

# Deep Learning Approaches for Air Quality Index Prediction: A Critical Review of Architectures and Applications

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*Abstract: Air pollution has emerged as a critical global environmental challenge, necessitating accurate and reliable Air Quality Index (AQI) prediction systems for public health protection and policy intervention. Traditional statistical and machine learning models often struggle to capture the nonlinear, non-stationary, and highly dynamic behavior of atmospheric pollutant time series. In recent years, deep learning (DL) techniques have demonstrated significant advancements in modeling complex spatiotemporal dependencies in AQI forecasting tasks. This review presents a comprehensive and critical analysis of state-of-the-art deep learning architectures used for AQI prediction, including Convolutional Neural Networks (CNNs), Recurrent Neural Networks (RNNs), Long Short-Term Memory networks (LSTM), Gated Recurrent Units (GRU), hybrid CNN–RNN models, attention mechanisms, and transformer-based frameworks. The study further evaluates data preprocessing strategies, feature engineering approaches, and the role of auxiliary meteorological and geospatial inputs in improving prediction performance. In addition, limitations such as overfitting, data scarcity, interpretability issues, and computational cost are critically discussed. Finally, future directions such as physics-informed deep learning, multimodal fusion models, and edge-deployable lightweight architectures are highlighted to guide further research in this domain.*

*Keywords: Air Quality Index, Deep Learning, LSTM, CNN, Transformer, Time Series Forecasting, Spatiotemporal Modeling*

**How to cite this article:** Ram Kumar Sah, Madhuvan Dixit. (2025). Deep Learning Approaches for Air Quality Index Prediction: A Critical Review of Architectures and Applications. *International Journal of Scientific Modern Research and Technology (IJS MRT)*, ISSN: 2582-8150, Volume-20, Issue-2, Number-3, Aug-2025, pp.14-21, URL: <https://www.ijsmrt.com/wp-content/uploads/2026/05/IJS MRT-25080203.pdf>

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IJS MRT-25080203

## I. INTRODUCTION

### Background

Air pollution has emerged as one of the most critical environmental and public health challenges of the modern era. Rapid urbanization, industrial expansion, vehicular emissions, and energy consumption have

significantly deteriorated atmospheric quality, particularly in developing regions. Exposure to polluted air is strongly associated with respiratory illnesses, cardiovascular diseases, neurological disorders, and increased mortality rates (Le et al., 2024).

To systematically quantify air pollution levels, the Air Quality Index (AQI) is widely used as a standardized indicator. AQI is derived from multiple pollutant concentrations, including particulate matter (PM<sub>2.5</sub> and PM<sub>10</sub>), nitrogen dioxide (NO<sub>2</sub>), sulfur dioxide (SO<sub>2</sub>), carbon monoxide (CO), and ozone (O<sub>3</sub>). However, AQI is not static; it exhibits strong spatiotemporal variability influenced by meteorological conditions, seasonal cycles, and human activities. From a data science perspective, AQI prediction is formulated as a multivariate time series forecasting problem, characterized by nonlinear interactions among pollutants and complex temporal dependencies (Fan et al., 2025).

### *Motivation*

Accurate AQI forecasting is challenging due to the nonlinear, dynamic, and interdependent nature of atmospheric processes. Air quality varies across multiple time scales and is strongly influenced by meteorological factors such as wind, temperature, and humidity. Sudden pollution spikes further complicate prediction. Traditional statistical models fail to capture these complexities, motivating the adoption of deep learning methods for improved accuracy and robust spatiotemporal modeling of air pollution data (Khan et al., 2023).

### *Contributions of the Review*

This paper provides a comprehensive and structured review of deep learning methodologies for AQI prediction. The key contributions are as follows:

- Systematic categorization of deep learning architectures used in AQI forecasting, including CNN, RNN, LSTM, GRU, hybrid CNN-RNN models, attention mechanisms, and transformer-based models.
- Critical comparative analysis of model performance in terms of accuracy, scalability, and computational complexity.
- Discussion of data preprocessing and feature engineering strategies, including handling missing data, normalization, and incorporation of meteorological variables.
- Identification of research gaps, particularly in interpretability, data scarcity, and

generalization across geographic regions.

- Future research directions, including physics-informed neural networks, multimodal fusion models, and lightweight edge-deployable architectures for real-time AQI prediction.

### *Organization of the Paper*

The remainder of this paper is organized, Section 2 describes the characteristics of AQI datasets, including pollutant variables, meteorological factors, and data challenges. Section 3 presents a detailed review of deep learning architectures used in AQI prediction, including CNN, RNN, LSTM, GRU, hybrid models, attention mechanisms, and transformers. Section 4 discusses evaluation metrics commonly used in AQI forecasting studies. Section 5 provides a comparative analysis of different deep learning models in terms of performance and complexity. Section 6 highlights real-world applications of AQI prediction systems in environmental monitoring and public health. Section 7 outlines key challenges and limitations in current research. Section 8 discusses future research directions and emerging trends. Section 9 concludes the paper with final observations and insights.

## II. DATA CHARACTERISTICS

AQI forecasting datasets typically include:

### *Pollutant Variables*

Pollutant variables are key components used to compute the Air Quality Index (AQI). PM<sub>2.5</sub> and PM<sub>10</sub> represent fine and coarse particulate matter that penetrate the respiratory system and affect health. NO<sub>2</sub>, SO<sub>2</sub>, CO, and O<sub>3</sub> are gaseous pollutants originating from vehicular emissions, industrial activities, and atmospheric reactions. These pollutants collectively determine air quality status and are essential inputs for modeling and predicting AQI in environmental monitoring systems (Kumar et al., 2024).

### *Meteorological Variables*

Meteorological variables play a crucial role in determining air quality conditions and pollutant behavior. Temperature influences chemical reaction

rates and pollutant formation. Humidity affects particulate matter through absorption and aerosol formation. Wind speed and direction control the transport and dispersion of pollutants across different regions, either diluting or concentrating them locally. Atmospheric pressure regulates vertical air movement and atmospheric stability, thereby affecting how pollutants accumulate or disperse in the environment over time (Jacobson, 2002).

#### *Temporal Structure*

The temporal structure of AQI data refers to how air quality values evolve over time in systematic and irregular patterns. Typically, AQI is recorded as hourly or daily time series, capturing fine-grained variations. It exhibits strong seasonal periodicity due to climate changes and recurring human activities. Additionally, abrupt event-driven spikes occur because of dust storms, industrial emissions, crop burning, or festivals, introducing sudden and extreme deviations in pollutant concentration levels (Chen, 2024).

#### *Challenges*

AQI datasets face multiple analytical challenges that complicate accurate modeling. Missing data and noise arise from sensor failures and environmental interference, reducing data reliability. Sensor inconsistency occurs due to calibration differences across monitoring stations, leading to biased readings. Multicollinearity exists when predictor variables are highly correlated, making feature interpretation difficult. Additionally, non-stationarity of distribution means pollutant patterns change over time, violating assumptions of many traditional statistical and machine learning models (Sellamuthu et al., 2024).

### III. DEEP LEARNING ARCHITECTURES

#### *Feedforward Neural Networks (FNN/DNN)*

Feedforward Neural Networks (FNNs), also known as Deep Neural Networks (DNNs) when multiple hidden layers are employed, are among the earliest deep learning models used for Air Quality Index (AQI) prediction. In these networks, information flows in a single direction from the input layer through one or more hidden layers to the output layer without any feedback connections. FNNs learn complex nonlinear relationships between input variables, such as

pollutant concentrations and meteorological parameters, and the target AQI value (Hampika, 2025). Their simple architecture, ease of implementation, and relatively low computational requirements make them suitable for basic forecasting tasks. However, FNNs process each observation independently and lack memory mechanisms to capture temporal dependencies. Consequently, they struggle to model sequential patterns and long-term trends present in AQI time-series data, often resulting in lower prediction accuracy compared to recurrent and hybrid deep learning architectures (Khan et al., 2023).

#### *Convolutional Neural Networks (CNNs)*

Convolutional Neural Networks (CNNs) are deep learning models originally developed for image processing but have been successfully adapted for Air Quality Index (AQI) prediction. CNNs use convolutional filters to automatically extract important features from input data by identifying local patterns and correlations among pollutant and meteorological variables. In AQI forecasting, CNNs can effectively learn relationships between factors such as PM<sub>2.5</sub>, PM<sub>10</sub>, temperature, humidity, and wind speed, helping to capture short-term pollutant interactions and spatial dependencies (Marpaung et al., 2024).

One of the major advantages of CNNs is parameter sharing, where the same filter is applied across the entire input, reducing the number of trainable parameters and computational complexity. This enables efficient feature extraction and faster training compared to fully connected networks. CNNs are also effective in reducing noise and identifying significant patterns from large environmental datasets (Deneu et al., 2021). However, CNNs are primarily designed to analyze spatial or local relationships and do not possess an inherent memory mechanism for sequential data. As a result, they have limited ability to capture long-term temporal dependencies and historical trends in AQI time series. For this reason, CNNs are often combined with recurrent architectures such as LSTM or GRU to improve forecasting performance by simultaneously learning spatial features and temporal dynamics. Such hybrid CNN-based models have demonstrated superior accuracy in air quality prediction applications (Ng et al., 2024).

### *Recurrent Neural Networks (RNNs)*

Recurrent Neural Networks (RNNs) are designed to process sequential data by retaining information from previous time steps through internal memory. In AQI prediction, they capture temporal relationships among pollutant measurements over time. However, traditional RNNs suffer from the vanishing gradient problem, which weakens learning during training and limits their ability to retain long-term dependencies, reducing forecasting accuracy for extended time-series patterns (Khan et al., 2023).

### *LSTM and GRU Models*

Long Short-Term Memory (LSTM) and Gated Recurrent Unit (GRU) are advanced recurrent neural networks designed to overcome the limitations of traditional RNNs. LSTM uses input, forget, and output gates to retain important information and capture long-term dependencies in AQI time-series data. GRU simplifies this architecture by combining gates, reducing computational complexity. Both models achieve high forecasting accuracy, although they require careful hyperparameter tuning and substantial training time (Ng et al., 2024).

### *CNN-LSTM Hybrid Models*

CNN-LSTM hybrid models combine the strengths of Convolutional Neural Networks (CNNs) and Long Short-Term Memory (LSTM) networks. CNN extracts meaningful spatial features and reduces noise from environmental data, while LSTM captures temporal dependencies and sequential patterns. This integrated approach effectively models AQI dynamics, resulting in higher prediction accuracy and consistently lower RMSE and MAE values than standalone CNN or LSTM models (Guo et al., 2025).

### *Attention Mechanisms*

Attention mechanisms enhance AQI prediction models by assigning different importance weights to historical time steps and input features. This enables the model to focus on critical pollution events and influential variables, improving forecasting accuracy and interpretability. By highlighting significant patterns, attention mechanisms provide better insights into model decisions. However, they increase computational complexity and may lead to overfitting

when trained on small or insufficient datasets (Hashim & Atia, 2025).

### *Transformer-Based Models*

Transformer models utilize self-attention mechanisms instead of recurrent structures to capture relationships among all input time steps simultaneously. This enables efficient parallel processing and superior modeling of long-range dependencies in AQI data. However, transformers require large training datasets and significant computational resources. In small or limited AQI datasets, they may not perform as effectively as LSTM-based models due to their high data and parameter requirements (My et al., 2025).

### *Hybrid and Ensemble Models*

Hybrid and ensemble models combine multiple forecasting techniques to leverage their individual strengths and overcome limitations. Architectures such as CNN-BiLSTM-Attention, CEEMDAN-based deep learning models, and ARIMA-CNN-LSTM frameworks improve feature extraction, temporal learning, and signal decomposition. By integrating complementary approaches, these models enhance robustness, reduce prediction errors, and achieve superior AQI forecasting accuracy under complex environmental conditions (Bahri & Vahidnia, 2022).

## IV. PERFORMANCE EVALUATION METRICS

Performance evaluation metrics are essential for assessing the accuracy and reliability of Air Quality Index (AQI) prediction models. These metrics quantify the difference between actual AQI values and predicted values, allowing researchers to compare different forecasting approaches objectively. Among the most commonly used metrics are Mean Absolute Error (MAE), Root Mean Square Error (RMSE), Mean Absolute Percentage Error (MAPE), and the Coefficient of Determination ( $R^2$  Score).

### *Mean Absolute Error (MAE)*

MAE measures the average magnitude of prediction errors without considering their direction. It calculates the absolute difference between actual and predicted AQI values and then computes their average.

$$MAE = \frac{1}{n} \sum_{i=1}^n |y_i - \hat{y}_i|$$

where:  $y_i$  = actual AQI value,  $\hat{y}_i$  = predicted AQI value,  $n$  = total number of observations

A lower MAE indicates better model performance. Since all errors are weighted equally, MAE provides an intuitive measure of average prediction accuracy. However, it does not emphasize large prediction errors.

#### Root Mean Square Error (RMSE)

RMSE is one of the most widely used metrics in AQI forecasting because it penalizes larger errors more heavily than MAE. It is calculated by squaring prediction errors, averaging them, and then taking the square root.

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2}$$

The squaring operation makes RMSE particularly sensitive to large deviations between actual and predicted AQI values. As a result, models producing occasional large errors receive higher RMSE values. Because severe AQI prediction errors can have significant environmental and public health implications, RMSE is often considered the most informative metric in air quality forecasting studies.

#### Advantages of RMSE:

- Strongly penalizes large forecasting errors.
- Useful for comparing deep learning models.
- Widely accepted in AQI prediction literature.

#### Limitation:

- Sensitive to outliers.

#### Mean Absolute Percentage Error (MAPE)

MAPE expresses prediction error as a percentage of the actual value, making results easier to interpret across different datasets.

$$MAPE = \frac{100}{n} \sum_{i=1}^n \left| \frac{y_i - \hat{y}_i}{y_i} \right|$$

MAPE indicates the average percentage deviation between predicted and actual AQI values. For

example, a MAPE of 5% means that predictions differ from actual observations by an average of 5%.

#### Advantages:

- Easy to understand and interpret.
- Enables comparison across datasets with different scales.

#### Limitations:

- Becomes unstable when actual AQI values are close to zero.
- Can produce misleading results for very small observations.

#### Coefficient of Determination ( $R^2$ Score)

The  $R^2$  Score measures how well a prediction model explains the variability in AQI data. It evaluates the proportion of variance in actual AQI values that is captured by the forecasting model.

$$R^2 = 1 - \frac{\sum (y_i - \hat{y}_i)^2}{\sum (y_i - \bar{y})^2}$$

where:  $\bar{y}$  = mean of actual AQI values

The  $R^2$  value typically ranges from 0 to 1:

- $R^2 = 1$ : Perfect prediction.
- $R^2 = 0$ : Model performs no better than predicting the mean.
- Higher  $R^2$  values: Better explanatory power.

#### Advantages:

- Measures goodness of fit.
- Indicates how much variability is explained by the model.

#### Limitation:

- Does not directly indicate prediction error magnitude.

## V. COMPARATIVE ANALYSIS OF ARCHITECTURES

The selection of an appropriate forecasting architecture plays a crucial role in determining the accuracy and reliability of Air Quality Index (AQI) prediction systems. Different models possess varying capabilities in capturing temporal dependencies, spatial relationships, and nonlinear interactions among environmental variables. Therefore, understanding the strengths and limitations of each architecture is essential for selecting the most suitable model for a particular forecasting scenario.

Table 1: Comparative analysis of architectures

Model Type	Temporal Learning	Spatial Learning	Accuracy	Complexity
ARIMA	Low	No	Low	Low
CNN	No	High	Medium	Medium
RNN	Medium	No	Medium	Medium
LSTM	High	No	High	High
CNN-LSTM	High	High	Very High	Very High
Transformer	Very High	High	High (data-dependent)	Very High

The table compares AQI prediction models based on learning capability, accuracy, and computational complexity. ARIMA shows limited performance due to its inability to capture nonlinear patterns. CNN excels in spatial feature extraction, while RNN and LSTM effectively model temporal dependencies. CNN-LSTM achieves the highest overall performance by combining spatial and temporal learning. Transformers provide excellent long-range dependency modeling but require large datasets and substantial computational resources for optimal performance.

## VI. APPLICATIONS OF AQI PREDICTION SYSTEMS

**Smart City Pollution Monitoring:** Deep learning-based AQI prediction systems are extensively used in smart cities to continuously monitor air quality levels. They analyze data from environmental sensors and forecast pollution trends, enabling city authorities to implement timely mitigation measures and improve urban environmental management.

**Health Risk Forecasting:** AQI prediction models help identify potential health risks associated with poor air quality. Early warnings can be issued to individuals suffering from asthma, COPD, cardiovascular diseases, and other respiratory disorders, allowing them to take preventive precautions.

**Environmental Policy Planning:** Governments and environmental agencies use AQI forecasts to design and evaluate pollution-control strategies. Predictive insights support evidence-based policymaking aimed at reducing emissions and improving long-term environmental sustainability.

**Industrial Emission Control:** Industries employ AQI prediction systems to monitor pollutant emissions and assess their environmental impact. These forecasts help optimize industrial operations, ensure regulatory compliance, and reduce harmful emissions.

**Real-Time Mobile AQI Applications:** Many mobile applications and web-based platforms integrate AQI forecasting models to provide real-time air quality information, pollution alerts, and health recommendations, helping citizens make informed decisions regarding outdoor activities and exposure to pollutants.

## VII. KEY CHALLENGES

### Data Challenges

AQI prediction models face significant data-related challenges. Sparse monitoring stations limit spatial coverage and may not accurately represent regional air quality conditions. Missing values caused by sensor failures reduce data reliability and model performance. Additionally, limited labeled datasets restrict effective training of deep learning models, often leading to reduced generalization capability and lower forecasting accuracy in real-world environmental applications.

### Model Challenges

Deep learning models for AQI prediction often face overfitting, where the model learns training data patterns too closely and performs poorly on unseen data. Their complex architectures also reduce interpretability, making decision processes difficult to understand. Furthermore, training and deploying deep models require substantial computational resources, memory, and processing time.

### Deployment Challenges

Deploying AQI prediction systems in real-world environments presents several challenges. Real-time forecasting requires rapid data processing and low-latency predictions. Edge devices, such as sensors and

mobile platforms, often have limited computational power and memory. Additionally, models trained in one city may not generalize effectively to other cities due to differences in pollution sources, climate, geography, and environmental conditions.

## VIII. FUTURE RESEARCH DIRECTIONS

### *Physics-Informed Deep Learning*

- Integrates atmospheric and environmental physics with deep learning models.
- Improves prediction reliability and scientific consistency.
- Enhances model generalization under varying environmental conditions.

### *Multimodal Fusion*

- Combines multiple data sources for comprehensive AQI forecasting.
- Integrates satellite imagery, sensor measurements, and meteorological variables.
- Improves prediction accuracy by capturing diverse environmental factors.

### *Lightweight Edge Models*

- Develops computationally efficient CNN-LSTM architectures.
- Enables deployment on mobile devices and IoT sensors.
- Supports real-time AQI prediction with low power consumption.

### *Uncertainty Quantification*

- Provides probabilistic rather than single-value forecasts.
- Estimates confidence levels and prediction uncertainty.
- Supports risk-aware decision-making in environmental monitoring and public health applications.

## IX. CONCLUSION

Deep learning has transformed Air Quality Index (AQI) prediction by effectively capturing the complex nonlinear relationships and spatiotemporal patterns present in environmental data. Advanced architectures such as LSTM, CNN-LSTM hybrids, and attention-

based models have demonstrated superior forecasting accuracy compared to traditional statistical and machine learning approaches. Among these, hybrid models provide the best balance between spatial feature extraction and temporal dependency learning. Despite these advancements, challenges related to data availability, model interpretability, computational complexity, and real-time deployment continue to limit widespread adoption. Future research should emphasize physics-informed learning, multimodal data integration, uncertainty-aware forecasting, and lightweight architectures to develop scalable, reliable, and efficient AQI prediction systems for practical environmental monitoring and public health applications.

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