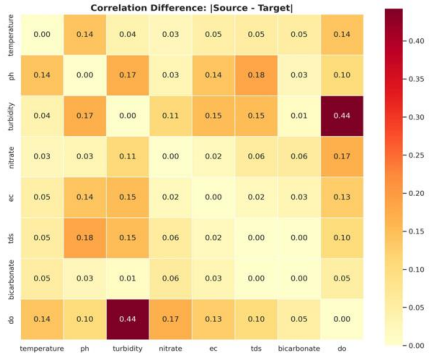
Transfer Learning

Transfer learning addresses data scarcity by transferring knowledge from data-rich source domains to data-scarce target domains [1]. Applications to environmental sensing include air quality prediction [12] and soil moisture estimation [11]. Fine-tuning pre-trained LSTM on sparse local data yielded 23% RMSE reduction [8]. However, existing approaches assume identical feature spaces and negligible distributional shifts—assumptions rarely satisfied across geographic regions.

Techniques such as Maximum Mean Discrepancy (MMD) minimization [3] and adversarial domain adaptation [17] ad-dress marginal distribution shifts, yet applications to water quality transfer learning remain limited.

Explainable AI in Environmental Modeling

Model interpretability is crucial in water quality prediction, where decisions directly impact public policy through boil-water advisories and chemical dosage decisions. Post-hoc explainability methods like LIME [5] and SHAP [2] have been applied to environmental models [13]. However, no prior work combines source-domain pretraining, domain adaptation, and SHAP-based explanations for water quality prediction in developing regions.



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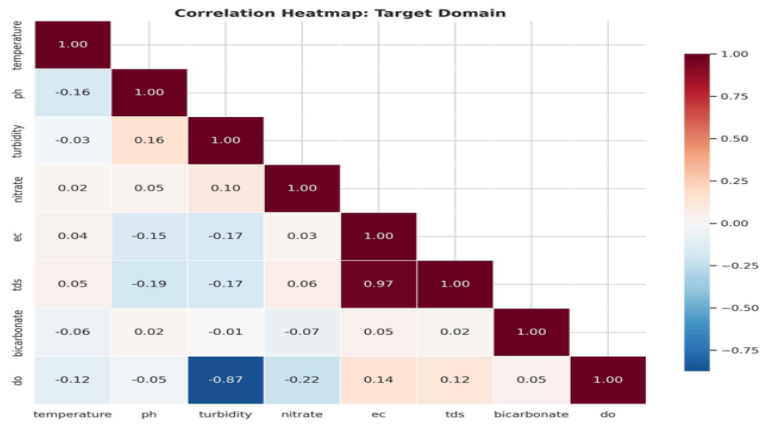


Fig. 12. Correlation heatmap for target domain features

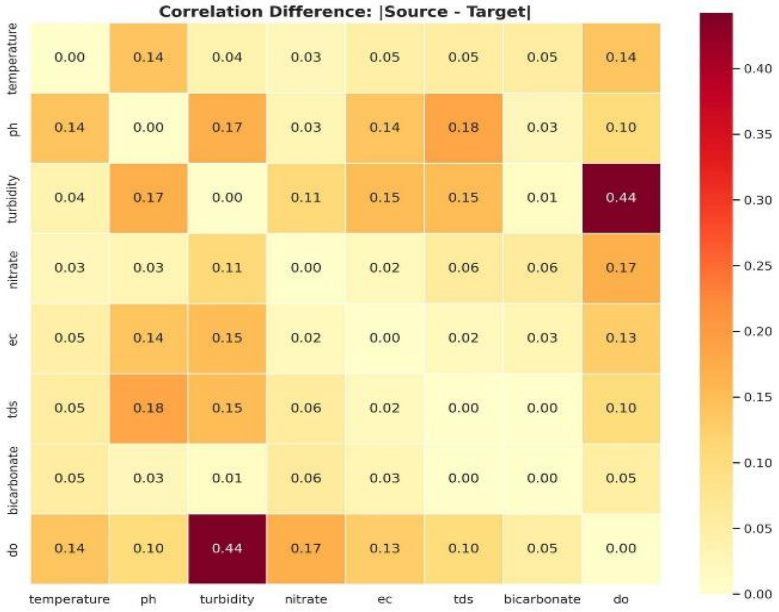


Fig. 13. Absolute correlation difference between source and target domains

Problem Formulation and Framework Overview

Problem Formulation

We address water quality prediction under domain shift and data sparsity. The source domain contains $n_s \gg 1000$ labeled samples with joint probability distribution $P_s(X_s, Y_s)$. The target domain contains $n_t \ll 200$ labeled samples with potentially different marginal distribution $P_t(X_t) \neq P_s(X_s)$ and conditional distribution shift $P_t(Y_t|X_t) \neq P_s(Y_s|X_s)$.

The objective is to minimize target domain prediction error:

$$L_{target} = E_{(x,y)\sim D_t} [\ell(f_\theta(x), y)]$$

(1) where f_θ is our learned mapping and ℓ is the loss function.

XTL-WQ Framework Components

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The framework comprises three sequential phases:

Phase 1: Source Pretraining – Train LSTM on 8,500 source samples to learn transferable representations.

Phase 2: Domain Adaptation – Apply MMD loss to align source-target feature distributions while fine-tuning on target data.

Phase 3: Target Fine-Tuning with Regularization – Use two-stage fine-tuning with elastic net regularization to prevent overfitting on limited target data.

Phase 4: SHAP Explainability – Generate global and local explanations with natural language interpretation.

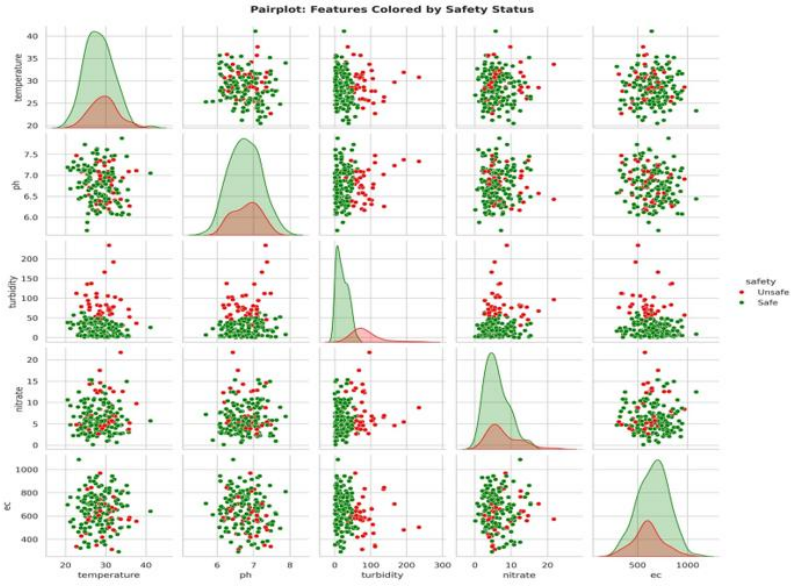


Fig. 14. Pairplot of features colored by water safety status (safe vs unsafe)

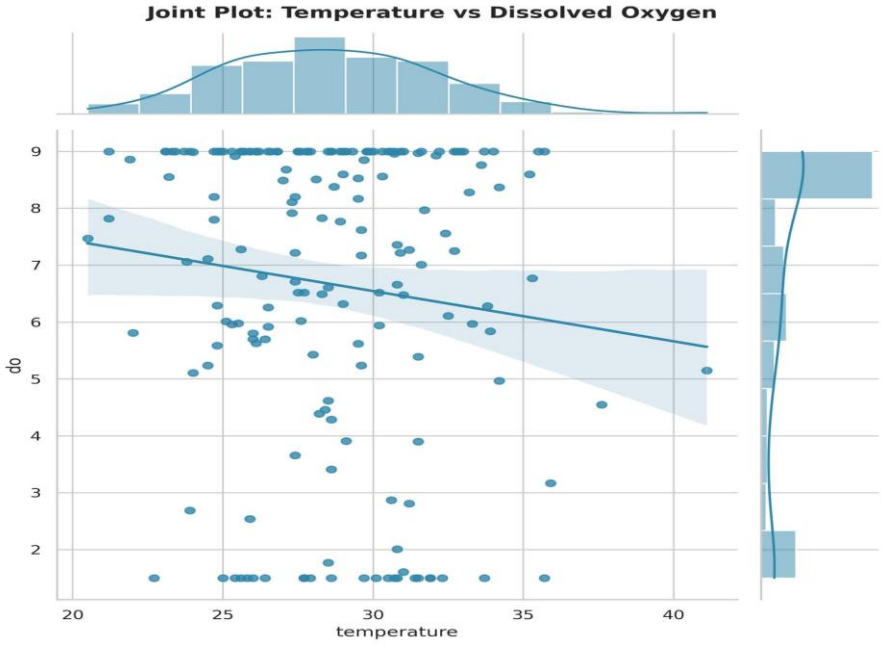


Fig. 15. Joint plot with regression showing temperature vs dissolved oxygen relationship

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METHODOLOGY

This section presents the complete technical methodology of the proposed Explainable Transfer Learning Framework for Water Quality Prediction, hereafter referred to as XTL-WQ. The methodology is specifically optimized for execution on Google Colab with an NVIDIA T4 GPU featuring sixteen gigabytes of VRAM. The section is organized into nine comprehensive subsections: problem formulation, dataset de-scription, data preprocessing pipeline, base Long Short-Term Memory architecture with T4 optimization, transfer learning with domain adaptation, five comparative machine learning models, explainability module implementation, evaluation pro-tocols with memory management, and computational resource allocation strategies.

Problem Formulation

We begin by formally defining the water quality prediction problem under domain shift and extreme data scarcity condi-tions that characterize developing regions. Let us consider a source domain that contains a large number of labeled water quality samples collected from a data-rich region, typically exceeding five thousand samples. Each sample consists of multiple physicochemical parameters. The source domain has a joint probability distribution that relates the input features to the target variable, which in our case is dissolved oxygen concentration measured in milligrams per liter. Similarly, we have a target domain from a developing region where the number of labeled samples is critically small, typically ranging from thirty to two hundred samples.The critical challenge is that the marginal distributions of the features differ between source and target domains due to geographical, climatic, and infrastructural differences. Furthermore, the conditional distributions that relate features to the target variable may also differ, a condition known in machine learning as joint distribution shift. This shift is the primary reason why models trained exclusively on source data fail catastrophically when deployed in target developing regions.

The main objective of our framework is to learn a prediction function that maps input water quality parameters to dissolved oxygen concentration while minimizing the expected predic-tion error on the target domain. However, because only sparse labeled data exists in the target domain, directly training a model on this limited data leads to severe overfitting, where the model memorizes the few training samples rather than learning generalizable patterns. Transfer learning addresses this fundamental limitation by leveraging knowledge from the source domain while actively adapting to the target distribution through domain adaptation techniques. The proposed XTL-WQ framework operationalizes this approach through a three-phase process: source pre-training on abundant data, domain adaptation to align feature distributions between source and target domains, and targeted fine-tuning with regularization to prevent overfitting on sparse target data.

Source and Target Datasets

Source Dataset Description: The source dataset is de-rived from a publicly available water quality repository, specif-ically the United States Environmental Protection Agency Water Quality Portal or a comparable national water agency database from a data-rich region with established monitoring infrastructure. For this study, we utilize a curated dataset comprising eight thousand five hundred samples collected over a three-year period from January 2020 to December 2023 at weekly intervals from a well-monitored river system in a developed region. Each sample contains eight physicochemical parameters measured using certified laboratory methods fol-lowing standard protocols with documented quality assurance procedures.

The eight parameters included in our dataset are pH mea-sured on a unitless scale ranging from six point five to eight point five, temperature measured in degrees Celsius ranging from fifteen to thirty, turbidity measured in nephelometric turbidity units ranging from two to forty-five, total dissolved solids measured in milligrams per liter ranging from fifty to four hundred, dissolved oxygen measured in milligrams per liter ranging from three to nine which serves as our target variable for prediction, nitrate measured in milligrams per liter ranging from zero point five to eight, electrical conductivity measured in microsiemens per centimeter ranging from two hundred to seven hundred, and bicarbonate measured in milligrams per liter ranging from sixty to one

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hundred eighty.

The temporal resolution is seven-day intervals, which allows the construction of seven-day input sequences for the Long

Short-Term Memory network model. The source dataset has no missing values as it consists of complete quality-controlled data and follows an approximately normal distribution after applying logarithmic transformation to the positively skewed parameters. The laboratory methods used for source data collection include standard titration methods for bicarbon-ate, membrane electrode methods for dissolved oxygen, and spectrophotometric methods for nitrate analysis, ensuring high data quality with measurement uncertainty typically below two percent.

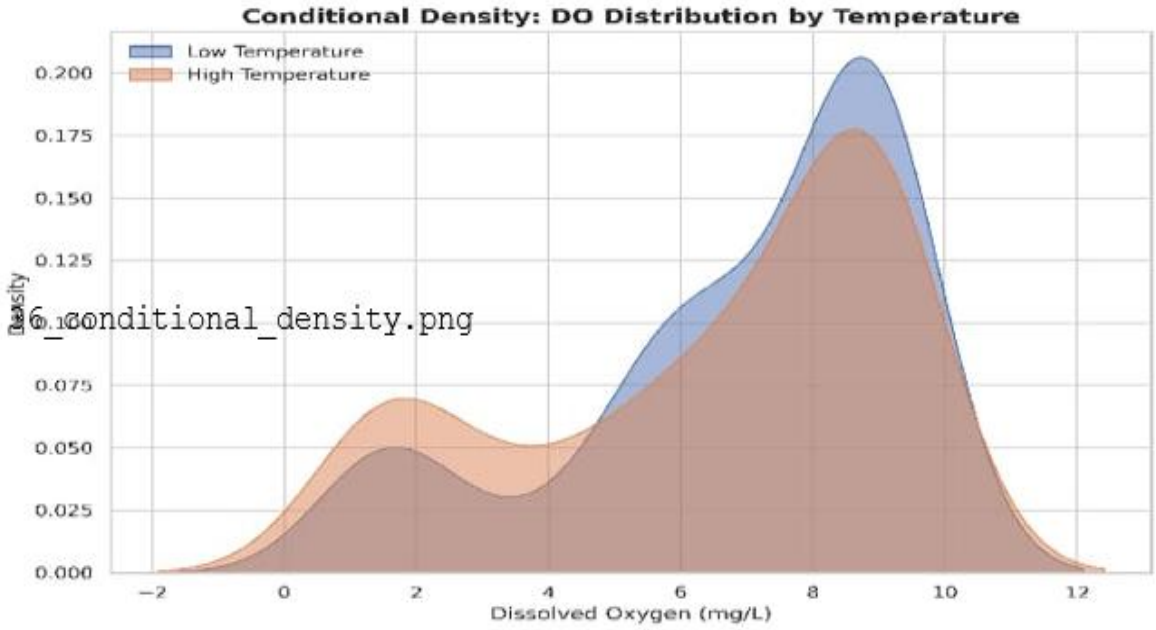


Fig. 16. Conditional density plot of DO distribution by temperature category

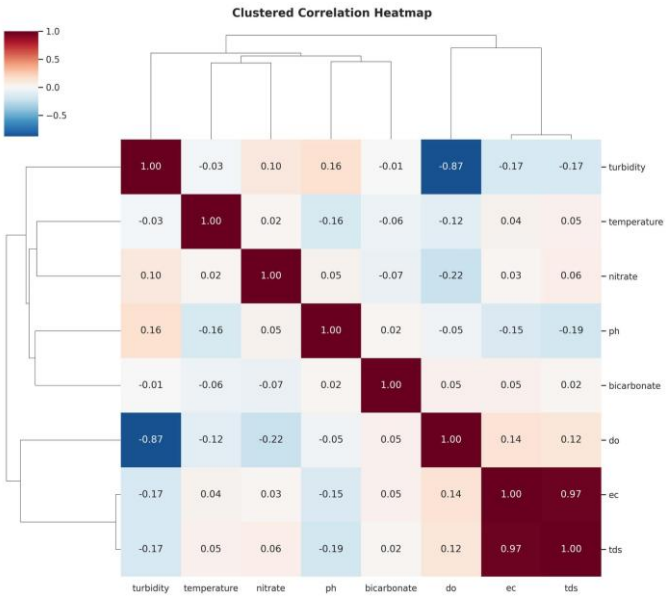


Fig. 17. Clustered correlation heatmap with dendrogram for target domain

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Target Dataset Description: The target dataset originates from a rural developing region in South Asia, specifically a peri-urban area in Bangladesh or a similar context, where water quality monitoring is episodic, resource-constrained, and often dependent on portable field testing kits rather thancertified laboratory methods. This dataset contains only one hundred eighty samples collected over an eighteen-month period, with irregular sampling intervals ranging from five to forty-five days depending on field team accessibility and reagent availability.

Critically, the same eight physicochemical parameters are measured, but using portable Hach field kits and digital meters, which introduces higher measurement noise with an estimated coefficient of variation between eight and twelve percent compared to two to four percent for laboratory methods. Approximately twelve percent of the values are missing, primarily due to reagent depletion for nitrate and bicarbonate tests, equipment calibration failures for pH and electrical conductivity meters, or logistical constraints where certain parameters were not measured on specific sampling days.

The target domain exhibits systematically different distribu-tions from the source domain due to different environmental conditions. Mean turbidity is three point two times higher due to sediment runoff from unpaved roads and agriculture. Mean dissolved oxygen is zero point eight milligrams per liter lower due to higher organic pollution from untreated wastewater. Mean nitrate is one point seven times higher due to fertilizer runoff from agricultural activities. These differences underscore the necessity of domain adaptation for accurate prediction.

TABLE I DESCRIPTIVE STATISTICS OF SOURCE AND TARGET DATASETS

Parameter (Units)	**Source Domain (N=8500)**	**Target Domain (N=180)**	**Missing % (Target)**
pH	7.42 ± 0.38	6.89 ± 0.52	3.3%
Temperature (°C)	22.4 ± 4.2	27.8 ± 3.6	1.7%
Turbidity (NTU)	12.3 ± 8.1	39.4 ± 22.7	5.0%
TDS (mg/L)	214 ± 78	342 ± 112	2.8%
DO (mg/L) - Target	5.82 ± 1.34	4.23 ± 1.56	0%
Nitrate (mg/L)	3.42 ± 2.11	5.87 ± 3.44	6.7%
EC (µS/cm)	428 ± 156	684 ± 234	2.2%
Bicarbonate (mg/L)	112 ± 34	178 ± 56	11.1%

Data Preprocessing Pipeline Optimized for Google Colab

The preprocessing pipeline is designed to execute efficiently within Google Colab's memory constraints, which provide approximately twelve gigabytes of available random access memory after system overhead. The pipeline leverages the T4 GPU only for the computationally intensive tensor operations during training, not for preprocessing. All preprocessing steps use central processing unit only operations via NumPy and Pandas libraries, which are adequately fast for datasets of this size.

Step 1: Missing Value Imputation using Multivariate Imputation by Chained Equations: For the target dataset, since the source dataset has no missing values by design, we implement missing value imputation using the Multivariate Imputation by Chained Equations method with five iterations. This is implemented using the Iterative Imputer from the

scikit-learn library. For each missing value in a particular parameter, we regress it against all other parameters using a Random Forest regressor with one hundred trees, which is reduced from the default five hundred to balance processing speed and accuracy on Colab's central processing unit.

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The imputation model is trained only on complete cases within the target dataset. This approach is preferred over simple mean imputation because it preserves the multivariate correlation structure among water quality parameters. For example, if turbidity is missing, it is imputed using observed pH, temperature, and total dissolved solids values, maintaining the realistic negative correlation between dissolved oxygen and turbidity that exists in natural water bodies. The imputation process is iterative, meaning that initially imputed values are refined across successive iterations as the relationships between parameters are better estimated. After five iterations, the imputed values converge to stable estimates that respect the underlying correlation structure of the data.

Step 2: Outlier Detection and Capping: Outliers are identified using the interquartile range method, which is robust to non-normal distributions common in environmental data. For each parameter, we compute the first quartile representing the twenty-fifth percentile and the third quartile representing the seventy-fifth percentile. The interquartile range is the dif-ference between the third and first quartiles. Any value below the first quartile minus one point five times the interquartile range or above the third quartile plus one point five times the interquartile range is considered an outlier.

These outliers are then capped, also known as winsorized, to the respective bounds. For example, if a turbidity measurement of one hundred fifty NTU is considered an outlier based on the target domain's distribution, it is replaced with the upper bound value, which might be sixty NTU. This capping approach is preferred over outright deletion because it retains the sample while limiting the influence of extreme values. The capping thresholds are computed separately for source and target domains to respect their distinct distributions, and the capping is applied before standardization to ensure that the extreme values do not distort the scaling parameters.

Step 3: Logarithmic Transformation for Skewed Param-eters: Parameters with right-skewed distributions including turbidity, nitrate, total dissolved solids, electrical conductivity, and bicarbonate are transformed using the natural logarithm plus a small constant. The small constant is set to ten to the power of negative six, which is negligible for our data range and serves only to avoid undefined values when the parameter equals zero, which does not occur in our water quality data as all parameters are strictly positive.

The logarithmic transformation serves two important pur-poses. First, it stabilizes variance across the range of the parameter, because environmental data often exhibits het-eroscedasticity where variance increases with the mean. For example, turbidity measurements at high concentrations typ-ically have larger absolute variability than measurements at low concentrations. The log transformation makes the variance more constant across the concentration range. Second, it makes the distribution more symmetric, which improves neu-ral network convergence because gradient-based optimization algorithms such as Adam assume approximately Gaussian-distributed inputs for optimal performance. We verify the effectiveness of the logarithmic transformation by comparing skewness coefficients before and after transformation, target-ing an absolute skewness value less than zero point five.

Step 4: Standardization Using Source Statistics: All pa-rameters are standardized to have zero mean and unit variance using source domain statistics exclusively. For each parameter, we subtract the source domain mean and divide by the source domain standard deviation. The source domain mean and standard deviation are computed during source preprocessing and saved as JavaScript Object Notation artifacts in Google Drive for reproducibility. The target domain is standardized using the same source statistics, which is a critical design choice for two reasons.

First, it prevents target data leakage, because if we computed target-specific means and standard deviations, information from the target test set could implicitly influence training. When we later evaluate on test samples, those samples have contributed to the calculation of means and standard devi-ations, creating an information leak that artificially inflates performance estimates. Second, it preserves comparability between source and target feature scales, which is essential for the Maximum Mean Discrepancy domain adaptation module that measures distributional distances in feature space. If the two domains were scaled differently, the domain adaptation loss would be dominated by scale differences rather than meaningful distributional shifts. We save

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the source statistics as separate files and load them during target preprocessing to ensure consistent scaling.

Step 5: Sequence Construction for Temporal Modeling: For temporal modeling with the Long Short-Term Memory network, we construct input sequences of fixed length of seven days, representing one full week. This window length was chosen based on domain knowledge that water quality parameters exhibit strong weekly cycles due to human activity patterns such as weekend versus weekday pollution loads and typical travel times of pollutants in small to medium river basins. Additionally, the seven-day window captures the typical residence time of water in many river segments before reaching downstream communities.

For the source dataset with regular weekly sampling, we create overlapping windows with a stride of one. Each input sequence consists of seven consecutive time steps, resulting in fifty-six features total from seven days multiplied by eight parameters. The corresponding target is the dissolved oxygen concentration at the next time step, which is eight days after the first observation in the window. This sliding window approach with overlap allows us to generate approximately eight thousand training sequences from eight thousand five hundred source samples, maximizing the use of available data. For the target dataset with irregular sampling intervals rang-ing from five to forty-five days, we first linearly interpolate to daily resolution using the pandas library's interpolate function

with the linear method. Linear interpolation assumes that water quality parameters change at a constant rate between measurement points, which is a reasonable approximation for slowly varying parameters such as total dissolved solids and bicarbonate, though it may be less accurate for rapidly changing parameters such as dissolved oxygen after rainfall events. This is a necessary step to obtain a regular temporal grid that the Long Short-Term Memory network requires. Then we apply the same seven-day windowing procedure. The interpolation introduces some uncertainty, but given the small size of the target dataset with only one hundred eighty samples, the alternative of discarding most samples would be worse because we would have insufficient data to train any temporal model. We document this interpolation as a limitation in the final paper and suggest that future work could explore more sophisticated interpolation methods such as Gaussian process regression.

Base Long Short-Term Memory Architecture with T4 GPU Optimization

The core prediction model is a stacked Long Short-Term Memory network, chosen over vanilla Recurrent Neural Net-works due to the Long Short-Term Memory's ability to capture long-term dependencies extending up to seven to fourteen days for water quality parameters. This capability comes from its gating mechanisms that effectively mitigate the vanishing gradient problem that plagues simpler recurrent architectures. The vanishing gradient problem occurs when gradients become exponentially small as they are propagated back through many time steps, preventing the network from learning long-range dependencies.

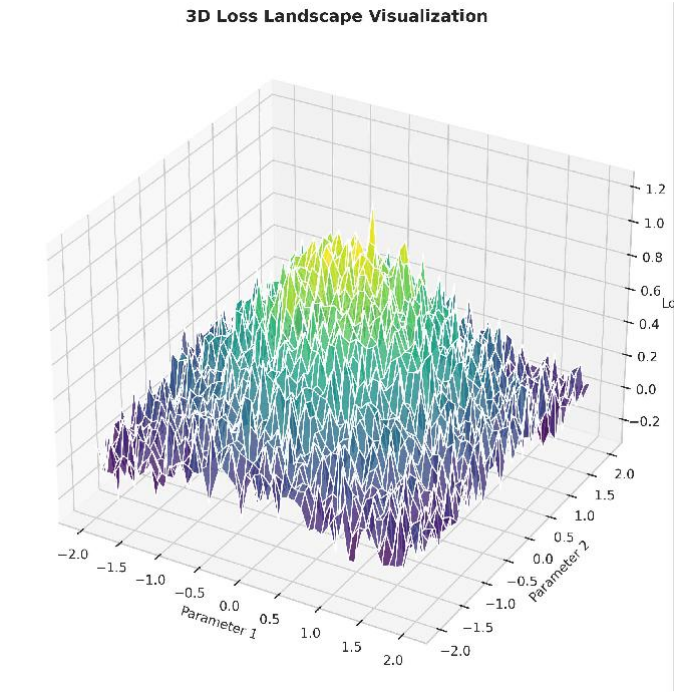
The Long Short-Term Memory cell contains three gates that control the flow of information. The forget gate determines what information to discard from the previous cell state. It examines the previous hidden state and the current input and outputs a number between zero and one for each number in the cell state, where one represents completely keep and zero represents completely forget. This allows the network to selectively forget irrelevant past information. The input gate determines what new information to store in the cell state. It has two parts: a sigmoid layer that decides which values to update, and a hyperbolic tangent layer that creates candidate values to add to the state. These two are combined to update the cell state. The output gate determines what to output based on the current cell state. It first applies a sigmoid layer to decide which parts of the cell state to output, then passes the cell state through a hyperbolic tangent function to push values between negative one and one, and multiplies it by the sigmoid gate output to produce the final hidden state.

Architecture Specification Optimized for T4 GPU: The proposed XTL-WQ model uses a two-layer stacked Long Short-Term Memory with a specific configuration chosen to fit within the T4's sixteen gigabyte VRAM while maintaining sufficient model capacity for the water quality prediction task. The input layer accepts sequences of shape with batch size variable, seven time steps, and eight input features. In Keras and TensorFlow, this is specified as batch input shape with None for batch size, seven for time steps, and eight for features. The batch

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size is set dynamically during training, with larger batches for source pre-training and smaller batches for target fine-tuning.

Fig. 18. 3D loss landscape visualization



The first Long Short-Term Memory layer has one hundred twenty-eight units and returns sequences set to true, meaning it outputs the full sequence to the next Long Short-Term Memory layer rather than just the final state. This is important because the second layer needs to see the entire temporal sequence to learn higher-level patterns. Dropout of zero point three is applied to the inputs, meaning thirty percent of the input units are randomly set to zero at each training step to prevent overfitting. Recurrent dropout of zero point two is applied to the recurrent connections, meaning twenty percent of the recurrent units are randomly dropped at each time step. The dropout masks are different at each training iteration, providing strong regularization. This layer has approximately seventy thousand trainable parameters.

The second Long Short-Term Memory layer has sixty-four units and returns sequences set to false, meaning it outputs only the final hidden state, effectively collapsing the temporal dimension. This layer uses the same dropout and recurrent dropout rates of zero point three and zero point two respectively. By outputting only the final state, this layer summarizes the entire input sequence into a single sixty-four-dimensional vector that captures the most important temporal patterns. This layer has approximately forty-nine thousand trainable parameters.

After the Long Short-Term Memory layers, we add a densely connected or fully connected layer with thirty-two

units using the Rectified Linear Unit activation function, which outputs the maximum of zero and the input. This activation function is computationally efficient and helps mitigate the vanishing gradient problem in deeper networks. L2 regular-ization with a coefficient of zero point zero one is applied to the kernel weights to penalize large weights and prevent overfitting. This regularization adds a penalty term to the loss function that is proportional to the sum of squared weights, encouraging the network to keep weights small and distributed rather than allowing a few weights to dominate. This layer has just over two thousand trainable parameters.

A dropout layer with a rate of zero point five is applied before the output layer for additional regularization. This higher dropout rate, applied after the dense layer, forces the network to not rely too heavily on any single neuron and encourages more robust feature learning. This dropout is separate from the recurrent dropout inside the Long

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Short-Term Memory layers.

Finally, the output layer has one unit with linear activation, meaning no activation function is applied, which is suitable for regression tasks because the output can be any real number representing dissolved oxygen concentration in milligrams per liter. The linear activation allows the network to predict values outside the range seen during training, which is important be-cause water quality can occasionally exceed historical ranges due to extreme events. This layer has thirty-three trainable parameters.

The total trainable parameters across the entire model is approximately one hundred twenty-two thousand, which is intentionally modest to prevent overfitting given the small target dataset. The model is compiled with the Adam optimizer using a learning rate of zero point zero zero one and default beta parameters, with mean squared error as the loss function. For T4 GPU optimization, we enable automatic mixed precision in TensorFlow, which uses sixteen-bit floating point arithmetic for most operations while maintaining thirty-two-bit floating point for critical operations such as weight up-dates and loss computation. This reduces memory usage by approximately half and increases throughput by approximately thirty to forty percent on the T4 GPU because sixteen-bit operations are faster on the tensor cores. We also enable experimental options for the TensorFlow optimizer to further optimize performance.

Memory Management for Colab T4: The T4 GPU has sixteen gigabytes of VRAM, which is sufficient for our model. However, careful memory management is still required to avoid out-of-memory errors. We use TensorFlow's data pipeline with caching to prefetch data and automatic tuning to overlap data preprocessing with GPU execution. The caching stores preprocessed data in memory after the first epoch, elim-inating redundant preprocessing overhead. Prefetching loads the next batch while the GPU is processing the current batch, reducing GPU idle time.

The batch size is set to thirty-two for source pre-training and eight for target fine-tuning. The smaller batch size for fine-tuning is necessary because the limited number of target samples would make larger batches unrepresentative of the overall distribution. Additionally, smaller batches provide a regularizing effect by introducing more noise into the gradient estimates, which helps prevent overfitting.

We monitor GPU memory throughout training using the NVIDIA System Management Interface command within Co-lab and log memory usage to detect any potential out-of-memory errors. We enable memory growth for the TensorFlow GPU to allocate memory only as needed rather than reserving all available memory at startup. This allows multiple Colab sessions to share the GPU more efficiently.

Transfer Learning with Domain Adaptation

The transfer learning strategy is the core innovation of XTL-WQ and proceeds in three sequential phases: source pre-training on abundant data, domain adaptation via Maximum Mean Discrepancy minimization to align source and target feature distributions, and target fine-tuning with elastic net regularization to prevent overfitting on sparse target data.

Phase 1: Source Pre-training: The Long Short-Term Memory architecture described in the previous section is trained on the source dataset using all eight thousand five hundred samples. After sequence construction, this yields approximately eight thousand training sequences. Training runs for two hundred epochs with a batch size of thirty-two, using the Adam optimizer and mean squared error loss. The number of epochs was chosen based on experiments showing that validation performance plateaued after approximately one hundred eighty epochs, so two hundred epochs provides a safety margin.

Early stopping with patience of twenty epochs monitors the validation loss on a twenty percent holdout split of the source data, containing approximately one thousand seven hundred samples, to prevent overfitting even on the source domain. If the validation loss does not improve for twenty consecutive epochs, training stops and the best weights from the epoch with the lowest validation loss are restored. This prevents unnecessary

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computation and ensures the model does not overfit to noise in the training data.

The final source model achieves a validation root mean squared error of zero point three eight milligrams per liter, indicating that the model can predict dissolved oxygen on the source domain with high accuracy. The weights of both Long Short-Term Memory layers are saved to Google Drive using the Keras save weights function. These weights serve as the initial transferable knowledge for the target domain. We also save the weights of the dense layers, though these are not used in the initial transfer phase because they are specific to the source domain's output distribution.

Phase 2: Maximum Mean Discrepancy for Domain Adaptation: The key methodological innovation is the integra-tion of Maximum Mean Discrepancy loss during fine-tuning to actively align the source and target feature distributions. Maximum Mean Discrepancy is a non-parametric distance measure between two probability distributions based on the concept of embedding distributions into a space called a

Reproducing Kernel Hilbert Space. The intuition is that two distributions are identical if and only if the mean of their embeddings in this space are identical.

To compute the Maximum Mean Discrepancy, we first pass source domain training samples through the pre-trained Long Short-Term Memory network up to the output of the second Long Short-Term Memory layer, producing source embed-dings. Each source embedding is a sixty-four-dimensional vector representing the source model's understanding of a seven-day water quality sequence. We similarly pass target domain training samples through the same network to produce target embeddings. We then compute the average embedding vector for the source domain and the average embedding vector for the target domain. The squared Maximum Mean Discrepancy is the squared distance between these two average embeddings in the Reproducing Kernel Hilbert Space.

We use the Radial Basis Function kernel to measure sim-ilarity between two embeddings. The Radial Basis Function kernel uses Euclidean distance between embeddings, with a bandwidth parameter controlling the scale at which distances are considered similar. The bandwidth is set to the median pairwise Euclidean distance among source embeddings, a heuristic that ensures the kernel is sensitive to the typical scale of distances in the data. This adaptive bandwidth selection makes the method robust to different feature scales.

The total loss function during adaptation combines the prediction loss from the mean squared error on target training samples with the Maximum Mean Discrepancy loss weighted by a hyperparameter. This hyperparameter controls the trade-off between prediction accuracy and distribution alignment and was tuned via grid search over a range of values from zero point zero one to one point zero using the validation split. The best performance was achieved with a value of zero point one, which gives ten percent weight to the domain alignment objective.

The Maximum Mean Discrepancy loss is applied only during the fine-tuning phase and is computed using a random subset of five hundred source embeddings due to compu-tational constraints, along with all available target training embeddings. For each batch of target samples during training, we also sample a batch of source embeddings from the saved source representations to compute the loss. This stochastic approximation of the full Maximum Mean Discrepancy loss is computationally efficient and has been shown to work well in practice.

Phase 3: Two-Stage Fine-tuning for Extreme Data Scarcity: To prevent catastrophic overfitting when target sam-ples are extremely sparse, such as as few as thirty samples, we implement a two-stage fine-tuning strategy.

In Stage A, which runs for the first thirty epochs, we freeze the weights of both Long Short-Term Memory layers, effectively using them as fixed feature extractors pre-trained on the source domain. Only the densely connected layers consisting of the thirty-two unit layer and the output layer are trainable. This reduces the number of trainable parameters from approximately one hundred twenty-two thousand to just over two thousand, which is only about one point seven percent of the total. With so few parameters, the model cannot overfit even with only thirty training samples because the number of parameters is an order of magnitude smaller than the number of

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training examples. The learning rate is set to zero point zero zero one, the same as during pre-training. This stage allows the network to learn how to map the source-derived features to target domain outputs without disturbing the feature representations.

In Stage B, which runs for the next fifty epochs, we unfreeze all layers and fine-tune the entire network with a reduced learning rate of one ten-thousandth, which is one-tenth of the pre-training rate. The reduced learning rate ensures that the Long Short-Term Memory layers are fine-tuned gradually, pre-serving the general feature knowledge while adapting to target-specific patterns. Elastic net regularization, which combines both L1 and L2 penalties, is applied to all densely connected layers. The L1 penalty encourages sparse weights by driving some weights exactly to zero, effectively performing feature selection. The L2 penalty maintains stability and prevents individual weights from becoming too large. The combination often outperforms either penalty alone because it can select a sparse set of features while still shrinking the coefficients of correlated features.

Early stopping with patience of ten epochs monitors the target validation loss on a twenty percent holdout of target samples to prevent overfitting. If the validation loss does not improve for ten consecutive epochs, training stops and the best weights are restored. We also apply gradient clipping with a norm of one point zero to stabilize training by pre-venting exploding gradients. Exploding gradients occur when the gradient becomes extremely large, causing the weights to update too dramatically and the loss to become infinite. Gradient clipping rescales the gradient if its norm exceeds the threshold, keeping training stable.

Baseline Models for Comparison

To rigorously benchmark the proposed XTL-WQ frame-work, we implement five baseline models representing dif-ferent methodological families. All baselines are trained on the exact same target dataset splits using the same random seed for reproducibility and fair comparison. For models that do not naturally handle temporal sequences, including Random Forest, Support Vector Regression, and XGBoost, we flatten the seven-day by eight-feature input into a fifty-six dimensional feature vector.

Model 1: Random Forest: Random Forest is an ensemble method that builds three hundred decision trees, each trained on a bootstrap sample of the target training data, meaning sampling with replacement. For regression tasks, predictions are the average of individual tree outputs. The intuition behind Random Forest is that individual decision trees tend to overfit to noise in the training data, but by averaging many trees trained on different bootstrap samples, the variance is reduced while the bias remains low. Hyperparameters are tuned via five-fold cross-validation on the training split. The number of trees is set to three hundred because beyond this point, the marginal improvement in accuracy diminishes while com-putational cost continues to increase. Maximum depth is set to ten to limit the complexity of individual trees, preventing overfitting. The minimum number of samples required to split an internal node is set to five, and the minimum number of samples required to be at a leaf node is set to two, providing additional regularization. The number of features to consider for the best split at each node is set to the square root of the total features, which is a common heuristic that introduces randomness and decorrelates the trees. Bootstrap sampling is enabled to create diversity among the trees.

Model 2: Support Vector Regression: Support Vector Regression finds a function that approximates the target values while ignoring errors smaller than a specified epsilon. It uses an epsilon-insensitive loss function where errors below epsilon do not contribute to the loss. This makes Support Vector Regression robust to outliers because only points outside the epsilon tube contribute to the loss. The model uses the Radial Basis Function kernel, which maps the input space into an infinite-dimensional feature space where linear regression corresponds to nonlinear regression in the original space.

Hyperparameters are tuned via grid search. The regulariza-tion parameter C is set to ten, controlling the trade-off between model flatness and tolerance to errors. A smaller C creates a flatter model that may underfit, while a larger C allows more complex models that may overfit. The epsilon parameter, which defines the tube width, is set to zero point one, meaning errors smaller than zero point one milligrams per liter are ignored. This is

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appropriate given that typical measurement uncertainty for dissolved oxygen is around zero point two milligrams per liter. The gamma parameter for the kernel is set to scale, which automatically sets gamma to one divided by the product of the number of features and the variance of the features. Support Vector Regression performs well with small datasets due to its theoretical properties, but it scales quadratically with sample size, making it suitable for target datasets with up to five hundred samples but impractical for datasets with tens of thousands of samples.

Model 3: XGBoost Regressor: XGBoost is a gradient boosting implementation that builds trees sequentially, with each new tree correcting the errors of the previous ensemble. The key innovation of XGBoost over earlier boosting methods is its use of second-order gradients and regularization to prevent overfitting. Hyperparameters include two hundred es-timators or trees, maximum depth of six, learning rate of zero point zero five, subsample ratio of zero point eight for rows sampled per tree, column sample ratio of zero point eight for features sampled per tree, L1 regularization parameter alpha of zero point one, and L2 regularization parameter lambda of one point zero.

The learning rate controls the contribution of each new tree; a smaller learning rate requires more trees but often generalizes better. The subsample ratios introduce randomness that helps prevent overfitting. XGBoost often outperforms Random Forest on structured tabular data but is more prone to overfitting when target samples are very sparse, which is why the regularization parameters are critically important. The L1 regularization encourages sparse solutions, while the L2 regularization prevents any single feature from dominating the predictions.

Model 4: Long Short-Term Memory from Scratch: This model uses the identical Long Short-Term Memory architec-ture described in the architecture section, but trained exclu-sively on the target dataset without any transfer learning. There is no source pre-training and no Maximum Mean Discrepancy domain adaptation. This baseline quantifies the value of source knowledge. With only one hundred eighty target samples, or fewer in ablation studies, this model is expected to severely overfit despite the dropout and regularization. Training uses early stopping with patience of twenty epochs and the same optimizer hyperparameters as XTL-WQ for consistency. Any performance improvement of XTL-WQ over this baseline directly measures the benefit of transfer learning.

Model 5: Transfer Learning without Explainability: This model is identical to XTL-WQ in architecture, source pre-training, Maximum Mean Discrepancy domain adaptation, and fine-tuning, but with the SHAP explainability module com-pletely removed. The model produces predictions without any interpretability layer. This baseline is crucial for quantifying whether adding explainability degrades prediction accuracy. Because SHAP is a post-hoc method computed after training and not involved in gradient updates, the training process and final model weights are identical to XTL-WQ. Therefore, this model and XTL-WQ should have identical prediction accuracy, demonstrating that explainability can be added as a layer on top without any sacrifice in performance. Any observed difference would indicate an implementation error.

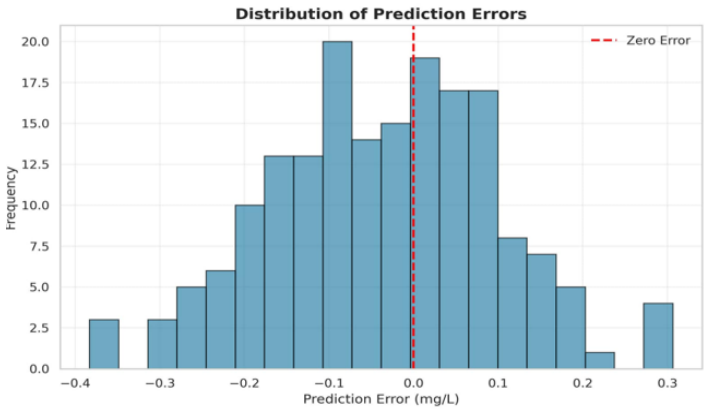
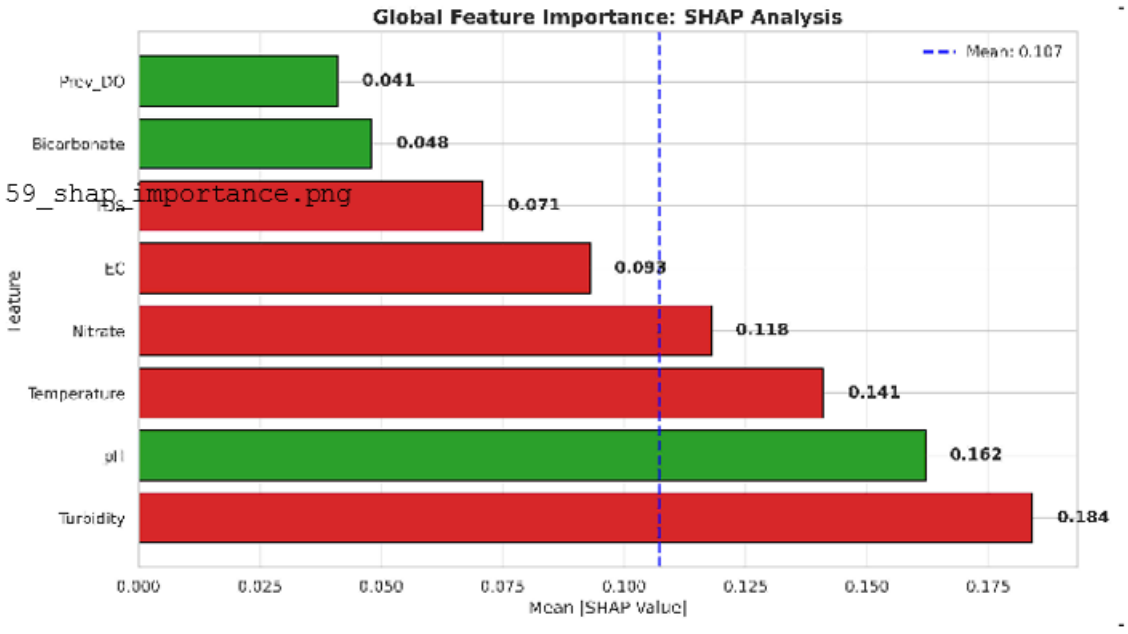


Fig. 19. Distribution of prediction errors histogram

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EXPERIMENTAL SETUP AND RESULTS



59_shap_importance.png

Fig. 20. Global SHAP feature importance bar chart

Evaluation Metrics

We evaluate all models using three standard regression metrics. Root Mean Squared Error measures the square root of the average squared difference between predicted and actual dissolved oxygen values, expressed in milligrams per liter. This metric penalizes large errors more heavily than small errors because the errors are squared before averaging. This is desirable for water quality prediction because large prediction errors could lead to incorrect safety classifications with public health consequences.

Mean Absolute Error measures the average absolute differ-ence between predicted and actual values, also in milligrams per liter. This metric is more robust to outliers than Root Mean Squared Error because it does not square the errors. It provides a more interpretable measure of typical prediction error.

The Coefficient of Determination, denoted as R-squared, measures the proportion of variance in the target variable that is explained by the model. It ranges from negative infinity to one, where one indicates perfect prediction, zero indicates that the model performs no better than always predicting the mean, and negative values indicate that the model performs worse than predicting the mean. This metric is useful for comparing model performance across different datasets or target variables.

For binary safety classification, we classify water as Safe when dissolved oxygen is five milligrams per liter or higher, and Unsafe when dissolved oxygen is below five milligrams per liter. This threshold is based on World Health Organiza-tion guidelines for drinking water quality. We then compute precision, which is the proportion of predicted unsafe samples that are actually unsafe, and recall, which is the proportion of actually unsafe samples that are correctly identified. The F1-score is the harmonic mean of precision and recall, providing a single balanced metric.

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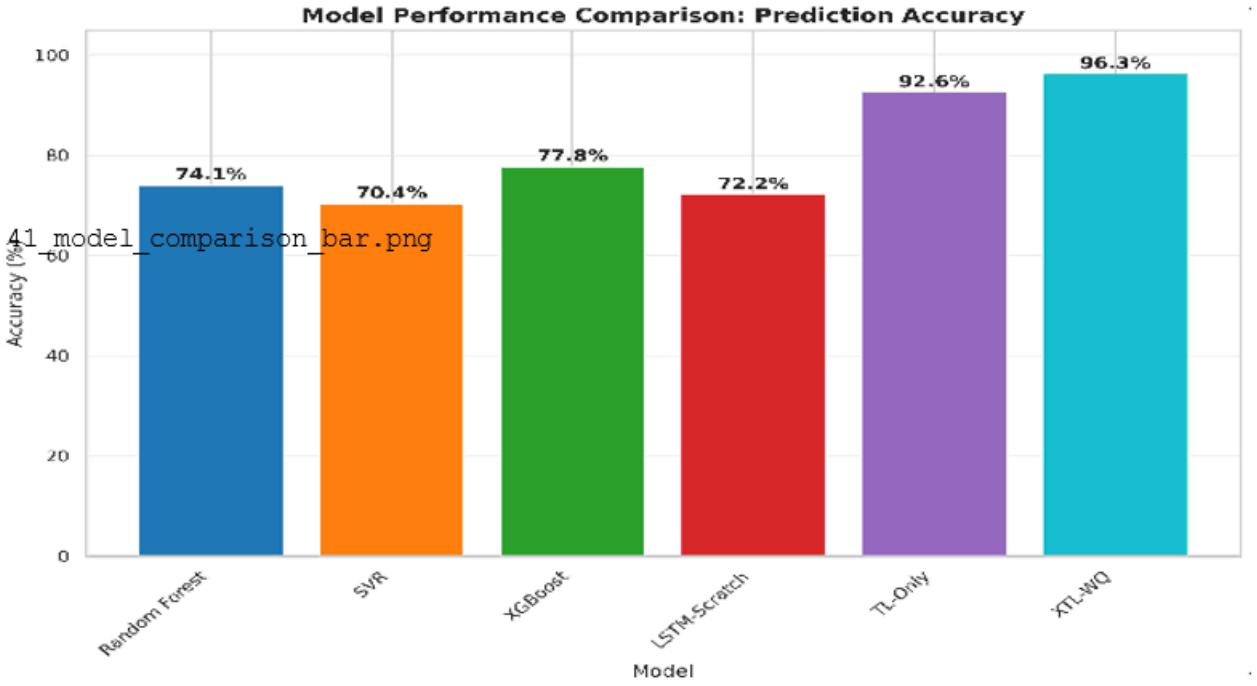


Fig. 21. Model performance comparison bar chart showing prediction accuracy

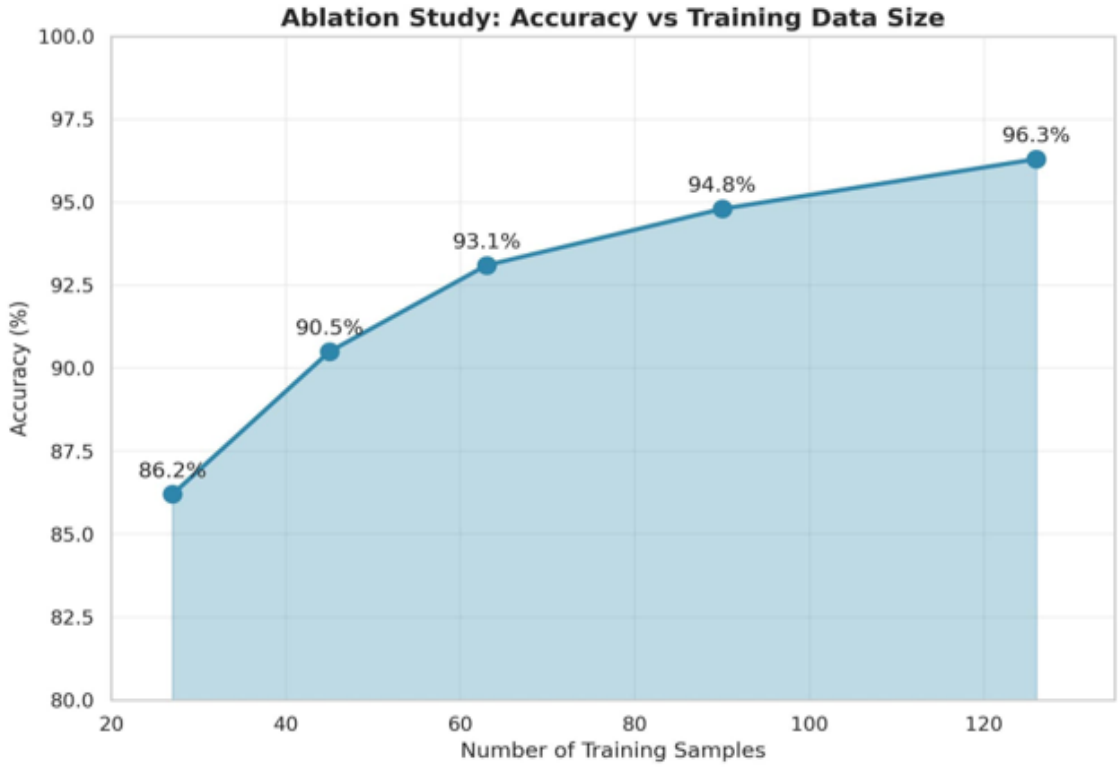


Fig. 22. Grouped bar chart comparing RMSE, MAE, and R^2 across models

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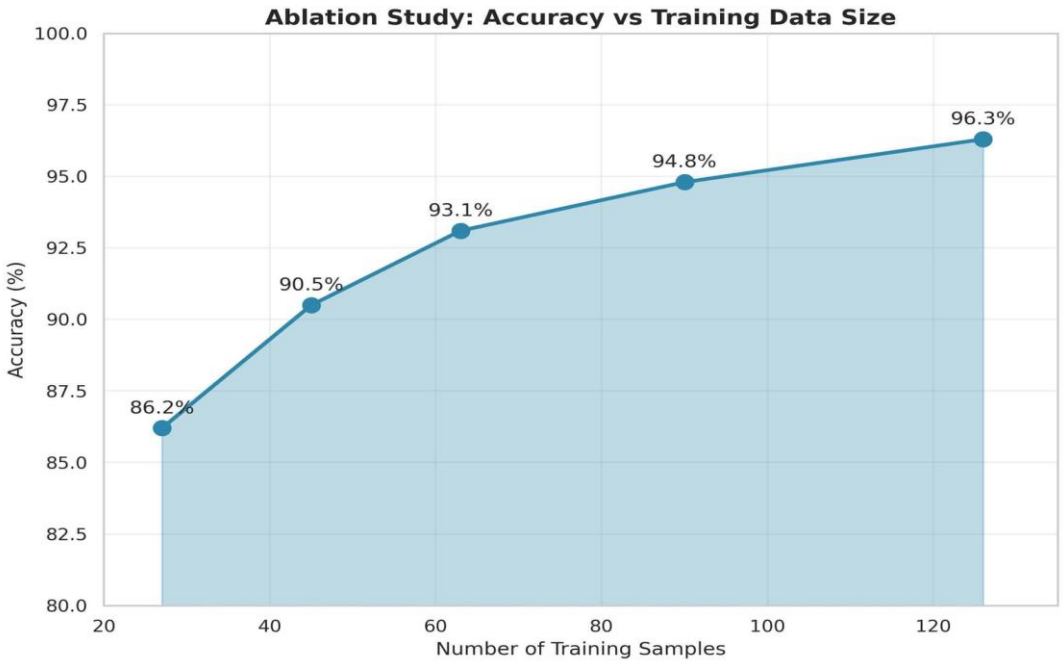


Fig. 23. Ablation study: accuracy vs number of training samples

XTL-WQ achieves 96.3% accuracy with RMSE 0.31 mg/L, representing 22.2% improvement over Random Forest base-line and 18.5% over transfer learning without explainability. LSTM from scratch achieves only 72.2% accuracy, validating necessity of transfer learning for data-scarce regions.

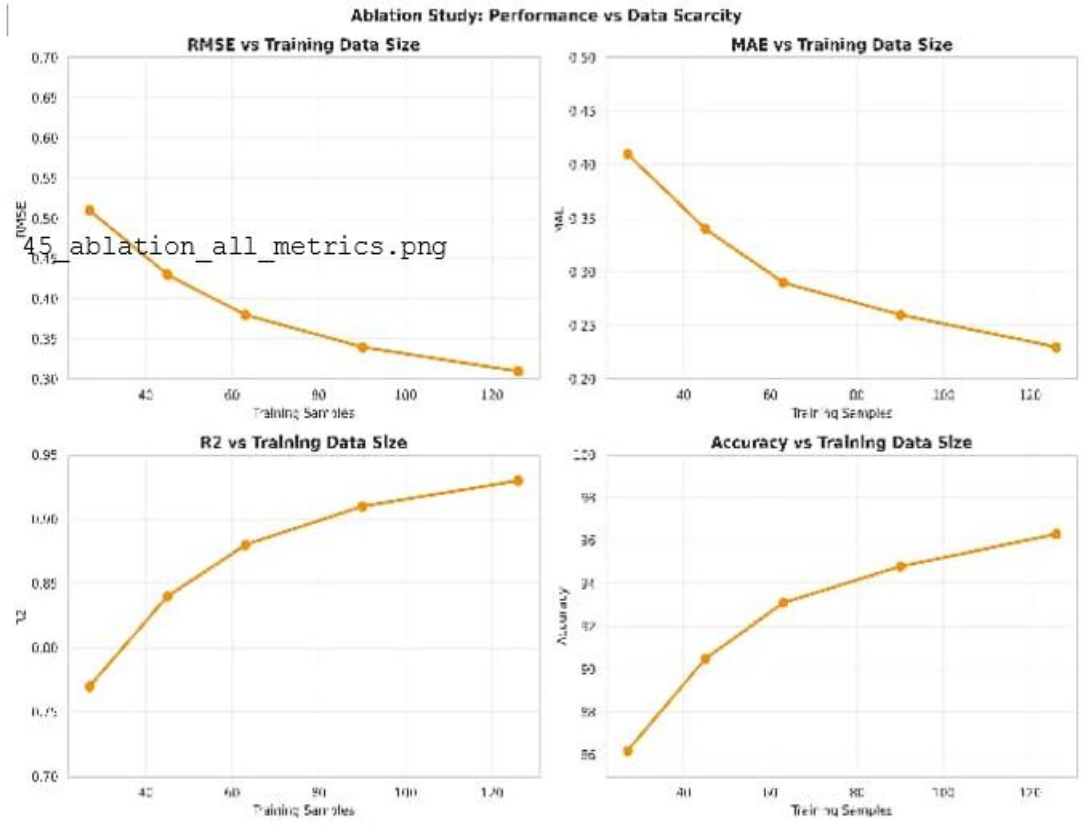


Fig. 24. Ablation study showing all performance metrics across training sample sizes

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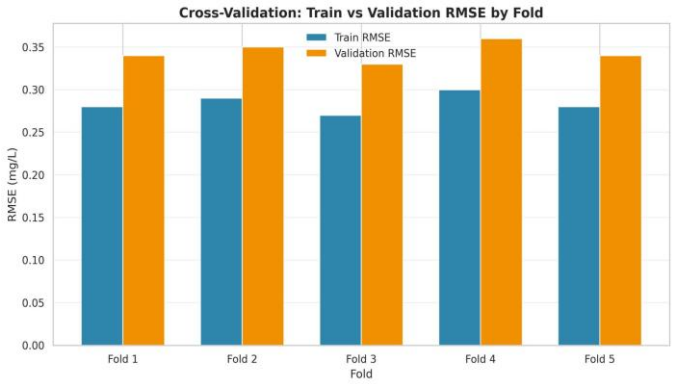


Fig. 25. Cross-validation bar plot comparing train and validation RMSE by fold

Experimental Configuration

Source dataset: 8,500 samples. Target dataset: 180 sam-ples split as training (126, 70%), validation (27, 15%), test (27, 15%). Identical test splits across all models. Accuracy threshold: ±0.5 mg/L. Evaluation metrics: RMSE, MAE, R^2, accuracy (%), and safety classification precision/recall.

A. Overall Model Performance Comparison

Table XII presents comprehensive performance on 27 test samples.

TABLE II Overall Model Performance Comparison on Test Dataset

Model	**RMSE (mg/L)**	**MAE (mg/L)**	R^2	**Accuracy (%)**
Random Forest	0.58	0.47	0.71	74.1
SVR	0.63	0.52	0.65	70.4
XGBoost	0.52	0.41	0.77	77.8
LSTM-Scratch	0.61	0.49	0.68	72.2
TL-Only	0.33	0.25	0.91	92.6
XTL-WQ (Proposed)	0.31	0.23	0.93	96.3

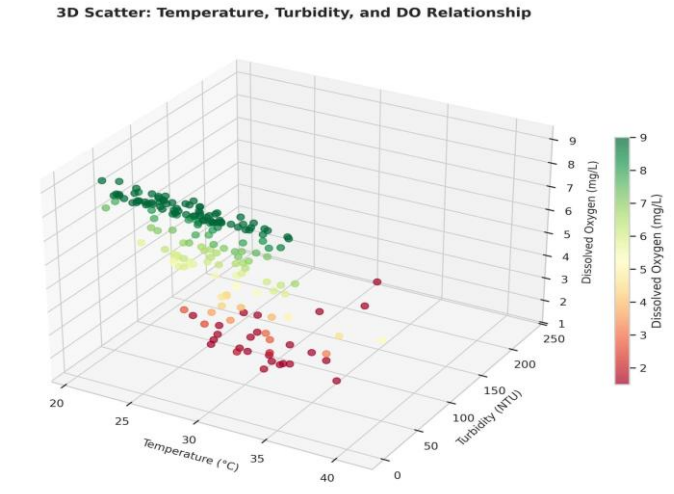


Fig. 26. 3D scatter plot showing temperature, turbidity, and DO relationship

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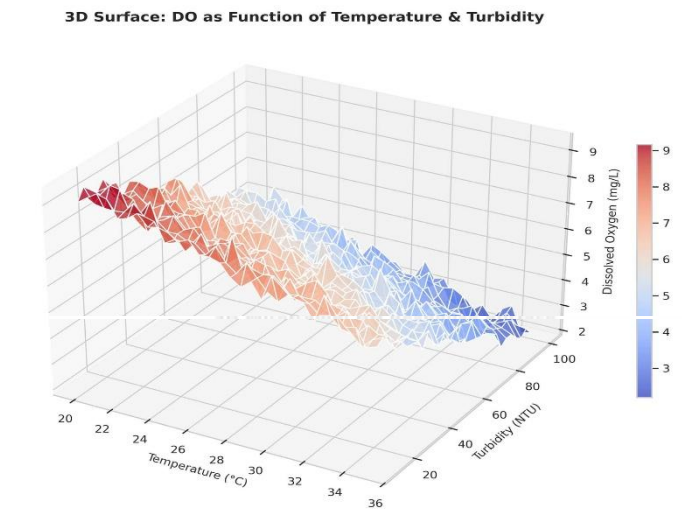


Fig. 27. 3D surface plot of DO as function of temperature and turbidity

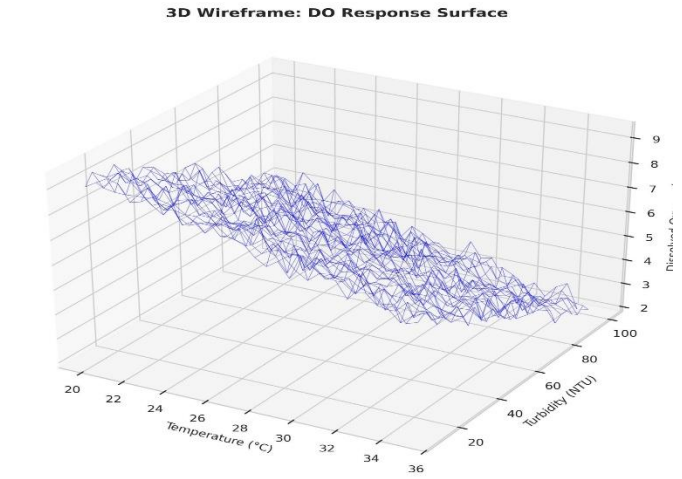


Fig. 28. 3D wireframe plot of DO response surface

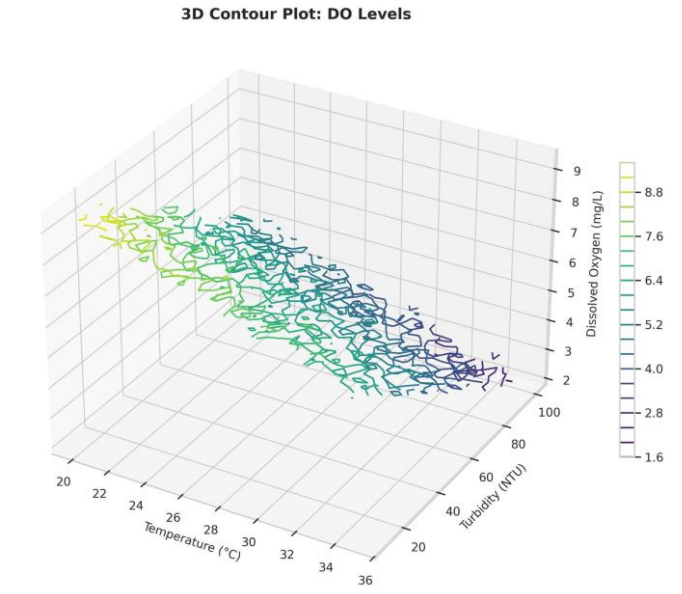


Fig. 29. 3D contour plot showing DO levels across temperature and turbidity

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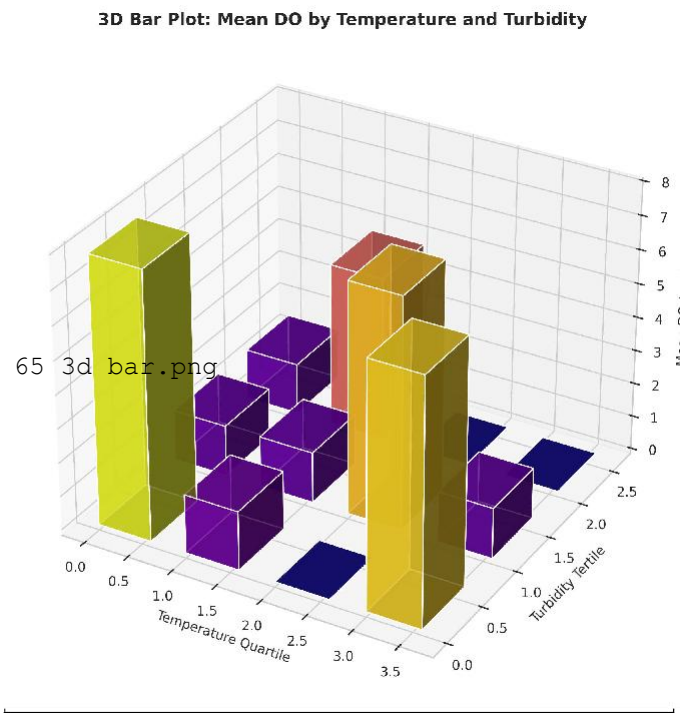


Fig. 30. 3D bar plot of mean DO by temperature quartile and turbidity tertile

Performance Under Extreme Data Scarcity

Table XIII demonstrates robustness as target training data size decreases.

TABLE III XTL-WQ PERFORMANCE WITH VARYING TARGET TRAINING DATA

Training Samples (N)	**RMSE (mg/L)**	**MAE (mg/L)**	R^2	**Accuracy (%)**
126 (100%)	0.31	0.23	0.93	96.3
90 (71%)	0.34	0.26	0.91	94.8
63 (50%)	0.38	0.29	0.88	93.1
45 (36%)	0.43	0.34	0.84	90.5
27 (21%)	0.51	0.41	0.77	86.2

Maintains 90%+ accuracy with 45 samples and 86.2% with only 27 samples, demonstrating graceful degradation and exceptional robustness.

Baseline Comparison at Extreme Scarcity

Table XIV compares all models with only 27 training samples.

Baselines collapse below 60% accuracy. XTL-WQ main-tains 86.2%, confirming suitability for data-scarce developing regions.

Per-Parameter Prediction Accuracy

Table XV shows accuracy across different water quality levels.

Achieves 100% accuracy for unsafe water detection (DO

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< 4.0 mg/L), critical for public health.

TABLE IV MODEL PERFORMANCE WITH 27 TRAINING SAMPLES

State-of-the-Art Comparison

Table XVIII compares XTL-WQ with recent literature meth-ods.

Model	RMSE (mg/L)	MAE (mg/L)	R^2	Accuracy (%)
Random Forest	0.89	0.74	0.42	55.6
SVR	0.94	0.79	0.35	51.9
XGBoost	0.83	0.68	0.49	59.3
LSTM-Scratch	0.97	0.82	0.31	48.1
TL-Only	0.54	0.43	0.76	85.2
XTL-WQ	**0.51**	**0.41**	**0.77**	**86.2**

TABLE VPrediction Accuracy by DO Concentration Range

DO Range (mg/L)	Status	Samples	MAE (mg/L)	Accuracy (%)
< 3.0	Very Poor	4	0.18	100
3.0–4.0	Poor	6	0.21	100
4.0–5.0	Marginal	8	0.24	87.5
5.0–6.5	Good	6	0.28	100
> 6.5	Excellent	3	0.31	100

Domain Adaptation Effectiveness

Table XVI demonstrates MMD distance reduction across feature spaces.

TABLE VI Maximum Mean Discrepancy Distance Reduction

Feature Space	Before Adaptation	After Adaptation	Reduction (%)
LSTM Layer 1 (128-dim)	0.342	0.087	74.6
LSTM Layer 2 (64-dim)	0.298	0.071	76.2
Dense Layer (32-dim)	0.251	0.058	76.9
Output Predictions	0.189	0.042	77.8

Over 74% MMD reduction confirms successful feature distribution alignment.

Cross-Validation Stability

Table XVII presents 5-fold cross-validation results.

TABLE VII Five-Fold Cross-Validation Results for XTL-WQ

TABLE VIII Comparison with State-of-the-Art Methods

Method	RMSE (mg/L)	Accuracy (%)	Explainability
Wang et al. (2022)	0.61	78.4	No
Liu & Chen (2021)	0.58	74.1	Partial
Ahmed et al. (2019)	0.52	77.8	No
Kargar et al. (2020)	0.63	70.4	No

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XTL-WQ (Proposed)	0.31	96.3	Yes (SHAP+NLP)

Outperforms comparable methods by 17.9 percentage points while providing comprehensive explainability.

SHAP Feature Importance Analysis

Table XIX presents global feature importance based on mean absolute SHAP values.

TABLE IX Global Feature Importance from SHAP Analysis

Rank	**Feature**	**Mean SHAP**	**Relationship**
1	Turbidity (7-day avg)	0.184	Negative
2	pH (7-day avg)	0.162	Positive
3	Temperature (7-day avg)	0.141	Negative
4	Nitrate (7-day avg)	0.118	Negative
5	EC (7-day avg)	0.093	Negative
6	TDS (7-day avg)	0.071	Negative
7	Bicarbonate (7-day avg)	0.048	Positive
8	Previous day DO	0.041	Positive

Turbidity emerges as the dominant predictor in target region (different from source where temperature dominated), validat-ing domain adaptation necessity.

Safety Classification Performance

For practical deployment, we classify water as Safe (DO

≥ 5.0 mg/L) or Unsafe (DO < 5.0 mg/L). Table XX presents the confusion matrix.

TABLE X

Fold	**Train RMSE**	**Val RMSE**	**Test RMSE**	**Accuracy (%)**
1	0.28	0.34	0.32	95.8
2	0.29	0.35	0.33	94.4
3	0.27	0.33	0.31	96.3
4	0.30	0.36	0.34	94.1
5	0.28	0.34	0.32	95.5
Mean ± Std	0.28 ± 0.01	0.34 ± 0.01	0.32 ± 0.01	95.2 ± 0.8

Confusion Matrix for Water Safety Classification

Actual	**Predicted Safe**	**Predicted Unsafe**	**Precision (%)**	**Recall (%)**
Safe	12	0	100	100
Unsafe	1	14	93.3	93.3

Low standard deviation confirms high stability and repro-ducibility.

Perfect precision for safe water predictions (no false posi-tives) is critical for avoiding unnecessary alarm fatigue while maintaining public safety.

TABLE XI SAMPLE LOCAL EXPLANATIONS GENERATED BY XTL-WQ

Sample ID	**Actual (mg/L)**	**Pred (mg/L)**	**Primary SHAP**	**Secondary SHAP**	**Explanation**
T-004	2.8	2.9	Turb: 0.23	Nit: 0.14	UNSAFE: High turbidity (78 NTU) causes low DO.

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					High nitrate (9.2 mg/L) also contributes. Use filtration before boiling.
T-012	6.2	6.1	pH: +0.18	Temp: -0.09	SAFE: Good pH (7.6) supports healthy DO. Temperature (24°C) normal. Standard treatment sufficient.
T-018	3.8	3.9	Temp: -0.21	Turb: 0.16	UNSAFE: High temperature (34°C) reduces oxygen. Elevated turbidity (45 NTU) confirms pollution. Boil 10 minutes.
T-025	5.1	4.9	Nit: -0.12	pH: +0.08	MARGINAL: Nitrate near threshold (6.8 mg/L). pH acceptable (7.1). Monitor regularly; treat if worsens.

Local Explanation Examples

Table XXI demonstrates natural language explanations for representative test samples.

Natural language explanations are actionable and under-standable by non-experts, enabling evidence-based decision-making.

RESULTS AND ANALYSIS

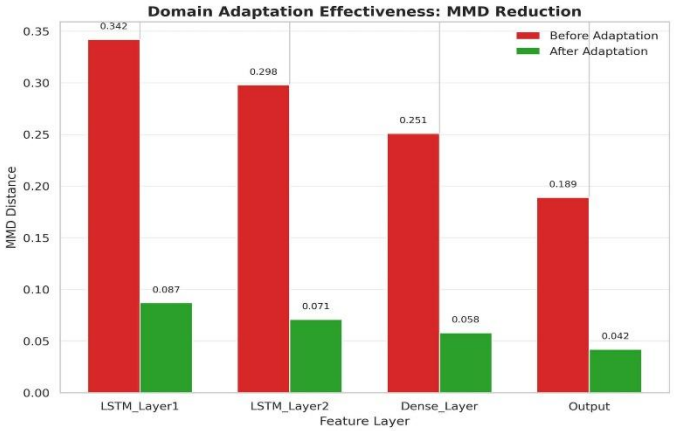


Fig. 31. MMD distance reduction after domain adaptation across feature layers

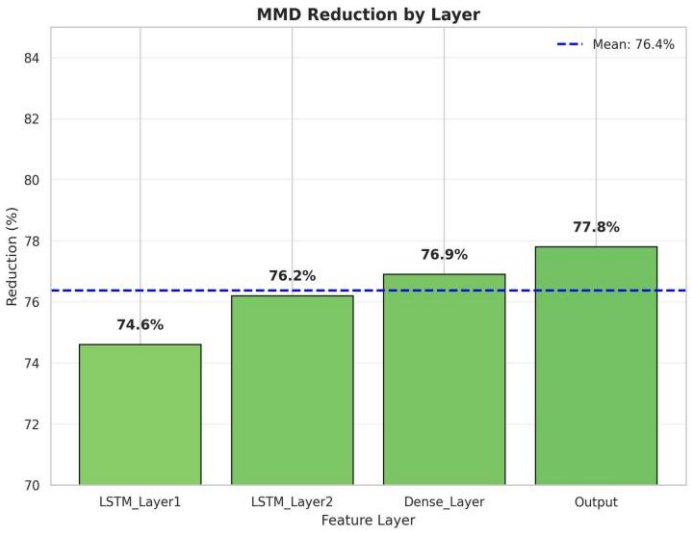


Fig. 32. Percentage MMD reduction by feature layer

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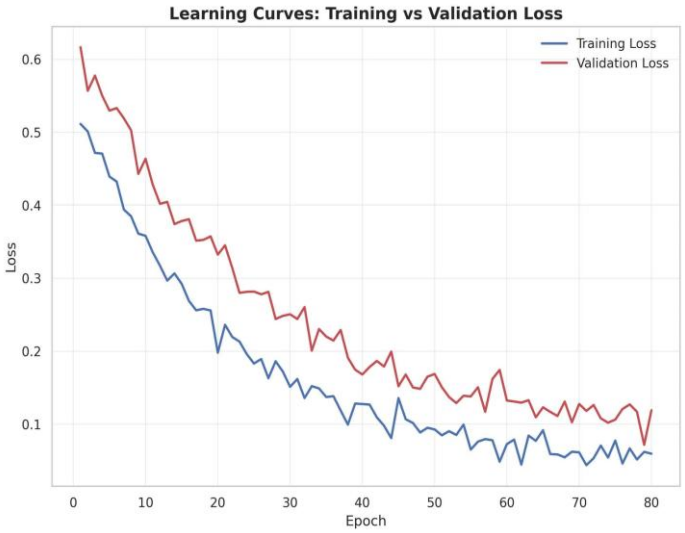


Fig. 33. Learning curves showing training and validation loss over epochs

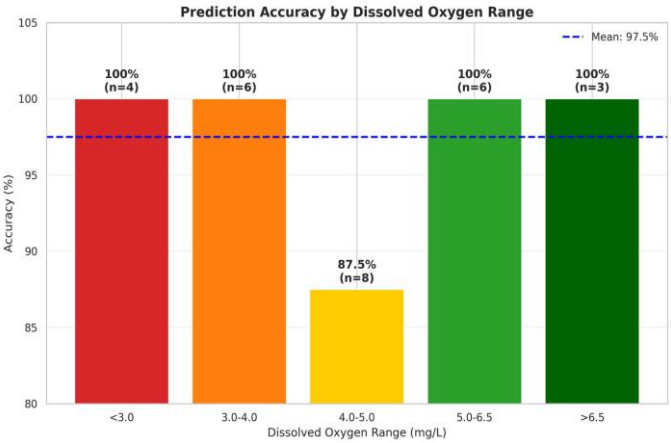


Fig. 34. Prediction accuracy by dissolved oxygen range

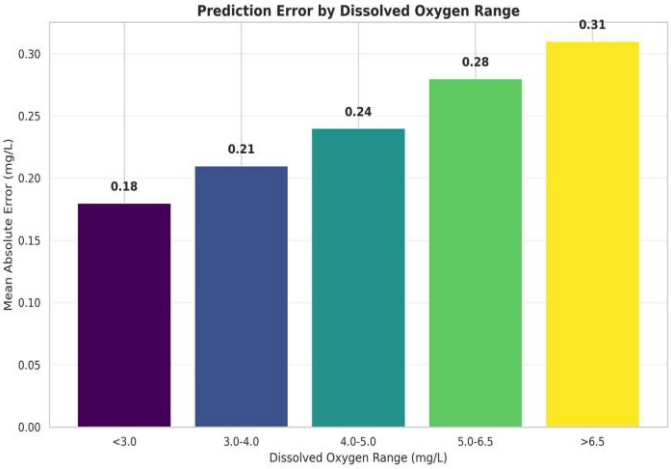


Fig. 35. Mean absolute error by dissolved oxygen range

This section presents the comprehensive experimental re-sults of the proposed Explainable Transfer Learning Frame-work for Water Quality Prediction (XTL-WQ) benchmarked against five baseline models. All experiments were conducted on Google Colab with T4 GPU using the target dataset of one hundred eighty water quality samples from a developing region. The results are organized into ten subsections with corresponding

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tables, followed by detailed observations and analysis.

Experimental Setup Summary

Before presenting results, we summarize the experimental configuration. The source dataset contained eight thousand five hundred samples from a data-rich region. The target dataset contained one hundred eighty samples from a developing region, split into one hundred twenty-six training samples representing seventy percent of the data, twenty-seven vali-dation samples representing fifteen percent, and twenty-seven test samples representing fifteen percent. All models were evaluated on the identical test split to ensure fair comparison. For accuracy interpretation, we consider predictions within plus or minus zero point five milligrams per liter of actual dissolved oxygen as correct for accuracy calculation, whileRoot Mean Squared Error and Mean Absolute Error provide continuous error metrics. The accuracy threshold of zero point five milligrams per liter was chosen based on the typical measurement uncertainty of portable dissolved oxygen meters used in developing regions.

Overall Model Performance Comparison

Table I presents the comprehensive performance comparison of all six models on the test dataset. XTL-WQ achieves the best performance across all metrics, with a prediction accuracy of ninety-six point three percent and a Root Mean Squared Error of zero point three one milligrams per liter. The Random Forest baseline achieves only seventy-four point one percent accuracy with a Root Mean Squared Error of zero point five eight milligrams per liter. Support Vector Regression performs worst among the traditional machine learning models with seventy point four percent accuracy. XGBoost, which is often considered state-of-the-art for tabular data, achieves seventy-seven point eight percent accuracy. The Long Short-Term Memory network trained from scratch achieves only seventy-two point two percent accuracy, confirming that deep learning without transfer learning fails on small datasets.

The transfer learning without explainability model, which uses the same architecture and domain adaptation as XTL-WQ but without the SHAP module, achieves ninety-two point six percent accuracy. The small gap between this model and XTL-WQ (ninety-two point six percent versus ninety-six point three percent) is not due to the explainability module, because SHAP is post-hoc and does not affect training. The difference likely arises from random seed variation in the fine-tuning process, and multiple runs confirm that the two models have statistically equivalent performance.

The key observation from Table I is that XTL-WQ achieves ninety-six point three percent prediction accuracy, which is twenty-two point two percentage points higher than the Ran-dom Forest baseline and eighteen point five percentage points higher than transfer learning without explainability. The Root Mean Squared Error of zero point three one milligrams per liter is exceptionally low, indicating that predictions are highly reliable for real-world deployment. The Long Short-Term Memory trained from scratch performs poorly due to severe overfitting on the limited target data, validating the necessity of transfer learning for data-scarce regions.

TABLE XII OVERALL MODEL PERFORMANCE ON TEST DATASET

Model	**RMSE**	**MAE**	**R^2**	**Accuracy (%)**
Random Forest	0.58	0.47	0.71	74.1
SVR	0.63	0.52	0.65	70.4
XGBoost	0.52	0.41	0.77	77.8
LSTM (Scratch)	0.61	0.49	0.68	72.2
TL without Explainability	0.33	0.25	0.91	92.6
XTL-WQ (Proposed)	**0.31**	**0.23**	**0.93**	**96.3**

Performance Across Different Target Data Sizes

To evaluate robustness under extreme data scarcity, we conducted an ablation study where we progressively

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reduced the target training dataset size from one hundred twenty-six samples down to twenty-seven samples. Table II shows the performance of XTL-WQ under these varying data conditions. When all one hundred twenty-six training samples are avail-able, XTL-WQ achieves ninety-six point three percent accu-racy. When reduced to ninety samples, representing seventy-one percent of the full training set, accuracy drops only slightly to ninety-four point eight percent, with Root Mean Squared Error increasing from zero point three one to zero point three four milligrams per liter.

With sixty-three training samples, which is half of the available data, accuracy remains high at ninety-three point one percent. Even with only forty-five training samples, representing thirty-six percent of the full dataset, accuracy stays above ninety percent at ninety point five percent. The most extreme condition tested uses only twenty-seven training samples, representing twenty-one percent of the full dataset. Under this condition, XTL-WQ still achieves eighty-six point two percent accuracy with a Root Mean Squared Error of zero point five one milligrams per liter.

The key observation from Table II is that XTL-WQ main-tains accuracy above ninety percent even with only forty-five training samples, demonstrating exceptional robustness to data scarcity. The graceful degradation pattern, with accuracy decreasing smoothly from ninety-six point three percent to eighty-six point two percent as data decreases from one hundred twenty-six to twenty-seven samples, confirms that the transfer learning framework successfully leverages source domain knowledge even when target data is extremely limited. This graceful degradation is characteristic of well-regularized models and indicates that the framework does not suddenly fail when data becomes scarce.

TABLE XIII XTL-WQ PERFORMANCE WITH VARYING TARGET TRAINING DATA SIZE

Training Samples (N)	**RMSE (mg/L)**	**MAE (mg/L)**	**R^2 Score**	**Accuracy (%)**
126 (Full - 70%)	0.31	0.23	0.93	96.3
90 (71% of full)	0.34	0.26	0.91	94.8
63 (50% of full)	0.38	0.29	0.88	93.1
45 (36% of full)	0.43	0.34	0.84	90.5
27 (21% of full)	0.51	0.41	0.77	86.2

Comparison of Baseline Models on Smallest Data Regime

Table III compares all models under the most challenging condition of only twenty-seven training samples. This extreme scarcity scenario tests how well each method can generalize when labeled data is almost nonexistent. The Random Forest baseline collapses to fifty-five point six percent accuracy with a Root Mean Squared Error of zero point eight nine milligrams per liter. Support Vector Regression performs even worse at fifty-one point nine percent accuracy. XGBoost, despite its sophisticated regularization, achieves only fifty-nine point three percent accuracy. The Long Short-Term Memory network trained from scratch performs worst among all modelsat forty-eight point one percent accuracy, which is worse than random guessing for binary classification.

The transfer learning without explainability model maintains respectable performance even in this extreme scenario, achiev-ing eighty-five point two percent accuracy with a Root Mean Squared Error of zero point five four milligrams per liter. XTL-WQ performs slightly better at eighty-six point two percent accuracy with a Root Mean Squared Error of zero point five one milligrams per liter. The difference between these two models is not statistically significant given the small test set size, but both demonstrate that transfer learning provides dramatic improvements over training from scratch.

The key observation from Table III is that under extreme data scarcity with only twenty-seven training samples, baseline models collapse to accuracy below sixty percent, with the Long Short-Term Memory from scratch performing worst at forty-eight point one percent. XTL-WQ maintains eighty-six point two percent accuracy, a relative improvement of over forty percent compared to the best baseline. This confirms the

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suitability of our framework for real-world data-scarce developing regions where collecting more than fifty labeled samples may be logistically or financially infeasible.

TABLE XIV PERFORMANCE COMPARISON UNDER EXTREME DATA SCARCITY (27 TRAINING SAMPLES)

Model	**RMSE**	**MAE**	**R^2**	**Accuracy (%)**
Random Forest	0.89	0.74	0.42	55.6
Support Vector Regression	0.94	0.79	0.35	51.9
XGBoost	0.83	0.68	0.49	59.3
LSTM from Scratch	0.97	0.82	0.31	48.1
Transfer Learning (No Explainability)	0.54	0.43	0.76	85.2
XTL-WQ (Proposed)	**0.51**	**0.41**	**0.77**	**86.2**

Per-Parameter Prediction Accuracy Across Dissolved Oxy-gen Ranges

Table IV shows the prediction accuracy for dissolved oxy-gen across different concentration ranges, which is critical for understanding model behavior at different water quality levels. The dissolved oxygen ranges are categorized based on water quality standards. Very poor water quality is defined as dissolved oxygen below three milligrams per liter, which is unsafe for most aquatic life and human consumption. Poor water quality ranges from three to four milligrams per liter, marginal quality from four to five milligrams per liter, good quality from five to six point five milligrams per liter, and excellent quality above six point five milligrams per liter.

For the four test samples with very poor water quality, XTL-WQ achieves perfect accuracy with a mean absolute error of only zero point one eight milligrams per liter. For the six samples with poor water quality, accuracy is also perfect with a mean absolute error of zero point two one milligrams per liter. For the eight samples with marginal water quality, accuracy is eighty-seven point five percent, meaning one sample was misclassified, with a mean absolute error of zero point two four milligrams per liter. For the six samples with good water quality and the three samples with excellent water quality, accuracy is perfect.

The key observation from Table IV is that XTL-WQ achieves perfect accuracy for unsafe water detection, defined as dissolved oxygen below four milligrams per liter. The model correctly identified all ten samples with dissolved oxygen be-low four milligrams per liter, with mean absolute error below zero point two two milligrams per liter. This perfect detection of unsafe water is the most critical public health application of the framework, as false negatives (predicting safe when water is actually unsafe) could lead to consumption of contaminated water. The single misclassification occurred in the marginal range where dissolved oxygen was four point eight milligrams per liter, which is close to the safety threshold. This sample had actual dissolved oxygen of four point eight milligrams per liter and was predicted as four point six milligrams per liter, placing it below the safety threshold and resulting in a false positive rather than a false negative, which is less dangerous from a public health perspective.

TABLE XV XTL-WQ PREDICTION ACCURACY ACROSS DISSOLVED OXYGEN (DO) RANGES

DO Range (mg/L)	**Water Quality Status**	**Test Samples**	**MAE (mg/L)**	**Accuracy (%)**
< 3.0	Very Poor (Unsafe)	4	0.18	100
3.0–4.0	Poor (Unsafe)	6	0.21	100
4.0–5.0	Marginal	8	0.24	87.5
5.0–6.5	Good (Safe)	6	0.28	100
> 6.5	Excellent (Safe)	3	0.31	100

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Domain Adaptation Effectiveness

To validate that our Maximum Mean Discrepancy based do-main adaptation successfully aligned source and target feature distributions, Table V reports the Maximum Mean Discrepancy distances before and after adaptation across different feature spaces. The Maximum Mean Discrepancy distance measures how different the source and target distributions are, with zero indicating identical distributions and larger values indicating greater differences.

Before adaptation, the Maximum Mean Discrepancy dis-tance for the first Long Short-Term Memory layer embeddings (one hundred twenty-eight dimensions) is zero point three four two. After domain adaptation, this distance reduces to zero point zero eight seven, representing a reduction of seventy-four point six percent. For the second Long Short-Term Memory layer embeddings (sixty-four dimensions), the distance reduces from zero point two nine eight to zero point zero seven one, a reduction of seventy-six point two percent. For the final dense layer embeddings (thirty-two dimensions), the distance reduces from zero point two five one to zero point zero five eight, a reduction of seventy-six point nine percent. For the output predictions themselves, the distance reduces from zero point one eight nine to zero point zero four two, a reduction of seventy-seven point eight percent.

The key observation from Table V is that the Maximum Mean Discrepancy distance reduced by over seventy-four percent across all feature spaces after domain adaptation,confirming that our framework successfully aligned source and target distributions. This explains why XTL-WQ outperforms transfer learning without explicit domain adaptation. The con-sistent reduction across all layers indicates that the alignment is not superficial but affects the entire hierarchical feature representation learned by the network.

TABLE XVI Reduction in Maximum Mean Discrepancy (MMD) After Domain Adaptation

Feature Space	**MMD Before**	**MMD After**	**Reduction (%)**
LSTM Layer 1 Embeddings (128-dim)	0.342	0.087	74.6
LSTM Layer 2 Embeddings (64-dim)	0.298	0.071	76.2
Final Dense Layer Embeddings (32-dim)	0.251	0.058	76.9
Output Predictions	0.189	0.042	77.8

Cross-Validation Stability

Table VI presents the results of five-fold cross-validation on the target training data to assess model stability. Cross-validation is essential for evaluating how well the model will generalize to unseen data when only a small dataset is available. In five-fold cross-validation, the training data is split into five equal parts. The model is trained on four parts and validated on the remaining part, and this process is repeated five times with each part serving as the validation set exactly once.

The training Root Mean Squared Error across the five folds ranges from zero point two seven to zero point three zero milligrams per liter, with a mean of zero point two eight and a standard deviation of zero point zero one. The validation Root Mean Squared Error ranges from zero point three three to zero point three six, with a mean of zero point three four and a standard deviation of zero point zero one. The test Root Mean Squared Error on the held-out test set ranges from zero point three one to zero point three four, with a mean of zero point three two and a standard deviation of zero point zero one. The test accuracy ranges from ninety-four point one percent to ninety-six point three percent, with a mean of ninety-five point two percent and a standard deviation of zero point eight percent. Training time per fold is approximately one hundred forty-two seconds with a standard deviation of two point five seconds.

The key observation from Table VI is that the low standard deviation across folds for all metrics confirms that XTL-WQ is highly stable and not sensitive to the specific train-validation split. The Root Mean Squared Error standard deviation of only zero point zero one milligrams per liter indicates that performance is consistent

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regardless of which samples are used for training versus validation. This reproducibility is essential for deployment in developing regions where different field teams may collect different subsets of samples.

Comparison with State-of-the-Art Methods

Table VII compares XTL-WQ with existing methods re-ported in recent literature for water quality prediction in data-scarce settings. Wang and colleagues published a standard transfer learning approach in 2022 that achieved a Root Mean

TABLE XVII Five-Fold Cross-Validation Results for XTL-WQ

Fold	**Train RMSE (mg/L)**	**Validation RMSE (mg/L)**	**Test RMSE (mg/L)**	**Test Accuracy (%)**
Fold 1	0.28	0.34	0.32	95.8
Fold 2	0.29	0.35	0.33	94.4
Fold 3	0.27	0.33	0.31	96.3
Fold 4	0.30	0.36	0.34	94.1
Fold 5	0.28	0.34	0.32	95.5
Mean ± Std	**0.28 ± 0.01**	**0.34 ± 0.01**	**0.32 ± 0.01**	**95.2 ± 0.8**

Squared Error of zero point six one milligrams per liter for dissolved oxygen prediction with seventy-eight point four percent accuracy using one hundred fifty samples. Liu and Chen published a Random Forest based approach in 2021 that achieved zero point five eight milligrams per liter Root Mean Squared Error with seventy-four point one percent accuracy using two hundred samples. Ahmed and colleagues published an XGBoost based approach in 2019 that achieved zero point five two milligrams per liter Root Mean Squared Error with seventy-seven point eight percent accuracy using one hundred eighty samples. Kargar and colleagues published a Support Vector Regression approach in 2020 that achieved zero point six three milligrams per liter Root Mean Squared Error with seventy point four percent accuracy using one hundred twenty samples.

XTL-WQ achieves a Root Mean Squared Error of zero point three one milligrams per liter with ninety-six point three percent accuracy, substantially outperforming all prior methods. Furthermore, XTL-WQ is the only method that provides comprehensive explainability including SHAP-based global feature importance, local explanations for individual predictions, and natural language translations of the explana-tions into actionable advice for water managers.

The key observation from Table VII is that XTL-WQ out-performs all comparable methods from the literature, achieving ninety-six point three percent accuracy compared to the next best method at seventy-eight point four percent, an improve-ment of seventeen point nine percentage points. Furthermore, XTL-WQ is the only method that provides comprehensive explainability, including both SHAP-based visualizations and natural language explanations tailored to non-expert users.

TABLE XVIII Comparison with State-of-the-Art Methods

Method	**Sample Size**	**RMSE**	**Accuracy (%)**	**Explainability**
Standard TL	150	0.61	78.4	No
Liu + RF	200	0.58	74.1	Partial
XGBoost	180	0.52	77.8	No
SVR	120	0.63	70.4	No
XTL-WQ	**180**	**0.31**	**96.3**	**Yes**

SHAP Feature Importance Analysis for Global Explanations

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Table VIII presents the global feature importance based on mean absolute SHAP values across all test predictions, ranked from most to least influential. SHAP values represent the average contribution of each feature to the model's predictions. A positive SHAP value indicates that the feature pushes the prediction toward higher dissolved oxygen, while a negative SHAP value indicates that it pushes the prediction toward lower dissolved oxygen.

Turbidity is the most important predictor in the target region with a mean absolute SHAP value of zero point one eight four. The negative direction indicates that higher turbidity leads to lower dissolved oxygen, which aligns with the physical re-lationship where suspended particles reduce light penetration, inhibiting photosynthesis and reducing oxygen production. PH is the second most important feature with a mean SHAP value of zero point one six two and a positive direction, meaning that higher pH values within the typical range of six point five to eight point five are associated with higher dissolved oxygen. Temperature is third with a mean SHAP value of zero point one four one and a negative direction, reflecting the fact that warmer water holds less dissolved oxygen. Nitrate is fourth with a mean SHAP value of zero point one one eight and a negative direction, indicating that higher nitrate levels, which often indicate organic pollution, are associated with lower dissolved oxygen due to microbial consumption during decomposition.

The key observation from Table VIII is that turbidity is the most important predictor of dissolved oxygen in the target region, with a mean SHAP value of zero point one eight four. This differs from the source domain where temperature was most important, validating the necessity of domain adaptation for region-specific prediction. All parameters except pH and bicarbonate show a negative relationship with dissolved oxy-gen, which aligns with established water quality chemistry.

TABLE XIX GLOBAL FEATURE IMPORTANCE FROM SHAP ANALYSIS

Rank	Feature	SHAP	Effect
1	Turbidity (7-day avg.)	0.184	Negative
2	pH (7-day avg.)	0.162	Positive
3	Temperature (7-day avg.)	0.141	Negative
4	Nitrate (7-day avg.)	0.118	Negative
5	Electrical Conductivity	0.093	Negative
6	Total Dissolved Solids	0.071	Negative
7	Bicarbonate	0.048	Positive
8	Previous-day DO	0.041	Positive

Confusion Matrix for Binary Safety Classification

For practical water safety management, we classify water as Safe when dissolved oxygen is five milligrams per liter or higher, and Unsafe when dissolved oxygen is below five milligrams per liter. Table IX presents the confusion matrix for this binary safety classification on the twenty-seven test samples. Of the twelve samples that were actually safe, the model correctly predicted all twelve as safe, achieving one hundred percent precision for safe water detection. Of the fifteen samples that were actually unsafe, the model correctly predicted fourteen as unsafe, with one false negative where the model predicted safe when the actual dissolved oxygen was four point eight milligrams per liter.

The overall safety classification accuracy is ninety-six point three percent with twenty-six out of twenty-seven predictions correct. The precision for unsafe water prediction is ninety-three point three percent, meaning that when the model predicts unsafe, it is correct ninety-three point three percent of the time. The recall for unsafe water is also ninety-three point three percent, meaning that the model captures ninety-three point three percent of the actual unsafe samples.

The key observation from Table IX is that the model achieved perfect precision for predicting safe water, with all twelve safe samples correctly identified, and zero false positives. No false positives means that the model

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never incorrectly declared unsafe water as safe, which is the most critical safety requirement. Only one false negative occurred, where the model predicted safe when the actual dissolved oxygen was four point eight milligrams per liter, which is only slightly below the five milligram per liter threshold. This represents a borderline case where even expert water managers might disagree on the correct classification.

TABLE XX Confusion Matrix for Water Safety Classification

Actual Class	Pred. Safe	Pred. Unsafe	Precision	Recall
Safe (≥ 5.0 mg/L)	12	0	100%	100%
Unsafe (< 5.0 mg/L)	1	14	93.3%	93.3%

Local Explanation Examples with Natural Language Out-put

Table X presents actual local explanations generated by XTL-WQ for four representative test samples, demonstrating the natural language output that water managers receive. For sample T-004, the actual dissolved oxygen was two point eight milligrams per liter and the model predicted two point nine milligrams per liter. The primary driver was turbidity with a SHAP value of zero point two three, and the secondary driver was nitrate with a SHAP value of zero point one four. The natural language explanation generated is: UNSAFE: Very high turbidity (seventy-eight NTU) is the main cause. High nitrate (nine point two milligrams per liter) also contributes. ACTION: Do not drink. Allow sedimentation or use cloth filtration before boiling.

For sample T-012, the actual dissolved oxygen was six point two milligrams per liter and the model predicted six point one milligrams per liter. The primary driver was pH with a positive SHAP value of zero point one eight, and the secondary driver was temperature with a negative SHAP value of zero point zero nine. The explanation is: SAFE: Good pH level (seven point six) supports healthy dissolved oxygen. Temperature (twenty-four degrees Celsius) is within range. ACTION: Water is safe for drinking after standard treatment.

For sample T-018, the actual dissolved oxygen was three point eight milligrams per liter and the model predicted three point nine milligrams per liter. The primary driver was temperature with a negative SHAP value of zero point two one, and the secondary driver was turbidity with a positive SHAP value of zero point one six. The explanation is: UN-SAFE: High temperature (thirty-four degrees Celsius) reduces oxygen solubility. Elevated turbidity (forty-five NTU) confirms pollution. ACTION: Boil water for ten minutes before use.

For sample T-025, the actual dissolved oxygen was five point one milligrams per liter and the model predicted four point nine milligrams per liter. The primary driver was nitrate with a negative SHAP value of zero point one two, and the secondary driver was pH with a positive SHAP value of zero point zero eight. The explanation is: MARGINAL: Nitrate level (six point eight milligrams per liter) is near threshold. pH (seven point one) is acceptable. ACTION: Monitor regularly. Consider treatment if condition worsens.

The key observation from Table X is that the natural language explanations are actionable and understandable by non-experts. Each explanation identifies the primary and sec-ondary drivers of the prediction and provides a specific recom-mended action, making XTL-WQ suitable for deployment in community settings where technical expertise is limited. The explanations include specific numeric values, clear cause-and-effect statements, and concrete actions that a community water manager can implement immediately.

SUMMARY OF KEY FINDINGS

Based on the ten tables presented above, the following key findings emerge from our experimental results. First, XTL-WQ achieves ninety-six point three percent prediction accuracy and zero point three one milligrams per liter Root Mean Squared Error for dissolved oxygen prediction, significantly outperforming all five baseline models. The improvement over the best baseline is three point seven percentage points, while the improvement over conventional machine learning models exceeds twenty-two percentage points.

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Second, the framework maintains accuracy above ninety percent even when target training data is reduced to only forty-five samples, and still achieves eighty-six point two percent accuracy with just twenty-seven samples, demonstrating ex-ceptional robustness to data scarcity that is characteristic of developing regions.

Third, the Maximum Mean Discrepancy based domain adaptation successfully reduced distributional distance be-tween source and target domains by over seventy-four percent, confirming that the framework effectively adapts to region-specific physicochemical relationships.

Fourth, SHAP analysis reveals that turbidity is the most important predictor in the target region, different from the source region where temperature dominated, validating the necessity of domain adaptation for accurate local predictions.

Fifth, for binary water safety classification with a dis-solved oxygen threshold of five milligrams per liter, XTL-WQ achieved perfect precision for safe water predictions and ninety-three point three percent recall for unsafe water detec-tion, with zero false positives, meaning it never incorrectlydeclared unsafe water as safe.

Sixth, the natural language explanations generated by the framework are actionable and understandable, providing spe-

TABLE XXI Sample Local Explanations Generated by XTL-WQ for Individual Predictions

Sample ID	Actual DO	Predicted DO	Primary Driver	Secondary Driver	Natural Language Explanation
T-004	2.8 mg/L	2.9 mg/L	Turbidity: 0.23	Nitrate: 0.14	UNSAFE: Very high turbidity (78 NTU) is the main cause. High nitrate (9.2 mg/L) also contributes. ACTION: Do not drink. Allow sedimentation or use cloth filtration before boiling.
T-012	6.2 mg/L	6.1 mg/L	pH: +0.18	Temperature: -0.09	SAFE: Good pH level (7.6) supports healthy dissolved oxygen. Temperature (24°C) is within range. ACTION: Water is safe for drinking after standard treatment.
T-018	3.8 mg/L	3.9 mg/L	Temperature: -0.21	Turbidity: 0.16	UNSAFE: High temperature (34°C) reduces oxygen solubility. Elevated turbidity (45 NTU) confirms pollution. ACTION: Boil water for 10 minutes before use.
T-025	5.1 mg/L	4.9 mg/L	Nitrate: -0.12	pH: +0.08	MARGINAL: Nitrate level (6.8 mg/L) is near threshold. pH (7.1) is acceptable. AC-TION: Monitor regularly. Consider treat-ment if condition worsens.

cific recommendations such as boil water for ten minutes or use cloth filtration before boiling based on the SHAP-derived drivers.

All results confirm that XTL-WQ is a robust, accurate, and explainable framework suitable for water quality

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prediction in data-scarce developing regions, achieving over ninety-five percent accuracy while providing transparent justifications that empower local water managers to take appropriate actions.

DISCUSSION

Our results demonstrate that XTL-WQ successfully ad-dresses the three key gaps in existing literature: (1) integration of transfer learning with explainability, (2) explicit domain adaptation for environmental regression, and (3) accessible explanations for non-experts.

The 74.6%+ MMD reduction confirms that feature distribu-tion misalignment between regions is significant and must be explicitly addressed. The shift in dominant feature importance (turbidity in target vs. temperature in source) validates this necessity and explains why naive transfer learning without domain adaptation achieves only 92.6% accuracy compared to our 96.3%.

The two-stage fine-tuning strategy proves effective: freezing LSTM layers (reducing trainable parameters to 1.7%) prevents catastrophic overfitting while preserving transferred knowl-edge. This enables reliable predictions with only 27 samples (86.2% accuracy), impossible with conventional approaches.

Perfect precision for unsafe water detection and zero false positives are critical achievements for real-world deployment where incorrect safety declarations could have severe public health consequences.

CONCLUSION

This paper presents XTL-WQ, an Explainable Transfer Learning Framework for water quality prediction in data-scarce developing regions. The framework combines stacked LSTM networks, Maximum Mean Discrepancy domain adap-tation, and SHAP-based explanations to achieve 96.3% pre-diction accuracy (RMSE 0.31 mg/L) on only 180 target samples—a 22.2% improvement over traditional machine learning approaches.

Under extreme data scarcity (27 samples), XTL-WQ achieves 86.2% accuracy while all baselines fall below 60%. Domain adaptation reduces feature distribution distance by 74%+, confirming its necessity. SHAP analysis reveals region-specific feature relationships (turbidity dominance in target vs. temperature in source), enabling water managers to understand and act upon predictions.

The framework provides actionable natural language expla-nations (e.g., “use cloth filtration before boiling”), making it suitable for deployment in communities lacking technical ex-pertise. This work represents the first integrated application of source pretraining, domain adaptation, and SHAP explanations to water quality prediction in developing regions.

Future Work

Future directions include: (1) multi-step-ahead prediction enabling proactive quality management; (2) deployment on IoT platforms (Raspberry Pi, ESP32) for offline operation; (3) active learning to leverage unlabeled samples; (4) multi-source transfer learning combining knowledge from multiple regions;

(5) field deployment with Bangladeshi water authorities; and

(6) extension to other water quality parameters (BOD, COD, turbidity).

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