

Predicting River Nitrate (NO₃) Concentrations Using Hybrid Deep Learning: Case Study of the Willamette River, Oregon

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Abstract—Predicting nitrate levels in rivers is vital for maintaining healthy ecosystems, as excessive nitrates can disrupt aquatic life and lead to harmful algal blooms. Accurate nitrate monitoring also ensures safe drinking water, protecting communities from health risks. To keep our rivers healthy, protect water resources, and ensure human safety, accurately measuring nitrate levels—a key sign of water quality—is essential. We developed three advanced models to predict hourly nitrate levels in the Willamette River in Portland, Oregon, using data from 2021–2022. These models were a Gated Recurrent Unit (GRU), a Convolutional Neural Network (CNN), and a new hybrid model combining both, called CNN-GRU. We tested their performance using metrics like correlation coefficient (R), Determination Coefficient (DC), and Root Mean Squared Error (RMSE). The models used six key water quality factors: river flow, turbidity (cloudiness), water velocity, specific conductance, dissolved oxygen, and water temperature. The hybrid CNN-GRU model performed best, with an R-value of 0.876, a DC of 0.761, and an RMSE of 0.086, outshining the standalone models. Among the individual models, GRU did better than CNN. We also found that turbidity was the most critical factor for predicting nitrate levels.

Keywords—water quality, nitrate prediction, deep learning, CNN, GRU

I. INTRODUCTION

Water scarcity has become a critical issue in the current global development landscape. Industrialization and urbanization have increased water pollution through the discharge of industrial and agricultural effluents into aquatic ecosystems [1]. This pollution exacerbates disease spread and biodiversity loss, making effective water resource management urgent in developing nations [2]. These countries can address pollution by monitoring physicochemical characteristics, key indicators of water quality [3]. Predicting water quality is essential for preventing and managing pollution and supporting water resource protection. Accurate predictions provide insights into pollution levels and trends, aiding strategic planning to mitigate water pollution [4]. However, the complex and interconnected nature of water quality data challenges accurate predictions [5]. Advanced algorithms are increasingly used to develop predictive models, enhancing strategies for pollution prevention and control [6].

Nitrate (NO₃) is a naturally occurring compound that originates primarily from the aerobic decomposition of organic nitrogen and microbial processes in the environment. It plays a vital role in various ecological and agricultural systems, significantly influencing nutrient dynamics, food production, water resource management, and the overall

stability of both natural and anthropogenically impacted ecosystems [7]. The concentration and mobility of nitrate within terrestrial and aquatic systems are central to nutrient cycling and agricultural productivity. However, elevated nitrate levels, particularly in surface water bodies such as streams and rivers, can have detrimental effects. These include the degradation of aquatic habitats, disruption of ecological balances, and serious health concerns for humans, especially when nitrate-contaminated water is consumed [8]. One of the challenges with nitrate is its high solubility and persistence in the environment. Because it readily leaches through soil layers and accumulates in groundwater and surface waters, it often contributes to declining water quality. This can lead to eutrophication—a process where nutrient overload stimulates excessive algal growth, depleting oxygen levels and harming aquatic life [9]. In response to these challenges, Machine Learning (ML) models have emerged as powerful tools for understanding and predicting complex interactions among water quality parameters. These models are particularly effective in identifying relationships that may not be evident through traditional statistical methods. For example, they can model the Water Quality Index (WQI), a composite indicator of overall water health, with high accuracy by analyzing large datasets of environmental variables [10]. Artificial intelligence (AI)-based approaches offer a cost-efficient alternative to conventional water quality assessment techniques, which typically require extensive laboratory testing and sophisticated instruments. These AI models excel at detecting nonlinear patterns, handling high-dimensional data, and identifying outliers or subtle changes in water quality indicators. As a result, they significantly enhance our ability to monitor, evaluate, and manage water quality in real time, supporting better decision-making and more sustainable resource management [11].

Nitrate (NO₃), formed through microbial decomposition of organic nitrogen, is highly soluble and mobile, making it a critical factor in water quality and nutrient balance. However, predicting nitrate levels remains challenging due to complex environmental interactions and the variability in data availability. This gap highlights the need for more efficient, site-specific models that can utilize short-term data for accurate predictions. Addressing this issue is essential to mitigating nitrate accumulation in surface and groundwater, which contributes to eutrophication and ecosystem degradation. In this context, leveraging deep learning methods for nitrate prediction offers a promising approach, enhancing water quality monitoring and supporting sustainable ecosystem management.

II. LITERATURE REVIEW

Accurate prediction of nitrate concentration is essential for effective water resource management and pollution control. Traditional methods for nitrate prediction rely on statistical and physical models, which often struggle with nonlinear relationships and complex temporal dependencies in water quality data [9].

Various methods have been employed to predict NO_3 concentrations in water, including Artificial Neural Networks (ANN) and Multilayer Perceptron (MLP) [12], Multilayer Neural Networks, General Regression Neural Networks (GRNN), and Radial Basis Function Neural Networks (RBFNN) [13]. Other approaches include Radial Basis Function Neural Networks (RBF-NN) combined with Multiple Linear Regression (MLR) [14], Binomial Regression Models (BRM) with Monte Carlo Markov Chain (MCMC) [15], Generalized Additive Models for Location, Shape, and Scale (GAMLSS) [16], as well as feature selection (FS) techniques integrated with eXtreme Gradient Boosting (XGBoost) and Random Forests (RF) [17]. Conventional nitrate prediction methods include regression models, autoregressive integrated moving average (ARIMA) models, and physically based hydrological models. While these methods have been widely used, they often fail to capture spatial and temporal variations effectively. Machine learning techniques such as Support Vector Machines (SVMs) and Random Forests (RFs) have improved prediction accuracy but still struggle with complex, high-dimensional datasets.

Deep learning, a transformative branch within the broader field of machine learning and artificial intelligence, has significantly advanced predictive modeling in environmental science, particularly in the domain of water quality forecasting [18]. Unlike traditional machine learning approaches, which often struggle with highly variable and non-linear data, deep learning models employ multilayered neural networks capable of identifying intricate and abstract patterns within large-scale, multidimensional datasets [19]. This capability is especially valuable in environmental applications, where water quality is influenced by a complex interplay of physical, chemical, and biological variables that conventional models frequently fail to capture adequately [20]. Among the most effective deep learning architectures are Convolutional Neural Networks (CNNs) and Gated Recurrent Units (GRUs). Each is uniquely suited to specific data structures: CNNs excel at extracting spatial features from grid-like data (such as images or spatial matrices), while GRUs are optimized for modeling sequential or time-dependent data, such as time-series measurements of water quality indicators. Traditionally, CNNs and GRUs have been deployed independently for forecasting applications. However, recent advancements in hybrid modeling techniques suggest that integrating the strengths of both architectures into a single CNN-GRU model can significantly enhance predictive performance by simultaneously capturing spatial and temporal dependencies [21]. Building on this emerging trend, the current study implemented a hybrid CNN-GRU model to forecast water levels in the Yangtze River. The results demonstrated that the hybrid model consistently outperformed standalone CNN and GRU models across key performance metrics, underscoring its superior capacity to handle complex, real-world environmental data [22]. This finding reinforces the potential of hybrid deep

learning architectures in water resource management, offering a robust solution for improving the accuracy and reliability of environmental forecasts.

While machine learning techniques have gained widespread adoption in environmental modeling, the application of deep learning approaches—particularly in the context of water quality prediction—remains relatively limited. A substantial number of existing studies rely on biological and chemical indicators, such as nitrate (NO_3) concentrations, as input data for training machine learning models. However, these models often struggle to achieve high predictive accuracy, with many reporting Nash-Sutcliffe Efficiency (NSE) values below 0.70, indicating only moderate performance [23, 24]. In contrast, the present study demonstrates a notable advancement by achieving an NSE score exceeding 0.75, signaling a more accurate and reliable model for predicting nitrate levels in river systems. This improvement underscores the potential of advanced modeling strategies in overcoming the limitations of conventional approaches. Moreover, to date, there has been no documented application of hybrid deep learning architectures—such as combined Convolutional Neural Networks (CNNs) and Gated Recurrent Units (GRUs)—specifically for forecasting nitrate concentrations in rivers. This study, therefore, breaks new ground by not only achieving higher predictive accuracy but also introducing a novel hybrid model that integrates both spatial and temporal learning capabilities. The results highlight the effectiveness of such models in capturing the complex dynamics of nitrate transport and transformation in aquatic environments, setting a foundation for future research in data-driven water quality assessment.

Deep learning models have gained traction in water quality prediction due to their ability to capture intricate patterns in large datasets. Researchers have traditionally used individual CNN and GRU models for time series forecasting [25, 26]. CNNs are widely used in spatial data processing and feature extraction. In nitrate prediction, CNNs can analyze spatially distributed data from in-situ measurements, identifying critical features that influence nitrate levels. GRUs are effective for time-series prediction as they handle long-term dependencies and mitigate vanishing gradient issues. By learning temporal correlations, GRUs enhance the ability to forecast future nitrate concentrations based on historical water quality data. Recent studies have demonstrated that hybrid models achieve superior performance in predicting water quality parameters [27, 28]. In addition, recent studies indicate that hybrid approaches integrating both CNN and GRU yield better predictive accuracy [22]. This research presents an innovative CNN-GRU hybrid model designed to forecast hourly nitrate (NO_3) concentrations in the Willamette River. The model's effectiveness is assessed against standalone CNN and GRU models, building on prior work in this domain. The GRU component enhances training speed and reduces computational demands, making it ideal for time series prediction, while the CNN layer effectively identifies local patterns within the data.

III. MATERIALS AND METHODS

A. Study Area and Dataset

The Willamette River runs 187 miles across northwestern Oregon, contributing 12 to 15 % of the Columbia River's total

flow. Data for a specific Willamette River station over the two-year period (2021–2022) were obtained from the United States Geological Survey (USGS) website (<https://waterdata.usgs.gov/nwis/sw>). Located at 45°31'5"N and 122°40'15"W, the USGS station (number 14211720) is in Portland. Fig. 1 shows the exact location of the gauging station and the geographic coverage of the Willamette River basin catchment area. The predictor variables include river discharge (Q; m³/s), mean water velocity (V; m/s), water temperature (T; °C), turbidity (TU; FNU), water pH, dissolved oxygen (DO; mg/L), specific conductance (SC; µS/cm), gauge height (GH; m), and chlorophyll (Chl; µg/L).

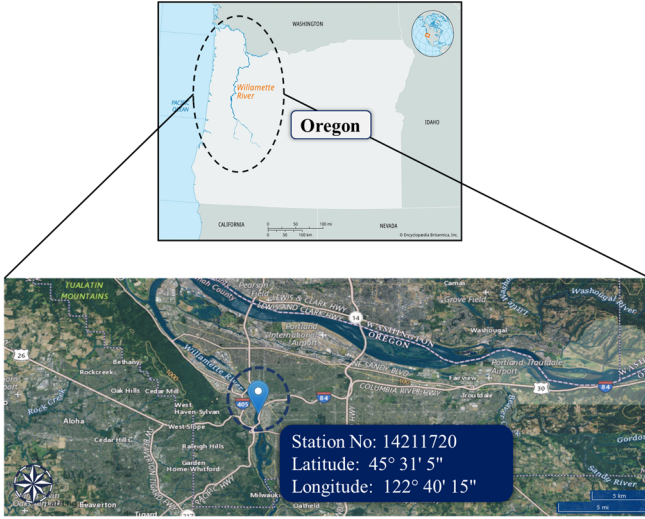


Fig. 1. Position of the analyzed USGS station.

B. Gated Recurrent Unit (GRU)

The GRU model streamlines recurrent neural networks by using two gates—the update gate and the reset gate—to efficiently manage long-interval time series predictions without additional memory cells. The update gate determines the retention of prior outputs, while the reset gate reads input sequences while ignoring previous states. This selective mechanism enables GRU to retain relevant data and discard unnecessary information. Its fixed parameter count across datasets offers advantages like faster convergence, improved CPU efficiency, and better generalization over other recurrent models.

The computation procedure of the memory unit is delineated through Eqs. (1–5).

$$r_t = \sigma(W_r \cdot [h_{t-1}, x_t]) \quad (1)$$

$$z_t = \sigma(W_z \cdot [h_{t-1}, x_t]) \quad (2)$$

$$\tilde{h}_t = \tanh(W_{\tilde{h}} \cdot [r_t \times h_{t-1}, x_t]) \quad (3)$$

$$h_t = (1 - z_t) \times h_{t-1} + z_t \times \tilde{h}_t \quad (4)$$

$$\tilde{y}_t = \sigma(W_o \cdot h_t) \quad (5)$$

In the equations above, r_t represents the reset gate's output at time t , z_t the update gate's output at time t , and h_t and h_{t-1} the outputs at times t and $t-1$, respectively. Furthermore, r denotes the activation function, and x_t represents the input at time t .

C. Convolutional Neural Network (CNN)

A CNN's architecture includes input, convolutional, pooling, fully connected, and output layers. The input layer introduces raw data, while the convolutional layer applies filters (kernels) to detect specific features, using an activation function like ReLU to address the vanishing gradient problem. The max-pooling layer extracts invariant features through non-linear down-sampling, reducing computational load. The fully connected layer links to the loss function to compute errors, and the dense layer aggregates high-level patterns for making predictions on sequential data [29, 30].

Conv1D (1-dimensional convolution) is a type of convolutional layer primarily used for processing sequential data, such as time series. It applies convolutional filters over 1D inputs to capture local patterns and relationships. By applying convolutional filters, CNN1D can identify patterns such as seasonal trends and sudden fluctuations in nitrate levels, making it particularly useful for environmental monitoring. The model is trained on past nitrate measurements, potentially incorporating additional factors like temperature and discharge, etc., to forecast future concentrations. Compared to recurrent models like LSTMs, CNN1D is computationally efficient and requires fewer parameters, making it suitable for real-time applications. With proper data preprocessing, hyperparameter tuning, and external feature integration, CNN1D can provide accurate and reliable predictions, aiding in water quality management and pollution control efforts.

D. Hybrid CNN-GRU Model

The combination of Convolutional Neural Networks (CNNs) and Gated Recurrent Units (GRUs) provides a powerful approach to time series analysis by leveraging their strengths. CNNs excel at extracting spatial patterns and local dependencies through convolutional layers, while GRUs effectively model temporal dependencies using gated mechanisms. In a hybrid CNN-GRU architecture, CNNs handle feature extraction, and GRUs manage sequence modeling, enhancing predictive accuracy in applications like weather forecasting, stock analysis, and environmental monitoring. This approach achieves efficient training, reduced complexity, and robust retention of temporal and spatial information, with ReLU activation applied throughout, except for the output layer, which uses linear activation for regression tasks.

In our study, we use the Mean Squared Error (MSE) as the loss function:

$$MSE = \frac{1}{N} \sum_{i=1}^N (Y_i - X_i)^2 \quad (6)$$

where Y_i demonstrates the predicted data, X_i depicts the observed data, and N represents all number of data.

E. Normalizing Data

A key step in applying intelligent methods is data preprocessing. To enhance modeling accuracy and speed, the diverse input data in this study were normalized using Eq. (7) within the range of 0.1 to 1. Ultimately, the processed data were utilized for modeling [31]

$$x_n = 0.1 + 0.9 \times \left(\frac{x - x_{min}}{x_{max} - x_{min}} \right) \quad (7)$$

where $x_{i \min}$ and $x_{i \max}$ are the minimum and maximum data in terms of value.

F. Model Performance Assessment

The data for the gauging station was split into two parts: the training set, covering January 2021 to June 2022 (18 months, or 75% of the total data), and the testing set, spanning July 2022 to December 2022 (6 months, or 25% of the data). We used the training data to build the models and the testing data to check how well those models performed. This split helped us thoroughly evaluate the models' reliability across different data sets. To measure how accurately the models estimated hourly NO_3 levels, we looked at three key stats: the correlation coefficient (R), the coefficient of determination (DC), and the root mean square error (RMSE).

$$R = \frac{\sum_{i=1}^N (V_o - \bar{V}_o) \times (V_p - \bar{V}_p)}{\sqrt{\sum_{i=1}^N (V_o - \bar{V}_o)^2 \times (V_p - \bar{V}_p)^2}} \quad (8)$$

$$DC = 1 - \frac{\sum_{i=1}^N (V_o - V_p)^2}{\sum_{i=1}^N (V_o - \bar{V}_p)^2} \quad (9)$$

$$RMSE = \sqrt{\sum_{i=1}^N \frac{(V_o - V_p)^2}{N}} \quad (10)$$

where V_o and V_p are the observed data and predicted data values, respectively. \bar{V}_o and \bar{V}_p are the average observed and predicted values, and N is the total amount of data.

G. Input Structures

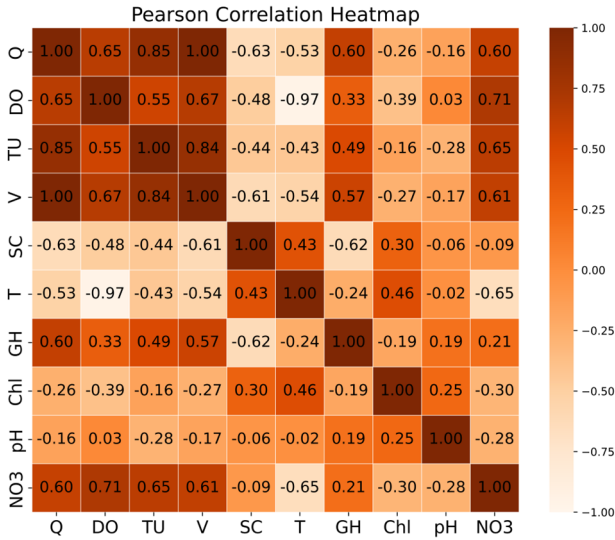


Fig. 2. Pearson correlation between nitrate and other water quality parameters.

Based on the association between nitrate (NO_3) and other input variables, eight models were developed. According to the correlation analysis, Dissolved Oxygen (DO) had the strongest relationship with nitrate. To prevent overfitting, the modeling approach first incorporated DO along with discharge (Q), a key surface water hydrologic variable. Pearson correlation map illustrated in Fig. 2. A Pearson correlation heatmap is a useful visualization tool for assessing the linear relationships between different water quality parameters with nitrate (NO_3). This heatmap is based on the Pearson correlation coefficient (r), which measures the strength and direction of the linear relationship between two continuous variables, with values ranging from -1 (strong

negative correlation) to +1 (strong positive correlation). In this study, the selected models were utilized as inputs for the hybrid CNN-GRU framework. An extensive comparative evaluation was carried out, juxtaposing the performance of this hybrid approach against standalone CNN and GRU models. Through a meticulous assessment based on key performance indicators (R, NSE, and RMSE), the research identified the most accurate model and the most effective strategy for predicting nitrate (NO_3) concentrations.

Through iterative testing, additional parameters were gradually introduced, culminating in the eighth model, which included all input variables for nitrate prediction in rivers. An overview of these models is provided in Table 1.

Table 1. The predictor variable combinations for deep learning models development

Model	Input	Target
N(I)	Q, DO	NO_3
N(II)	Q, DO, TU	NO_3
N(III)	Q, DO, TU, V	NO_3
N(IV)	Q, DO, TU, V, SC	NO_3
N(V)	Q, DO, TU, V, SC, T	NO_3
N(VI)	Q, DO, TU, V, SC, T, GH	NO_3
N(VII)	Q, DO, TU, V, SC, T, GH, Chl	NO_3
N(VIII)	Q, DO, TU, V, SC, T, GH, Chl, pH	NO_3

IV. RESULTS AND DISCUSSION

The performance of hybrid CNN-GRU models, as well as standalone CNN and GRU models with different input combinations, was evaluated using statistical metrics including R, NSE, and RMSE across both training and testing phases. The results of the most optimally structured models during these stages are summarized in Table 2.

Table 2. Results of the best model performance at each station

Method	Model	Train			Test		
		R	DC	RMSE	R	DC	RMSE
CNN	N(I)	0.760	0.556	0.149	0.738	0.541	0.119
	N(II)	0.861	0.730	0.116	0.827	0.677	0.100
	N(III)	0.871	0.746	0.113	0.839	0.680	0.099
	N(IV)	0.955	0.910	0.067	0.862	0.735	0.090
	N(V)	0.950	0.902	0.070	0.867	0.751	0.087
	N(VI)	0.954	0.909	0.067	0.859	0.738	0.090
	N(VII)	0.961	0.923	0.062	0.840	0.697	0.097
	N(VIII)	0.965	0.931	0.058	0.775	0.529	0.120
GRU	N(I)	0.901	0.812	0.097	0.854	0.715	0.094
	N(II)	0.903	0.814	0.097	0.858	0.716	0.093
	N(III)	0.920	0.846	0.088	0.884	0.748	0.088
	N(IV)	0.952	0.906	0.068	0.864	0.739	0.089
	N(V)	0.957	0.914	0.065	0.867	0.753	0.089
	N(VI)	0.958	0.917	0.064	0.872	0.742	0.087
	N(VII)	0.966	0.933	0.058	0.851	0.724	0.092
	N(VIII)	0.975	0.949	0.050	0.797	0.547	0.118
CNN-GRU	N(I)	0.896	0.803	0.099	0.862	0.733	0.091
	N(II)	0.916	0.839	0.090	0.868	0.736	0.090
	N(III)	0.918	0.844	0.088	0.879	0.744	0.089
	N(IV)	0.968	0.936	0.056	0.859	0.735	0.090
	N(V)	0.967	0.934	0.057	0.876	0.761	0.086
	N(VI)	0.968	0.937	0.056	0.861	0.734	0.090
	N(VII)	0.975	0.948	0.050	0.818	0.641	0.105
	N(VIII)	0.978	0.954	0.048	0.759	0.500	0.124

Across all approaches and conditions, the fifth N(V) model consistently outperforms the other models, as shown in the tables. The DC evaluation parameter values for the CNN-GRU, GRU, and CNN models are 0.761, 0.753, and 0.751, respectively. This indicates that the metrics Q, DO, TU, V, SC, and T are effective in accurately forecasting NO_3 concentrations.

The table demonstrates that river nitrate (NO_3) level modeling heavily depends on DO and Q, both of which are included in all input structures. For example, with assessment metrics of $R = 0.738$, $\text{DC} = 0.541$, and $\text{RMSE} = 0.119$, the CNN approach performs relatively well in model one (N(I)). However, this model has considerable uncertainty due to its limited input dimensions, which makes training more challenging. Therefore, the first model requires a greater number of epochs than the others. Additional parameters—TU, V, SC, and T—are progressively added to reduce model uncertainty and produce more accurate and reliable findings. A clear trend is observed in the steady increase of the DC evaluation parameter across models. For instance, in the CNN technique, the DC value increases to 0.677, 0.680, 0.735, and 0.751, respectively, when the parameters TU, V, SC, and T are included. This trend also applies to other approaches.

Furthermore, the optimization process utilized the Adaptive Moment Estimation (Adam) optimizer, while Mean Squared Error (MSE) served as the fitness function for all algorithms. Fig. 3 illustrates the loss function graphs for the best-performing model, N(V), across all deep learning approaches.

Deep learning models, particularly those used for time-series prediction tasks such as nitrate concentration forecasting, require careful configuration of numerous parameters to achieve optimal performance. A critical aspect of this process involves tuning hyperparameters, which significantly influence model accuracy, convergence speed, and generalization capability.

In the GRU model, key hyperparameters include the number of neurons in the Hidden Layers (HN), Activation Function (AF), Batch Size (BS), number of Training Epochs (EP), and Learning Rate (LR). Similarly, the CNN model depends on its own set of architectural hyperparameters, such as the number of Convolutional Filters (HF), Kernel Size (KS), Stride (S), and Pooling Size (PS). These parameters control how features are extracted and processed, directly affecting the model's ability to capture spatial and temporal patterns.

For the hybrid CNN-GRU model, the architecture incorporates components from both individual models, including convolutional layers, pooling layers, and recurrent hidden layers. Consequently, the hybrid model inherits a combined set of hyperparameters from its CNN and GRU components, requiring integrated tuning strategies to balance performance across both feature extraction and sequence modeling stages.

To ensure fair comparison and consistency, the same set of hyperparameters was applied to both the proposed models and the benchmark comparison model. Hyperparameter optimization was conducted through an extensive trial-and-error process during a preliminary experimental phase, where each parameter was varied individually while holding others constant. This approach allowed for a more controlled assessment of each hyperparameter's influence on model behavior.

The ranges for selected hyperparameters were as follows:

- Hidden layer neurons (HN): [4, 8, 16, 32, 64, 128, 256, 512]
- Activation function (AF): [tanh, ReLU]
- Batch size (BS): [4, 8, 16, 32, 64, 128, 256, 512]
- Epochs (EP): [50, 100, 150, 200]

- Learning rate (LR): [0.001, 0.0001]
- Hidden layer filters (HF): [4, 8, 16, 32, 64, 128, 256, 512]
- Kernel size (KS): [1, 2, 3, 4, 5]
- Pooling size (PS): [1, 2, 3, 4, 5]

Experimental results demonstrated that a kernel size of 2 and a pooling size of 1 were optimal for the Conv1D and MaxPooling layers, respectively. The stride parameter, which determines the step size of the convolutional filter across the input, was fixed at 1 in all CNN-based models to preserve temporal resolution.

Furthermore, a learning rate of 0.0001 yielded the most stable performance across most model configurations. However, in certain cases—such as the first model configuration (N(I))—the learning rate was increased to 0.001 to mitigate overfitting issues, particularly when the input dimension was small and the model had a tendency to memorize rather than generalize.

These findings underscore the importance of deliberate and data-informed hyperparameter tuning in achieving reliable and accurate model performance, particularly when employing complex hybrid architectures in environmental prediction tasks.

Loss function plots are used to visualize how a machine learning model's error changes over time during training. Typically, these plots show the loss on the y-axis and the number of iterations or epochs on the x-axis. A decreasing loss curve indicates that the model is learning effectively, while a stagnant or increasing loss may suggest issues like overfitting or poor optimization. Comparing training and validation loss curves helps identify whether a model is generalizing well to unseen data. If the validation loss starts increasing while the training loss continues to decrease, it often signals overfitting. The plots are shown in Fig. 3.

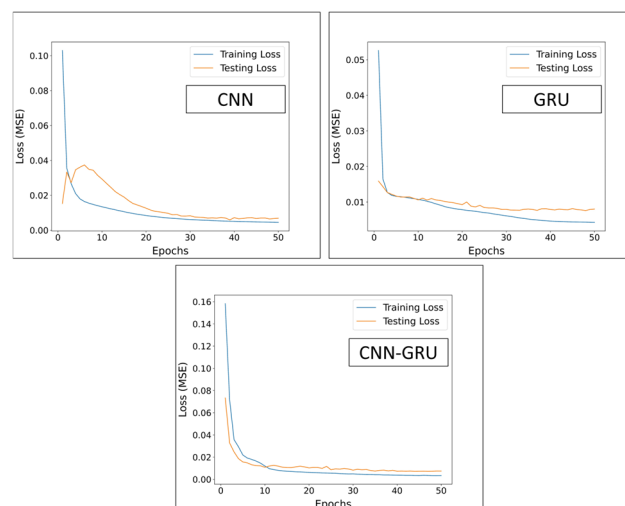


Fig. 3. Loss function graphs for deep learning models used in this study for model N(V).

A consistent trend of achieving optimal performance across various variable combinations (from model one to eight) is observed when evaluating the results from different models. Compared to standalone CNN and GRU models, the comparative study demonstrates the superior efficacy of the proposed hybrid GRU-LSTM model. For example, the CNN-GRU hybrid outperforms GRU and CNN, which achieve DC values of 0.753 and 0.751, respectively, in the most effective

input combination model (N(V)), with a DC of 0.761.

Although hybrid models require more epochs and have longer runtimes, they consistently produce more robust, precise, and reliable results than solo models under the same conditions. Among solo models, GRU outperforms CNN. Fig. 4 illustrates how various deep learning models compare in forecasting nitrate levels for the optimal input combination (model N(V)).

In the eighth model configuration (N(VIII)), the inclusion of the pH parameter led to a noticeable deterioration in model performance across all architectures. Specifically, there was a sharp decline in both the correlation coefficient (R) and Nash-Sutcliffe Efficiency (NSE), accompanied by a significant rise in Root Mean Squared Error (RMSE). The evaluation metrics for this configuration reveal the extent of the impact: for the CNN-GRU model, R dropped to 0.759, NSE fell to 0.500, and RMSE increased to 0.124. Similarly, the CNN model recorded $R = 0.775$, $NSE = 0.529$, and $RMSE = 0.120$, while the GRU model showed slightly better results with $R = 0.797$, $NSE = 0.547$, and $RMSE = 0.118$.

These findings suggest that the pH parameter does not contribute meaningfully to the prediction of nitrate (NO_3) concentrations in this riverine system. In fact, its inclusion appears to introduce noise or redundancy that adversely affects model accuracy. This underscores the importance of carefully selecting relevant input variables during model development to avoid performance degradation.

Looking ahead, future efforts in nitrate prediction should consider the integration of spatio-temporal modeling approaches that combine Geographic Information Systems (GIS), remote sensing technologies, and in situ hydrological measurements. Such multi-dimensional data fusion can better account for the spatial heterogeneity and temporal dynamics of nitrate pollution in river basins. Moreover, leveraging advanced machine learning techniques with spatial awareness can enhance prediction accuracy and enable the identification of nitrate pollution hotspots. These insights can inform more effective, geographically targeted intervention strategies to reduce nutrient loading and protect water quality in aquatic ecosystems.

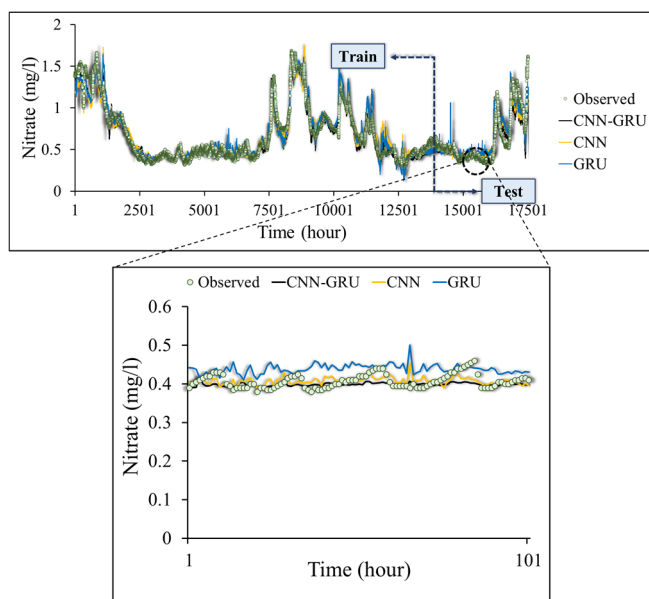


Fig. 4. Performance evaluation of various deep learning models for NO_3 prediction.

The results indicate that each modeling approach, characterized by its unique combination of input variables, brings distinct advantages to the task of nitrate (NO_3) prediction. This diversity in performance highlights the critical role that temporal information plays in accurately modeling nitrate dynamics. To gain deeper insight into the relative importance of the input parameters and better understand their individual contributions, a basic sensitivity analysis was conducted. For this purpose, the most accurate configuration—referred to as N(V)—which incorporates six different input features, was chosen as the basis for further evaluation. The CNN-GRU architecture underpinning this model was then systematically altered: each input parameter was removed one at a time, and subsequently reintroduced, to isolate and examine its specific impact on the model's predictive capability. This step-by-step analysis provided a clearer picture of how each variable influences nitrate modeling, enabling a more nuanced understanding of the model's inner workings.

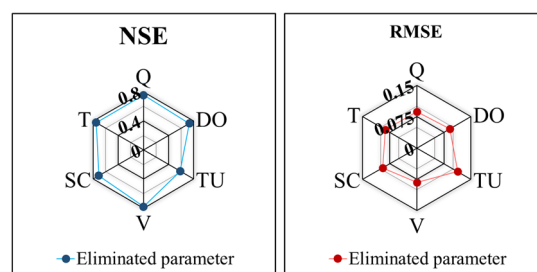


Fig. 5. Results of sensitivity analysis obtained from the employed CNN-GRU.

The exclusion of individual input parameters had a noticeable impact on the predictive performance of the CNN-GRU model. To quantitatively assess the significance of each parameter, two evaluation metrics were employed: Root Mean Squared Error (RMSE) and Nash-Sutcliffe Efficiency (NSE). The outcomes of this sensitivity analysis are illustrated in Fig. 5, where variations in RMSE and NSE represent the changes in model accuracy associated with the removal of each input.

This analysis provides valuable insight into how each variable contributes to the overall modeling process. Among all inputs, Turbidity (TU) emerged as the most influential factor in predicting nitrate concentrations. Its exclusion led to a substantial decrease in model performance, with NSE dropping by 0.21 and RMSE increasing by 0.034, indicating a significant loss in predictive accuracy. Specific Conductance (SC) and Dissolved Oxygen (DO) were identified as the next most critical parameters. When removed, they caused moderate degradations in model accuracy, with NSE reductions of 0.087 and 0.063, respectively. Meanwhile, Discharge (Q) and water Temperature (T) showed similar levels of influence, with their absence causing approximately a 10% rise in RMSE. In contrast, mean water Velocity (V) had a minimal effect on model performance when excluded, suggesting that it contributes little to the predictive capability of the model in this context. These findings highlight the uneven importance of different input variables, emphasizing the need to prioritize high-impact parameters—such as turbidity, specific conductance, and dissolved oxygen—when developing nitrate forecasting models.

V. CONCLUSION

Accurately forecasting river water quality is essential for sustainable freshwater management and ecosystem health preservation. It provides key insights for informed decision-making and proactive environmental risk mitigation. However, modeling and predicting river water quality parameters remain a challenge. Nitrate (NO₃) dynamics involve complex interactions of biological and environmental factors, many not fully understood. Collecting data to simulate these processes is difficult, and developing accurate mathematical models is often highly complex. As a result, commonly used physical-based models, despite their widespread use in predicting nitrate and other water quality indicators, tend to oversimplify these intricate processes and often fail to deliver accurate NO₃ predictions.

This research seeks to create a novel hybrid CNN-GRU model for forecasting nitrate (NO₃) concentrations in the Willamette River by incorporating various hydro-chemical parameters. A comparative analysis is conducted to assess the performance of the standalone CNN and GRU models, which serve as the foundational components of the hybrid approach.

The results indicate that model five, integrating Q, DO, TU, V, SC, and T, achieves the highest accuracy in predicting NO₃ levels. Conversely, model eight, which incorporates all possible input variables, performs the least effectively, primarily due to the inclusion of GH, pH, and Chl. Notably, DO enhances model performance due to its strong correlation with NO₃, whereas pH significantly reduces accuracy. Sensitivity analysis shows that excluding turbidity leads to a 0.21 decrease in NSE and a 0.034 increase in RMSE, highlighting turbidity as the most critical factor for NO₃ prediction.

The hybrid model outperformed its individual counterparts within the deep learning framework. Interestingly, the CNN-GRU approach proved to be the most effective. Furthermore, among the individual models, the GRU performed better than the CNN in terms of prediction accuracy.

CONFLICT OF INTEREST

The authors declare no conflict of interest.

AUTHOR CONTRIBUTIONS

I.F. conceptualized the study and supervised the research; S.D. handled data curation, software, validation, and visualization; both authors contributed to writing and editing and approved the final version of the article.

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