Multivariate Time-Series Forecasting of Boiler Water Conductivity in Power Plant Using Machine Learning

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***Abstract*— Water quality is a critical parameter for maintaining the reliable operation of power plants, particularly in the water–steam cycle and Heat Recovery Steam Generator (HRSG) systems. This study develops a predictive monitoring approach based on multivariate time-series forecasting to predict HP Drum Water conductivity using 35,064 hourly observations, of which 34,083 valid observations remained after preprocessing. Three models, namely Extreme Gradient Boosting (XGBoost), Long Short-Term Memory (LSTM), and Gated Recurrent Unit (GRU), were evaluated at forecasting horizons of 1, 6, and 24 h. The results show that XGBoost achieved the best performance at the 1-h horizon, with an RMSE of 3.3193, an MAE of 1.6358, and an R^2 of 0.9379. LSTM achieved the best performance at the 6-h and 24-h horizons, with R^2 values of 0.7256 and 0.5966, respectively. SHapley Additive exPlanations (SHAP) analysis identified current conductivity as the most influential feature. The predictive monitoring system also detected two early-warning events when conductivity exceeded the statistical threshold of approximately 44–45, demonstrating its potential to support predictive water-quality monitoring and earlier operational decision-making.**

Keywords — Conductivity, Predictive Monitoring, Multivariate Time-Series Forecasting, XGBoost, LSTM, GRU.

I. INTRODUCTION

Power plants are complex industrial systems characterized by strong interactions among thermal, mechanical, electrical, and working-fluid conditions. In power plants employing a water–steam cycle, water and steam conditions must be maintained within specified operating ranges to ensure stable power generation and reliable equipment operation under their intended design conditions. One continuously monitored water-quality parameter is conductivity, which reflects the ability of a solution to conduct electrical current and is indirectly associated with the concentration of dissolved ions in water. Changes in conductivity therefore provide important information for monitoring systems because they may indicate variations in water quality as well as changes in operating conditions. In power plant environments, conductivity does not behave as an independent variable. Its dynamics may occur simultaneously with variations in make-up water flow, steam flow, condensate flow, and Heat Recovery Steam Generator (HRSG) operating conditions. Consequently, conductivity analysis should consider not only its temporal behavior but also its interactions with other operational variables [1] .

Industrial monitoring systems generally rely on current parameter values and compare them with predefined limits or alarm thresholds. This approach is effective for identifying conditions that have already occurred; however, it has limited capability to provide information about conditions that may develop in the near future. From an operational perspective, the ability to anticipate parameter trends before significant changes occur can provide operators with additional time to perform further analysis and support timely decision-making [2]. The availability of historical data generated by power plant sensors and control systems enables the development of data-driven approaches. Power plant sensor data inherently exhibit multivariate time-series characteristics, as each observation is temporally ordered and consists of multiple interrelated operating parameters. This characteristic provides opportunities for applying machine learning and deep learning methods to capture nonlinear relationships and temporal patterns embedded in historical operational data.

One machine-learning algorithm with strong capability for learning nonlinear relationships in tabular data is XGBoost. This model constructs a sequence of decision trees iteratively, allowing errors produced by previous trees to be corrected by subsequent ones. In contrast, Long Short-Term Memory (LSTM) and Gated Recurrent Unit (GRU) are extensions of Recurrent Neural Networks (RNNs) specifically designed for sequential data processing. Both models incorporate memory mechanisms that enable relevant historical information to be retained and utilized when predicting subsequent observations [3]. However, forecasting studies using industrial data should not focus solely on minimizing prediction error. The developed models should also be evaluated across multiple forecasting horizons, feature configurations, and historical look-back lengths to assess their robustness under different predictive settings. In addition, the black-box nature of machine learning and deep learning models raises interpretability concerns, since operators require not only accurate predictions but also information regarding which variables contribute most strongly to changes in the predicted output [4] .

Based on these challenges, this study develops an explainable multivariate time-series forecasting framework for predicting conductivity in power plant systems. Three models, namely XGBoost, Long Short-Term Memory (LSTM), and Gated Recurrent Unit (GRU), are compared under identical experimental conditions. The study further evaluates the effects of feature engineering, forecasting horizon, look-back window length, and model residual characteristics. Shapley Additive Explanations (SHAP) analysis is then employed to identify the variables that contribute most strongly to conductivity prediction. [5] .

The contribution of this study lies in integrating multivariate forecasting, feature engineering, multi-horizon evaluation, robustness analysis, and explainable artificial intelligence using actual power plant operational data. Accordingly, the study not only identifies the algorithm with the lowest prediction error but also evaluates model consistency and interpretability as a basis for developing a predictive monitoring system.

II. Material and Methode

A. Research Framework

The research workflow was systematically designed to illustrate the relationships among data processing, modeling, performance evaluation, model interpretation, and predictive monitoring implementation. The complete research framework is presented in Fig. 1.

Fig. 1 illustrates the research framework used to develop a predictive monitoring system for power plant conductivity. The study begins with the collection of historical power plant data from the data information system of PT Indonesia Power Priok, followed by data validation to ensure data completeness, consistency, value ranges, and data types. Data cleaning is then performed to handle missing values, identify abnormal observations, and correct data inconsistencies. The next stage involves exploratory data analysis to examine temporal patterns, data distributions, inter-variable relationships, and variations in operating parameters. The resulting information is subsequently used for temporal feature engineering by constructing time-based features, lag features, rolling statistics, and relevant temporal-change features. This stage aims to provide a more informative data representation for the forecasting models. In the modeling stage, three approaches are implemented and compared: Extreme Gradient Boosting (XGBoost), Long Short-Term Memory (LSTM), and Gated Recurrent Unit (GRU). The forecasting performance of the three models is then evaluated at multiple prediction horizons to assess their accuracy and consistency over different future time intervals.

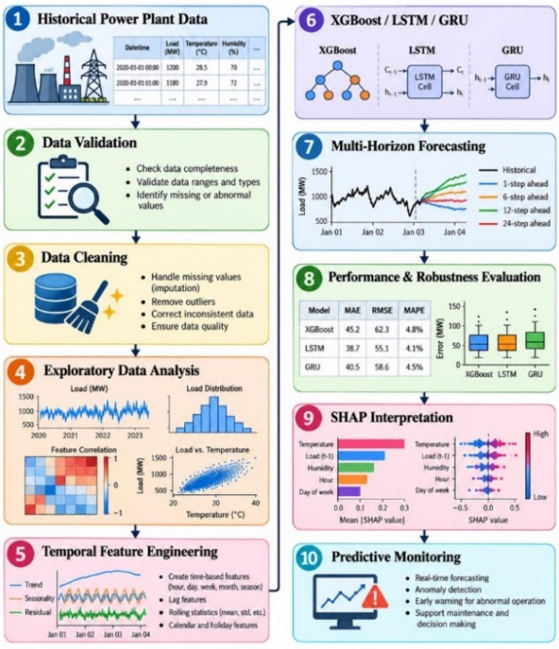


Fig 1. Research framework for multivariate time-series forecasting and predictive monitoring of power plant conductivity.

The three models are employed for multi-horizon forecasting at different prediction horizons to evaluate their ability to capture both short-term and longer-term variations in conductivity. Model performance is assessed using several evaluation metrics, including Mean Squared Error (MSE), Root Mean Squared Error (RMSE), Mean Absolute Error (MAE), Mean Absolute Percentage Error (MAPE), and the coefficient of determination R^2 together with robustness analysis under different temporal configurations. Subsequently, SHapley Additive exPlanations (SHAP) are used to interpret the contribution of each input variable to the prediction results. The overall findings are then utilized to support a predictive monitoring system capable of assisting operational condition monitoring, identifying abnormal trends, and enabling earlier operational decision-making.

B. Extreme Gradient Boosting Model

Extreme Gradient Boosting (XGBoost) is an extension of the gradient boosting approach that constructs a predictive model by combining multiple regression trees. Unlike neural network models that process data sequentially, XGBoost incorporates temporal information through features that are explicitly reconstructed into a tabular representation, such as lag features, rolling means, and changes in conductivity. The XGBoost prediction can be represented as shown in (1) [6] .

$$\hat{y}_i = \sum_{k=1}^{k} f_k(x_i) \quad (1)$$

Where K denotes the total number of trees and f_k represents the function generated by the k – th tree. The XGBoost objective function can then be expressed as shown in (2).

$$Obj = \sum_{i=1}^{n} l(y_i, \hat{y}_i) + \sum_{k=1}^{K} \Omega(f_k) \quad (2)$$

Where l denotes the loss function, while Ω represents the regularization component used to control model complexity [7] .

In this study, XGBoost is employed as a machine learning model to investigate whether explicitly reconstructed operational information and temporal features can provide competitive forecasting performance compared with recurrent neural network models. This approach captures nonlinear relationships among operational variables, historical conductivity values, lag features, and rolling statistics without requiring an internal sequential architecture. The performance of XGBoost is subsequently compared at identical forecasting horizons using the same evaluation metrics. This comparison is intended to assess whether explicit temporal feature engineering can provide an effective alternative to the direct temporal representation learning performed by deep learning models.

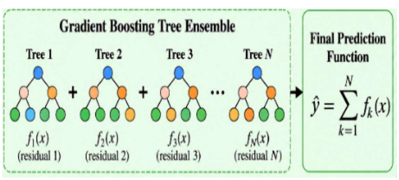


Fig. 2 XGboost learning process

The figure illustrates the XGBoost learning mechanism as a gradient boosting method that sequentially constructs multiple decision trees. The process begins with Tree 1, which generates an initial prediction. The difference between the actual value and the first prediction forms a residual, which is then used as correction information for Tree 2. The same process continues through Tree 3 up to Tree K, where each new tree is trained to reduce the prediction error produced by the ensemble of previous trees. Through this mechanism, the model does not rely on a single decision tree but combines multiple weak learners to produce a more accurate final prediction.

In the final stage, the outputs of all trees are combined to form the final prediction function, as expressed in (1). In this study x represents the set of input features, including power plant operational variables and temporal features, whereas $\widehat{y_i}$ denotes the predicted conductivity value. The iterative addition of trees enables XGBoost to capture nonlinear relationships among the input variables while progressively reducing prediction errors. Therefore, XGBoost is suitable for feature-based time-series forecasting within a predictive monitoring system for power plant water quality.

C. *LSTM Model*

Long Short-Term Memory (LSTM) is an extension of the Recurrent Neural Network (RNN) designed to overcome the limitations of conventional RNNs in retaining information over long data sequences. In time-series data, the state of a variable at a given time is generally influenced by patterns observed at previous time steps. Therefore, LSTM is well suited for modeling power plant operational data because it can preserve historical information through memory cells while controlling information flow using a set of gates. In this study, LSTM is employed to learn the temporal relationships between historical conductivity values and power plant operating variables to generate future conductivity predictions [8] .

At each time step t, the LSTM receives two main sources of information: the current input vector $x(t)$ and the hidden state from the previous time step h_{t-1} . This information is processed through three main mechanisms: the forget gate, input gate, and output gate. The forget gate determines which components of the historical information remain relevant and should be retained in the memory cell. This mechanism can be represented as shown in (3).

$$f_t = \sigma(W_f|h_{t-1}, x_t| + b_f) \tag{3}$$

The value of f_t ranges from 0 to 1 due to the use of the sigmoid activation function. A value close to 0 indicates that the previous information tends to be discarded, whereas a value close to 1 indicates that the information is retained. In the context of this study, this mechanism enables the model to determine whether previous conductivity patterns and operating conditions remain relevant for subsequent predictions. This selective retention of information helps the LSTM reduce the influence of irrelevant historical patterns while preserving temporal dependencies that contribute to forecasting accuracy. As a result, the model can adaptively balance short-term fluctuations and longer-term trends in conductivity during the prediction process.

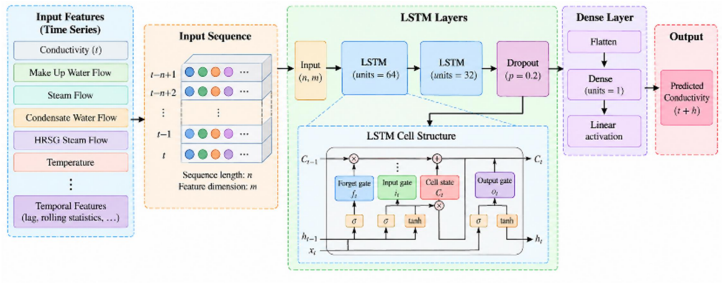


Fig. 3 Architecture of the LSTM conductivity forecasting model

Fig. 3 illustrates the LSTM architecture used for conductivity prediction. The input data, consisting of power plant operating variables and temporal features, are arranged as an input sequence before being processed by the LSTM layer. At each time step, the LSTM cell regulates information flow through the forget, input, and output gates to retain relevant historical patterns. The resulting temporal representation is then passed through dropout and dense layers to generate the conductivity prediction at the specified forecasting horizon.

D. *GRU Model*

Gated Recurrent Unit (GRU) is a variant of the Recurrent Neural Network (RNN) designed to learn temporal dependencies in sequential data. Compared with LSTM, GRU has a simpler architecture because it does not employ a separate cell state. Historical information is stored and updated directly through the hidden state using two main mechanisms, namely the update gate and the reset gate. The update gate determines the extent to which previous information is retained or replaced by new information, as expressed in (4) [9] .

$$z_t = \sigma(W_z x_t + U_z h_{t-1} + b_z) \tag{4}$$

Next, the reset gate controls the extent to which historical information is used when constructing the candidate hidden state. The previous information and the new candidate are then combined to form the final hidden state, as expressed in (5).

$$h_t = (1 - z_t) \odot h_{t-1} + z_t \odot \widetilde{h_t} \tag{5}$$

where x_t denotes the input vector at time – t, $h_{t-1}$is the previous hidden state, h_t is the current hidden state, z_t represents the update gate, r_t represents the reset gate, and $\widetilde{h_t}$ denotes the candidate hidden state.

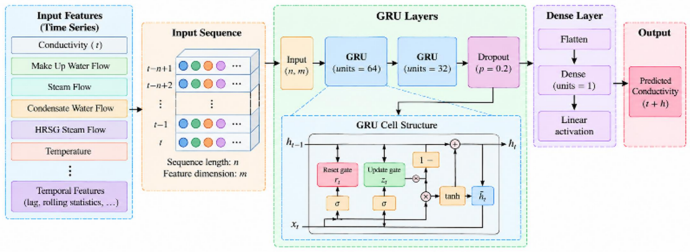


Fig. 4 Architecture of the GRU conductivity forecasting model

The parameters W, U, and b represent the weights and biases learned during the training process, while σ denotes the sigmoid activation function and $\odot$ represents element-wise multiplication.

Fig. 4 illustrates the GRU architecture used for conductivity prediction. The input data, consisting of historical conductivity values, power plant operating variables, and temporal features, are arranged as an input sequence before being processed by the GRU layer. At each time step, the GRU employs the reset and update gates to select relevant historical information and combine it with new information. The resulting temporal representation is subsequently passed through dropout and dense layers to generate the conductivity prediction at the specified forecasting horizon. Compared with LSTM, the simpler GRU structure generally requires fewer parameters, making it suitable as a comparative model for multivariate time-series forecasting.

E. *Explainable Artificial Intelligence Using SHAP*

To improve model interpretability, SHapley Additive exPlanations (SHAP) are employed as an Explainable Artificial Intelligence (XAI) method to quantify the contribution of each feature to the model output. In this study, SHAP is primarily applied to the XGBoost model using TreeSHAP because it is specifically designed for tree-based models. In general, the model prediction can be expressed as shown in (6).

$$f_x = \varphi_0 + \sum_{j=1}^{M} \varphi_j \qquad (6)$$

where f_x denotes the model prediction, φ_0 represents the baseline prediction, φ_j denotes the contribution of the j – th feature, and M is the total number of features. A positive SHAP value indicates that a feature increases the predicted conductivity, whereas a negative value indicates a contribution toward a lower prediction. The larger the absolute SHAP value, the greater the contribution of the corresponding feature to the model output [10] .

In this study, SHAP is used to identify the most influential features and the direction of their contributions to conductivity prediction. The resulting interpretation is treated as a predictive association rather than evidence of a causal relationship between operational parameters and conductivity. This analysis also improves transparency by showing how individual input variables contribute to variations in the predicted output.

III. Result and Discussion

The Results and Discussion section evaluates the performance of Extreme Gradient Boosting (XGBoost), Long Short-Term Memory (LSTM), and Gated Recurrent Unit (GRU) for conductivity prediction using historical power plant operational data. The evaluation includes data characteristics after preprocessing, forecasting performance at multiple prediction horizons, robustness analysis, and feature-contribution interpretation using SHapley Additive exPlanations (SHAP). Model performance is compared using Mean Squared Error (MSE), Root Mean Squared Error (RMSE), Mean Absolute Error (MAE), Mean Absolute Percentage Error (MAPE), and the coefficient of determination R^2 to identify the most accurate and stable model for supporting predictive monitoring of power plant water quality.

A. *Dataset Characteristics and Data Quality*

The initial data assessment showed that the dataset consisted of 35,064 observations recorded at hourly intervals. For the target variable, HP Drum Water 1 Conductivity, 514 missing values (1.466%), 31 zero-valued observations (0.088%), and 436 negative observations were identified. Accordingly, 467 conductivity observations were considered invalid because they contained zero or negative values. After scale conversion and data cleaning, 34,083 valid conductivity observations were retained. Descriptive statistics after preprocessing showed a mean value of 20.0679, a standard deviation of 13.3206, a minimum of 0.001, and a maximum of 240.000. The median value was 20.4700, while the first and third quartiles were 13.7555 and 25.5155, respectively, indicating that most conductivity values were concentrated within this range.

Before preprocessing, the target variable contained 514 missing values and 467 invalid observations, resulting in a total of 981 observations requiring data handling. Zero and negative values were first treated as missing values, after which invalid target observations were excluded from the modeling dataset to ensure that no missing values remained in the target variable used for forecasting. The preprocessing stage retained 34,083 valid observations, corresponding to approximately 97.20% of the original dataset. The cleaning procedure was performed while preserving the chronological order of the data to maintain the temporal structure required for subsequent lag-feature construction, rolling statistics, and input-sequence generation for the XGBoost, LSTM, and GRU models.

B. *Feature Engineering Analysis*

Temporal feature testing was conducted to verify whether historical information derived from conductivity data could capture short-term patterns, daily patterns, and volatility relevant to the forecasting process. Fig. 5 shows that the lag-1 feature closely follows the actual conductivity pattern, whereas lag-24 exhibits larger deviations of approximately 10–20 units during several periods, indicating that the two features represent short-term dependency and daily behavior, respectively. The 24-h rolling mean smooths conductivity fluctuations within an approximate range of 9–45, compared with actual values ranging from approximately 6 to 50, while the ±1 rolling standard deviation band becomes wider during periods of higher volatility. These results indicate that the combination of lag features and rolling statistics effectively represents persistence, local trends, and conductivity volatility as informative inputs for the forecasting models.

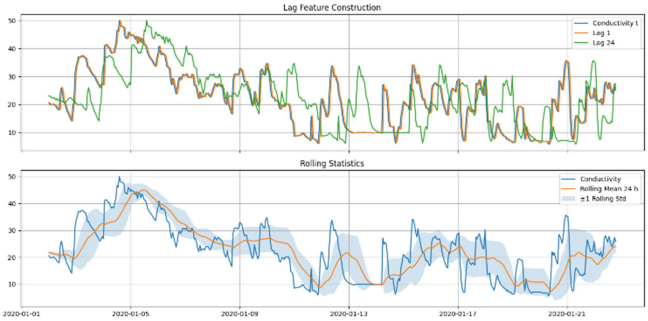


Fig. 5 Construction of lag features and 24-h rolling statistics for conductivity time-series data.

C. Feature Engineering Analysis

Multi-horizon forecasting was conducted to evaluate the ability of the models to maintain prediction accuracy as the forecasting horizon increased from 1 h to 6 h and 24 h. Fig. 6 shows that XGBoost achieved the best performance at the 1-h horizon and closely followed the actual conductivity pattern over an approximate range of 7–46. During most periods, the visual difference between actual and predicted values remained relatively small, at approximately 1–3 units, including during increases to around 45–46. This indicates that XGBoost is effective for short-term forecasting because recent historical information remains highly relevant to near-future conductivity changes.

At the 6-h and 24-h horizons, LSTM provided the best performance; however, the predictions became progressively smoother as the forecasting horizon increased. At the 6-h horizon, predicted values were generally within the range of 20–31, causing several actual peaks of approximately 40–46 to be underestimated by about 10–17 units. At the 24-h horizon, the prediction range narrowed further to approximately 18–28, while the actual values continued to fluctuate up to around 45–46. These results indicate that longer forecasting horizons favor the prediction of general trends rather than short-term extreme variations. Therefore, XGBoost is more suitable for short-term forecasting, whereas LSTM demonstrates greater stability for longer forecasting horizons.

The results in Table I further confirm that model performance decreases as the forecasting horizon increases. At the 1-h horizon, XGBoost achieved the best performance with an RMSE of 3.3193, an MAE of 1.6358, and an \(R^2\) of 0.9379, outperforming both LSTM and GRU. At the 6-h horizon, LSTM became the best-performing model with an RMSE of 6.9747, an MAE of 4.9273, and an \(R^2\) of 0.7256. LSTM remained superior at the 24-h horizon, with an RMSE of 8.4230, an MAE of 6.0815, and an \(R^2\) of 0.5966. The decrease in \(R^2\) from approximately 0.94 at the 1-h horizon to approximately 0.60 at the 24-h horizon indicates increasing prediction uncertainty as the forecasting horizon becomes longer.

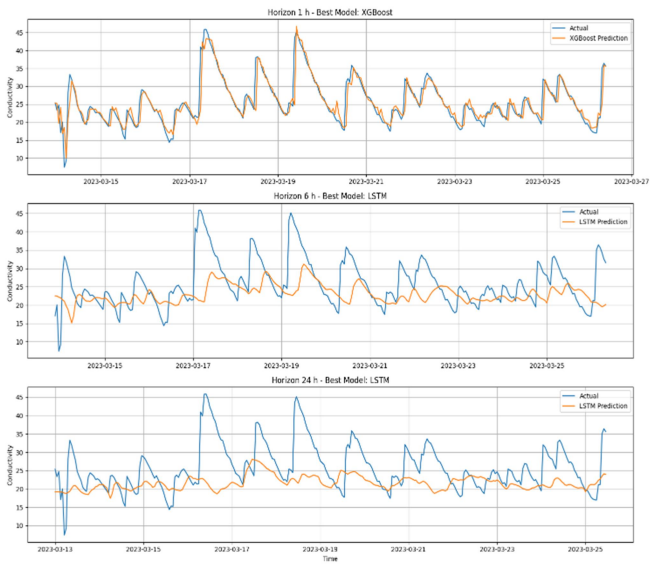


Fig. 6 Actual and predicted conductivity for the best-performing model at 1-h, 6-h, and 24-h forecasting horizons.

TABLE I. PERFORMANCE COMPARISON OF XGBOOST, LSTM, AND GRU AT DIFFERENT FORECASTING HORIZONS.

Horizon_h	*Model*	*MSE*	*RMSE*	*R^2*
1	XGBoost	0.00134	0.03656	0.93788
1	LSTM	0.00170	0.04121	0.92107
1	GRU	0.00195	0.04414	0.90943
6	XGBoost	0.00703	0.08383	0.67329
6	LSTM	0.00590	0.07682	0.72563
6	GRU	0.00650	0.08060	0.69800
24	XGBoost	0.01025	0.10124	0.51957
24	LSTM	0.00861	0.09277	0.59659
24	GRU	0.01017	0.10083	0.52344

Overall, XGBoost is more effective for very short-term prediction, whereas LSTM demonstrates relatively more stable performance at the 6-h and 24-h horizons. The increase in RMSE and the decrease in R^2at longer forecasting horizons indicate that prediction uncertainty increases as the forecasting interval becomes longer. These findings suggest that model selection should consider the forecasting horizon applied within the predictive monitoring system for power plant water quality.

D. SHAP-Based Feature Interpretation

SHapley Additive exPlanations (SHAP) analysis was conducted to identify the features that contributed most strongly to the XGBoost predictions and to examine the direction of their influence on predicted conductivity. Fig. 7 shows that CONDUCTIVITY is the most dominant feature, with SHAP values ranging approximately from −0.18 to 0.48, which is substantially wider than those of the other features that are generally concentrated around zero. Higher conductivity values tend to produce positive SHAP values, thereby increasing the predicted output, whereas lower conductivity values tend to contribute negatively. This indicates that the current conductivity condition provides the most influential information for short-term prediction.

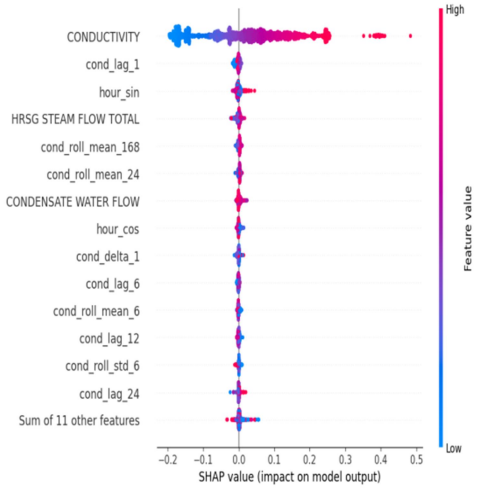


Fig. 7 SHAP summary plot showing the contribution of input features to XGBoost conductivity prediction

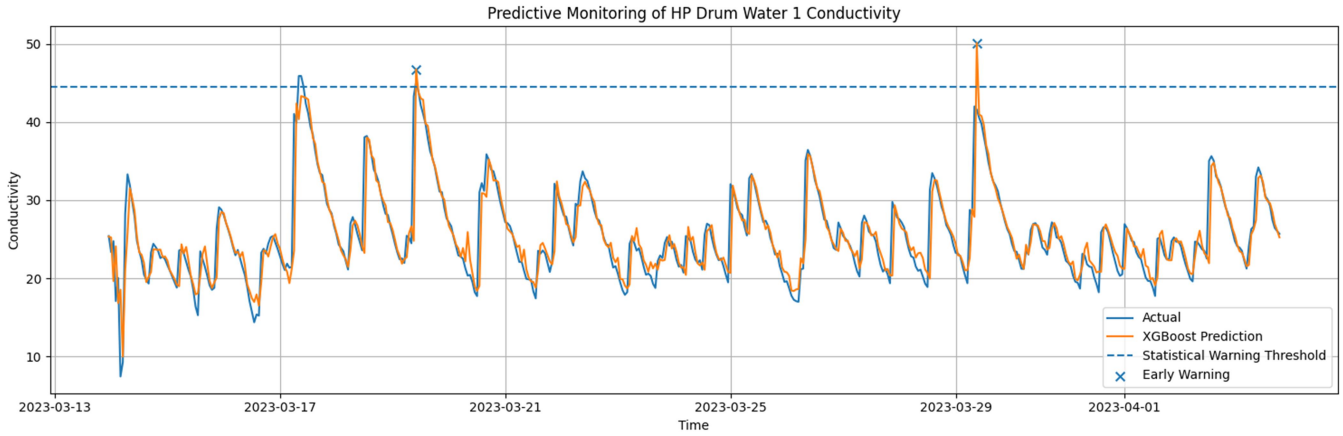


Fig. 8 Predictive monitoring of HP Drum Water 1 conductivity using XGBoost with statistical early-warning threshold.

The subsequent features, including cond_lag_1, hour_sin, HRSG STEAM FLOW TOTAL, and the 24-h and 168-h rolling means, provide smaller contributions, with SHAP values generally ranging from approximately −0.03 to 0.05. Although their influence is lower than that of the current conductivity value, these features still provide complementary information related to temporal patterns, operating conditions, and historical trends. Therefore, the SHAP results indicate that the model prediction is primarily driven by the current conductivity condition, while temporal and operational features provide additional predictive information.

Predictive monitoring was evaluated to assess the ability of the best-performing model to track changes in conductivity while detecting conditions that exceeded a statistical warning threshold. Fig. 8 shows that the XGBoost predictions closely follow the actual pattern during most of the evaluation period, particularly when conductivity ranges from approximately 18 to 35. The statistical warning threshold is approximately 44–45, and predicted values exceeding this limit are identified as early-warning conditions. Approximately two warning events are observed in the displayed period, occurring when conductivity increases to around 46–47 and 50. These results indicate that XGBoost can not only provide accurate short-term predictions but also support the early identification of abnormal increases in conductivity.

IV. Conclusion

This study develops a predictive monitoring approach for forecasting HP Drum Water conductivity using XGBoost, LSTM, and GRU. From the initial 35,064 observations, 34,083 valid data points were retained after preprocessing. The evaluation results show that XGBoost achieved the best performance at the 1-h horizon, with an RMSE of 3.3193, an MAE of 1.6358, and an R2R2 of 0.9379, whereas LSTM outperformed the other models at the 6-h and 24-h horizons, with R2R2 values of 0.7256 and 0.5966, respectively. These results indicate that prediction accuracy decreases as the forecasting horizon increases. SHAP analysis shows that the current conductivity value is the most influential feature, while lag features, rolling statistics, and HRSG Steam Flow provide additional contributions. The predictive monitoring system was also able to detect approximately two early-warning conditions when conductivity exceeded the statistical threshold of around 44–45. Overall, XGBoost is more suitable for short-term forecasting, whereas LSTM demonstrates greater stability at longer forecasting horizons.

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