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MACHINE LEARNING-BASED AIR POLLUTION PREDICTION MODELS: A COMPREHENSIVE REVIEW

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ABSTRACT

Air pollution remains a critical global environmental health challenge, contributing to millions of premature deaths annually. Traditional deterministic and statistical models (e.g., chemical transport models, linear regression) often struggle with capturing the complex, non-linear, and spatiotemporal dynamics of air pollutants. In recent years, machine learning (ML) has emerged as a powerful paradigm for air quality prediction, offering superior accuracy and computational efficiency. This review synthesizes the state-of-the-art ML-based prediction models, categorizing them into shallow models (e.g., Random Forest, Support Vector Machines) and deep learning architectures (e.g., Recurrent Neural Networks, Long Short-Term Memory networks, Convolutional Neural Networks, and hybrid models). We critically evaluate their performance in predicting criteria pollutants (PM2.5, PM10, NO2, O3, SO2, CO) across different temporal and spatial scales. Furthermore, we propose innovative graphical and schematic models illustrating data fusion pipelines, spatiotemporal attention mechanisms, and explainable AI frameworks. Key findings indicate that hybrid deep learning models integrating meteorological, traffic, and satellite aerosol data consistently outperform classical methods. However, challenges persist regarding data sparsity, model interpretability, and generalizability across diverse geographic regions. Future directions include federated learning, graph neural networks, and real-time IoT integration.

KEYWORDS: Air pollution prediction, machine learning, deep learning, spatiotemporal modeling, LSTM, CNN, PM2.5 forecasting, explainable AI, hybrid models

1. INTRODUCTION

Air pollution is recognized as one of the most pressing environmental and public health crises of the 21st century. The World Health Organization (WHO) estimates that exposure to ambient and household air pollution contributes to approximately 7 million premature deaths annually, making it the fourth leading risk factor for mortality globally (WHO, 2021). The Global Burden of Disease Study 2019 reported that fine particulate matter (PM2.5) alone was responsible for over 4.1 million deaths and 147 million disability-adjusted life years (DALYs) worldwide (Murray et al., 2020). Beyond mortality, chronic exposure to air pollution is associated with respiratory diseases (asthma, chronic obstructive pulmonary disease), cardiovascular disorders (myocardial infarction, stroke), neurological impairments (including Alzheimer's and Parkinson's diseases), and adverse pregnancy outcomes (Landrigan et al., 2018; Schraufnagel et al., 2019; Fu et al., 2022).

The six criteria pollutants regulated by environmental agencies globally—PM2.5 (particulate matter with aerodynamic diameter $\leq$ 2.5 µm), PM10 ($\leq$ 10 µm), ground-level ozone (O3), nitrogen dioxide (NO2), sulfur dioxide (SO2), and carbon monoxide (CO)—exhibit complex spatiotemporal dynamics governed by emission sources (traffic, industry, biomass burning, natural dust), meteorological conditions (wind speed and direction, temperature inversions, humidity, precipitation), topography (valleys, coastal areas, urban canyons), and atmospheric chemical reactions (Seinfeld & Pandis, 2016; Kroll et al., 2020). For instance, secondary pollutants like O3 are not emitted directly but form photochemically from precursor gases (NOx and volatile organic compounds) under sunlight, leading to distinct diurnal and seasonal patterns (Monks et al., 2015). The interplay of these factors renders air pollution time series highly non-linear, non-stationary, and cross-correlated across multiple spatial scales (from street canyons to continental plumes) (Viana et al., 2014).

Accurate prediction of air pollutant concentrations is a societal and scientific imperative. Reliable forecasts—ranging from hourly to daily horizons—enable: (i) early warning systems for vulnerable populations (e.g., asthmatics, elderly, children), triggering protective behavioral changes (Brůha et al., 2020); (ii) proactive public health advisories and school closures during severe smog episodes (D'Amato et al., 2020); (iii) optimized urban traffic management and industrial emission controls (Baklanov et al., 2018); and (iv) long-term policy evaluation and land-use planning (Karner et al., 2010). Many countries have established national air quality indices (AQI) and real-time monitoring networks, yet prediction capabilities remain heterogeneous, especially in low- and middle-income countries where monitoring infrastructure is sparse (Martin et al., 2019).

1.1 Traditional Prediction Approaches and Their Limitations

Historically, air pollution prediction has been approached through three methodological families: deterministic chemical transport models (CTMs), statistical time series models, and hybrid physical-statistical systems.

Deterministic CTMs—such as the Community Multiscale Air Quality (CMAQ) model, Weather Research and Forecasting coupled with Chemistry (WRF-Chem), and CHIMERE—solve systems of partial differential equations that describe emission, advection, diffusion, deposition, and chemical transformation of pollutants (Byun & Schere, 2006; Grell et al., 2005; Menut et al., 2013). These models provide mechanistic insights and can simulate "what-if" emission reduction scenarios. However, they suffer from several critical limitations: (i) extremely high computational cost, often requiring supercomputing clusters for regional forecasts (Zhang et al., 2012); (ii) dependence on accurate, high-resolution emission inventories that are outdated or unavailable in many regions (Kuenen et al., 2014); (iii) uncertainty in chemical mechanisms and boundary layer parameterizations (Solazzo et al., 2012); and (iv) systematic biases that require post-processing statistical corrections (Delle Monache et al., 2006). Studies have shown that CTMs can yield mean fractional errors exceeding 50% for PM2.5 and 70% for O3 in complex terrain (Timmermans et al., 2017).

Statistical time series models offer a computationally efficient alternative. Classical methods include multiple linear regression (MLR), autoregressive integrated moving average (ARIMA), seasonal ARIMA (SARIMA), and exponential smoothing (Bruno & Cocchi, 2002; Slini et al., 2006). These models assume linearity, stationarity (or stationarity after differencing), and Gaussian error distributions. In practice, air pollution series violate these assumptions: they exhibit non-linear responses to meteorology (e.g., threshold effects where wind speed below 1 m/s sharply increases concentrations), heteroscedasticity (variance changing with pollution level), and long-memory dependence (Chelani, 2012). ARIMA models, for example, typically achieve R^2 values below 0.6 for next-day PM2.5 prediction, which is insufficient for operational early warning (Kumar & Goyal, 2018; Liu et al., 2020).

Hybrid physical-statistical models attempt to combine CTM output with statistical bias correction (e.g., Kalman filtering or quantile mapping), but they inherit the fundamental errors of the CTM and remain computationally intensive (Djalalova et al., 2015).

1.2 Rise of Machine Learning in Environmental Modeling

Machine learning (ML) has emerged as a transformative paradigm capable of overcoming many limitations of traditional methods. ML algorithms are data-driven, non-parametric, and exceptionally adept at learning complex, high-dimensional, non-linear relationships without explicit physical equations (Reichstein et al., 2019). In the context of air pollution prediction, ML offers several compelling advantages: (i) ability to model non-linear interactions between dozens of predictors (e.g., wind speed × temperature × traffic volume); (ii) flexibility to incorporate heterogeneous data types (numeric, categorical, spatial grids, text from social media); (iii) computational efficiency at inference time (milliseconds per prediction after training); and (iv) adaptability to new data via online learning or transfer learning (Bellinger et al., 2017; Wei et al., 2019).

The earliest applications of ML for air quality date to the 1990s, using artificial neural networks (ANNs) with a single hidden layer. Gardner and Dorling (1998) demonstrated that ANNs could predict daily maximum O3 concentrations with correlation coefficients of 0.85, outperforming regression models. Subsequently, support vector machines (SVMs) were applied to PM10 forecasting, capitalizing on their kernel trick to map data into higher-dimensional feature spaces (Vong et al., 2012; Ortiz-García et al., 2010). Decision tree ensembles—particularly Random Forest (RF) and Gradient Boosted Regression Trees (GBRT)—gained popularity due to their robustness to outliers, built-in feature selection, and interpretable variable importance measures (Li et al., 2017; Kaminska, 2019). RF models have been shown to achieve 15–25% lower root mean square error (RMSE) than ANNs for multi-step ahead predictions (Zhao et al., 2019).

1.3 Deep Learning Revolution

The advent of deep learning (DL) —characterized by multi-layered architectures that automatically learn hierarchical feature representations—has fundamentally advanced the state of the art. Unlike shallow ML models that require hand-engineered features, DL models can discover latent spatiotemporal patterns directly from raw inputs (LeCun et al., 2015). Recurrent neural networks (RNNs) , particularly Long Short-Term Memory (LSTM) networks, are specifically designed for sequential data and can capture long-range temporal dependencies spanning dozens of time steps (Hochreiter & Schmidhuber, 1997). For air pollution, where today's concentration correlates strongly with that of 24–48 hours ago, LSTMs have achieved remarkable accuracy. Freeman et al. (2018) reported that a stacked LSTM reduced RMSE by 38% compared to ARIMA for 24-hour ahead PM2.5 prediction in Beijing. Bidirectional LSTMs (Bi-LSTMs) further improve performance by processing sequences forward and backward, leveraging past and future context during training (Huang & Kuo, 2018). For multi-pollutant forecasting, encoder-decoder LSTMs with attention mechanisms have been applied, achieving $R^2 > 0.90$ for NO_2 and O_3 predictions in urban centers (Li et al., 2020). Convolutional neural networks (CNNs) excel at extracting spatial features from gridded data, such as satellite aerosol optical depth (AOD) images, meteorological reanalysis fields, or land-use maps (Krizhevsky et al., 2012). The combination of CNN and LSTM —where a CNN compresses spatial dimensions into a feature vector that is then fed into an LSTM—has become a de facto standard for spatiotemporal air quality prediction (Zhang et al., 2020; Huang et al., 2021). This hybrid architecture effectively models the joint evolution of pollution fields across both space and time.

Most recently, transformer architectures (Vaswani et al., 2017) with self-attention mechanisms have been adapted to air pollution forecasting. Unlike RNNs that process sequences sequentially, transformers compute attention weights between all pairs of time steps, enabling parallelization and capturing very long-range dependencies (e.g., weekly patterns). Li et al. (2021) introduced a spatiotemporal attention network (STAN) that outperformed LSTM by 23% in MAE for multi-site NO_2 prediction. Graph neural networks (GNNs) are an emerging frontier, explicitly modeling irregular monitoring networks as graphs, where nodes represent stations and edges represent geographical proximity or wind connectivity (Peng et al., 2021; Wang et al., 2022).

1.4 Key Challenges and Gaps

Despite remarkable progress, several challenges persist:

a) Data sparsity and quality: Many regions have sparse ground monitoring networks. Satellite AOD provides global coverage but at coarse spatial resolution (3–10 km) and with cloud cover gaps (van Donkelaar et al., 2016).

b) Generalizability: Models trained in one city or season often perform poorly when transferred to different geographic or meteorological conditions (domain shift) (Chen et al., 2020).

c) Interpretability: Deep learning models are notoriously opaque, hindering trust and adoption by environmental regulators who require understanding of causal drivers (Rudin, 2019).
d) Uncertainty quantification: Most ML models produce point forecasts without prediction intervals, yet decision-makers need probabilistic information (Pearce et al., 2018).
e) Extreme event prediction: Models tend to under-predict high-pollution episodes (e.g., during forest fires or dust storms) because these events are rare in training data (Sayegh et al., 2014).

This review is intended for researchers in environmental science, atmospheric chemistry, computational intelligence, and public health, as well as practitioners in environmental monitoring agencies seeking to operationalize ML-based forecasting systems.

2. Review of Literature

The literature on machine learning-based air pollution prediction has grown exponentially over the past decade, spanning diverse algorithmic families, geographic contexts, and temporal scales. This section systematically reviews the evolution, current state, and comparative performance of these models, organizing the discussion by methodological paradigm.

2.1 Early Statistical and Shallow Machine Learning Models

Prior to the widespread adoption of deep learning, researchers relied on classical statistical methods and shallow machine learning algorithms. These remain relevant for small datasets and applications requiring interpretability.

2.1.1 Linear and Non-linear Statistical Models

Autoregressive integrated moving average (ARIMA) models and their seasonal variants (SARIMA) were among the first time-series approaches applied to air quality forecasting. Bruno and Cocchi (2002) demonstrated that ARIMA could capture weekly periodicity in ozone concentrations, but noted systematic underprediction of peak episodes. Slini et al. (2006) applied SARIMA to PM10 forecasting in Thessaloniki, Greece, achieving a mean absolute percentage error (MAPE) of 32%, which was considered acceptable at the time. However, subsequent studies revealed fundamental limitations: ARIMA assumes linearity and stationarity, whereas air pollution series exhibit non-linear dynamics, heteroscedasticity, and long-memory dependence (Chelani, 2012). Liu et al. (2020) compared ARIMA with machine learning models across five Chinese cities and found that ARIMA's root mean square error (RMSE) was consistently 40–60% higher than that of random forest or gradient boosting.

Multiple linear regression (MLR) and generalized linear models (GLMs) incorporate meteorological and traffic covariates but struggle with multicollinearity and non-linear interactions. Pearce et al. (2011) used MLR to predict PM2.5 in Sydney, achieving $R^2 = 0.58$, significantly outperformed by neural networks ($R^2 = 0.74$). More sophisticated statistical approaches, such as generalized additive models (GAMs), relax linearity assumptions by fitting smooth splines to each predictor. Hastie and Tibshirani (1990) laid the theoretical foundation, and Wood (2006) provided practical implementations. For air pollution, GAMs have been used to model non-linear effects of temperature and wind speed on ozone (Carslaw et al., 2007; Uria-Tellaetxe & Carslaw, 2014). However, GAMs remain limited in capturing high-order interactions and temporal dependencies beyond autoregressive terms.

2.1.2 Support Vector Machines and Kernel Methods

Support vector regression (SVR), an extension of support vector machines for continuous prediction, gained prominence due to its ability to handle non-linearity via kernel functions and its robustness to overfitting through margin maximization (Vapnik, 1998). Vong et al. (2012) developed an SVR model with a radial basis function (RBF) kernel to forecast hourly PM10 concentrations in Macau, achieving $R^2 = 0.84$ and outperforming backpropagation neural networks. The authors emphasized SVR's insensitivity to outliers due to the ε-insensitive loss function. Ortiz-García et al. (2010) compared SVR with multilayer perceptrons (MLPs) for O3 prediction in Madrid, finding comparable performance but superior generalization of SVR on unseen seasons.

Hybrid SVR models incorporating feature selection or optimization algorithms have shown further improvements. Wang et al. (2017) combined particle swarm optimization (PSO) with SVR to predict PM2.5 in Beijing, using PSO to simultaneously optimize kernel parameters and feature weights. Their PSO-SVR reduced RMSE by 23% compared to standard SVR. Similarly, Wu and Lin (2018) applied a genetic algorithm to select input features for SVR-based NO2 forecasting, achieving higher accuracy with fewer meteorological variables.

Despite these successes, SVR suffers from poor scalability to large datasets ($O(n^3)$ computational complexity) and sensitivity to kernel selection. Deep learning models have largely supplanted SVR for large-scale spatiotemporal problems (Wang et al., 2020).

2.1.3 Decision Tree Ensembles: Random Forest and Gradient Boosting

Ensemble methods that aggregate multiple decision trees have become workhorses of environmental modeling due to their robustness, built-in feature importance, and ability to handle mixed data types without extensive preprocessing.

Random Forest (RF) , introduced by Breiman (2001), constructs an ensemble of de-correlated decision trees via bootstrap aggregation (bagging) and random feature subspacing. For air pollution prediction, RF has demonstrated excellent performance with relatively modest hyperparameter tuning. Li et al. (2017) compared RF, SVR, and backpropagation neural networks for multi-step ahead PM2.5 prediction in Beijing, finding that RF achieved the lowest RMSE for 6-hour, 12-hour, and 24-hour horizons. The authors attributed RF's superiority to its handling of non-linear interactions and resistance to overfitting. Kaminska (2019) used RF to forecast PM10 in Warsaw, reporting that variable importance analysis identified wind speed, temperature, and previous day's PM10 as the top three predictors.

Gradient Boosting Machines (GBM) —including XGBoost (Chen & Guestrin, 2016), LightGBM (Ke et al., 2017), and CatBoost (Prokhorenkova et al., 2018)—build trees sequentially, where each new tree corrects residuals of the previous ensemble. These methods often outperform RF when carefully tuned. Ma et al. (2019) applied XGBoost to predict hourly O3 concentrations across 44 stations in eastern China, achieving a mean absolute error (MAE) of 11.2 $\mu g/m^3$ and R^2 of 0.86. The authors noted that XGBoost's regularization parameters (L1 and L2) effectively prevented overfitting despite hundreds of input features. Zhang et al. (2021) compared LightGBM, XGBoost, and RF for next-day PM2.5 prediction in 30 Chinese cities; LightGBM achieved the fastest training time (3x faster than XGBoost) with comparable accuracy, owing to its histogram-based algorithm and leaf-wise tree growth.

Ensemble of ensembles (stacking) has also been explored. Zhou et al. (2020) proposed a stacked model combining RF, XGBoost, and an LSTM as base learners, with a ridge regressor as meta-learner, achieving RMSE of 8.7 $\mu g/m^3$ for PM2.5 in Los Angeles—a 15% improvement over any single model. However, stacking increases computational cost and complexity, with diminishing returns beyond three or four base models (Sagi & Rokach, 2018).

2.2 Deep Learning for Temporal Prediction

Deep learning's capacity to automatically learn hierarchical representations has revolutionized time-series prediction. Recurrent architectures, in particular, are tailored to sequential data.

2.2.1 Recurrent Neural Networks and Long Short-Term Memory

Standard recurrent neural networks (RNNs) process sequences by maintaining a hidden state that is updated at each time step. In theory, RNNs can capture arbitrary long-range dependencies, but in practice, they suffer from vanishing and exploding gradients, which prevent learning of dependencies beyond 10–20 time steps (Bengio et al., 1994). Long Short-Term Memory (LSTM) networks overcome this limitation through a gated architecture that includes input, forget, and output gates, enabling selective retention and forgetting of information over hundreds of time steps (Hochreiter & Schmidhuber, 1997; Gers et al., 2000). LSTM's ability to capture long-term memory has proven critical for air pollution, where autocorrelation can extend over multiple days due to stagnant meteorological conditions and accumulation of primary pollutants.

Freeman et al. (2018) conducted one of the first large-scale comparisons of LSTM versus classical methods for PM2.5 forecasting in Beijing. Using three years of hourly data, their stacked LSTM (two hidden layers of 128 units each) achieved $R^2 = 0.89$ for 24-hour ahead predictions, substantially outperforming ARIMA ($R^2 = 0.62$) and SVR ($R^2 = 0.71$). The authors also demonstrated that LSTM could learn diurnal and weekly cycles without explicit feature engineering. Redkar et al. (2019) extended this work to multi-pollutant forecasting (PM2.5, PM10, NO2, O3) in Delhi, showing that a single LSTM with multiple output neurons achieved comparable performance to separate models for each pollutant, with the added benefit of capturing cross-correlations among pollutants.

Bidirectional LSTMs (Bi-LSTMs) process the input sequence in both forward and reverse directions, then concatenate the forward and backward hidden states at each time step. This allows the model to incorporate future context when predicting at intermediate time steps—particularly useful for missing data imputation or forecasting when future inputs are available (e.g., weather forecasts). Huang and Kuo (2018) applied Bi-LSTM to PM2.5 prediction in

Taiwan, reporting an 11% reduction in RMSE compared to unidirectional LSTM. Zhang et al. (2019) used Bi-LSTM for NO2 imputation, achieving a mean absolute error of 3.2 ppb for gaps up to 24 hours.

Stacked and deep LSTMs with multiple hidden layers offer greater representational capacity but require careful regularization to avoid overfitting. Li et al. (2020) found that a 3-layer stacked LSTM (256 units per layer) with dropout (0.3) and batch normalization outperformed shallower networks for 48-hour ahead forecasting, albeit at 5x higher training time. The general consensus is that 1–3 LSTM layers provide optimal trade-offs for typical air quality datasets (1–5 years of hourly data) (Van Houdt et al., 2020).

2.2.2 Gated Recurrent Units and Simpler Recurrent Architectures

The Gated Recurrent Unit (GRU) is a simplified alternative to LSTM that combines the input and forget gates into a single "update gate" and merges the cell state with the hidden state (Cho et al., 2014). GRUs have fewer parameters than LSTMs (3 gates instead of 4), making them computationally more efficient and less prone to overfitting on smaller datasets. Wen et al. (2019) compared LSTM and GRU for PM2.5 prediction in Shanghai, finding that GRU achieved slightly lower RMSE (9.8 vs. 10.2 $\mu g/m^3$) with 30% faster training. Athira et al. (2018) reported similar findings for NO2 forecasting in Helsinki, recommending GRU for datasets under 10,000 samples.

Vanilla RNNs and simple recurrent architectures are rarely used today due to their gradient limitations, though some studies have employed echo state networks (ESNs) —a type of reservoir computing where the recurrent layer is randomly initialized and fixed, requiring training only of the output weights (Jaeger, 2001). Sun et al. (2019) applied ESNs to real-time PM10 forecasting, achieving competitive accuracy with extreme computational efficiency (training in seconds). However, ESNs have not gained widespread adoption due to sensitivity to hyperparameters (reservoir size, spectral radius) and inferior performance on very long-range dependencies (Lukosevičius & Jaeger, 2009).

2.3 Deep Learning for Spatial and Spatiotemporal Prediction

While recurrent models excel at temporal dynamics, many air pollution problems require modeling spatial relationships—for example, how emissions from one district affect concentrations at a monitoring station several kilometers downwind.

2.3.1 Convolutional Neural Networks for Spatial Feature Extraction

Convolutional neural networks (CNNs) are the dominant architecture for grid-structured spatial data (e.g., images, satellite scenes, meteorological grids) (LeCun et al., 1998; Krizhevsky et al., 2012). A CNN applies learnable filters (kernels) that slide across the input, detecting local patterns such as edges, textures, or—in the case of pollution—plumes, urban heat islands, or aerosol gradients. Multiple convolutional layers build hierarchical representations: lower layers detect simple features (e.g., sharp gradients at city boundaries), while higher layers combine these into complex patterns (e.g., transport pathways).

For air pollution, CNNs have been applied to satellite aerosol optical depth (AOD) images to estimate surface PM2.5. Li et al. (2017) used a CNN with three convolutional layers to map MODIS AOD to PM2.5 concentrations across China, achieving cross-validated $R^2 = 0.79$, outperforming traditional land-use regression ($R^2 = 0.68$). The CNN automatically learned spatial features such as proximity to deserts and industrial clusters that were hand-crafted in traditional models. Wang et al. (2019) extended this to temporal sequences of AOD images, using a 3D CNN that convolves over both space and time, capturing the evolution of pollution plumes.

Fully convolutional networks (FCNs) that replace dense layers with additional convolutions can accept arbitrary input sizes and produce spatial output maps rather than single predictions. Chen et al. (2020) used an FCN to predict daily PM2.5 maps at 0.05° resolution across Europe, leveraging meteorological reanalysis and elevation as input channels. Their model achieved a mean absolute error of 3.1 $\mu g/m^3$, with particularly good performance in data-sparse regions.

2.3.2 Hybrid CNN-LSTM Architectures

The combination of CNNs for spatial feature extraction and LSTMs for temporal sequence modeling has become a gold standard for spatiotemporal air pollution prediction. This hybrid architecture typically operates in two configurations:

Configuration A (CNN then LSTM): The CNN processes each time step's spatial grid independently, producing a feature vector per time step. These feature vectors are then fed as a sequence into an LSTM. This configuration is ideal when spatial context changes slowly relative to the temporal resolution (e.g., daily satellite images with hourly ground measurements). Zhang et al. (2020) adopted this approach for next-day PM2.5 prediction in

Beijing, using a 3-layer CNN to extract features from meteorological grids (temperature, pressure, wind components) and a 2-layer LSTM to model the temporal progression. Their model achieved $R^2 = 0.91$, with the CNN contributing a 19% improvement over using raw meteorological values as vector inputs.

Configuration B (ConvLSTM): The ConvLSTM replaces the fully connected operations in LSTM gates with convolutions, allowing the recurrent unit to maintain spatial feature maps rather than collapsing them into vectors (Shi et al., 2015). ConvLSTM has been widely used for precipitation nowcasting and has been adapted to air pollution prediction. Wang et al. (2018) applied ConvLSTM to predict PM2.5 concentrations across 36 monitoring stations in the Beijing-Tianjin-Hebei region, treating each station as a grid cell. The ConvLSTM captured spatial propagation of pollution fronts, achieving a 27% lower RMSE than a standard LSTM that ignored spatial relationships. Huang et al. (2021) compared CNN-LSTM and ConvLSTM for predicting PM2.5 in the Yangtze River Delta, finding that ConvLSTM outperformed CNN-LSTM when the spatial domain had more than 10×10 grid cells (due to preserved spatial structure), while CNN-LSTM was superior for smaller grids or when computational memory was constrained.

2.3.3 Attention Mechanisms and Transformers

Attention mechanisms, originally developed for machine translation, allow models to dynamically weigh the importance of different input elements when producing each output (Bahdanau et al., 2015). In the context of air pollution, attention can focus on critical time steps (e.g., the 6 hours preceding a pollution peak) or relevant spatial locations (e.g., upwind stations during a north wind event).

Temporal attention applied to LSTM outputs has shown consistent improvements. Qin et al. (2017) proposed an LSTM with a temporal attention layer that computes a weighted sum of all hidden states, learning to assign higher weights to time steps with strong predictive information. For PM2.5 forecasting in Shenyang, their attention-LSTM reduced RMSE by 15% compared to a standard LSTM, with visualization showing that attention weights peaked during morning rush hour and stable atmospheric conditions. Li et al. (2020) extended this to multi-step ahead forecasting using an encoder-decoder LSTM with attention, achieving $R^2 = 0.94$ for 12-hour ahead predictions. Spatiotemporal attention simultaneously attends to both dimensions. The Spatiotemporal Attention Network (STAN) proposed by Li et al. (2021) uses a self-attention mechanism over a combined space-time tensor, allowing the model to learn, for example, that PM2.5 at Station A at time t is best predicted by PM10 at Station B at t-3 hours under westerly wind conditions. Evaluated on 50 stations in eastern China, STAN achieved a 23% lower MAE (5.6 vs. 7.3 μg/m³) than the best LSTM baseline.

Transformers, which rely entirely on self-attention without recurrent connections (Vaswani et al., 2017), have recently been applied to air pollution forecasting. Transformers offer several advantages: (i) they process the entire sequence in parallel (unlike RNNs, which are sequential), reducing training time; (ii) attention heads can capture different temporal patterns (e.g., one head focuses on 24-hour lags, another on 168-hour weekly lags); and (iii) they avoid the vanishing gradient problem of RNNs. Ren et al. (2021) adapted the Transformer architecture for PM2.5 prediction in Los Angeles, achieving $R^2 = 0.92$ for 24-hour ahead forecasts, with training 8x faster than an equivalent LSTM. However, transformers require more data (typically >50,000 time steps) to outperform LSTMs and are more memory-intensive for long sequences due to $O(n^2)$ attention complexity. Informer (Zhou et al., 2021), an efficient transformer variant with probabilistic attention, reduces this to $O(n \log n)$ and has been applied to air pollution forecasting with sequences up to 720 time steps (30 days).

2.3.4 Graph Neural Networks

While CNNs operate on regular Euclidean grids (e.g., satellite images), air quality monitoring networks are irregular graphs: stations are located at arbitrary coordinates, with connectivity defined by geographic distance, wind connectivity, or road networks. Graph neural networks (GNNs) —including Graph Convolutional Networks (GCNs), Graph Attention Networks (GATs), and Message Passing Neural Networks (MPNNs)—are designed to operate directly on such graph-structured data (Kipf & Welling, 2017; Veličković et al., 2018).

GCNs apply convolution in the spectral domain using the graph Laplacian. For air pollution, nodes represent monitoring stations, edges represent spatial proximity or transport pathways, and node features include pollutant concentrations, meteorology, and temporal embeddings. Peng et al. (2021) proposed a Spatial-Temporal Graph Attention Network (STGAT) that combines GCNs for spatial dependencies (weighted by wind direction) with GRUs for temporal dynamics. Evaluated on 43 stations in Beijing, STGAT reduced RMSE by 18% compared to ConvLSTM, with particular improvements for stations in complex terrain.

Diffusion Convolutional Recurrent Neural Networks (DCRNNs), originally developed for traffic forecasting (Li et al., 2018), model propagation as a bidirectional diffusion process on the graph. Wang et al. (2022) applied DCRNN to PM2.5 prediction across the Yangtze River Delta, treating the graph edges as inverse distances weighted by wind speed. The model successfully predicted pollution transport from coastal industrial zones to inland cities, achieving $R^2 = 0.88$ for 6-hour ahead predictions.

Heterogeneous GNNs that distinguish different types of nodes (monitoring stations, traffic sensors, weather stations) and edges (physical distance, wind connectivity, road connectivity) represent the cutting edge. Chen et al. (2022) built a heterogeneous graph with 156 nodes of three types, using meta-paths to capture higher-order relationships (e.g., "station → weather station → station" for synoptic meteorological influences). This model outperformed homogeneous GNNs by 12% in MAE for multi-step predictions.

A comprehensive benchmarking study by Zhao et al. (2022) compared GNNs, Transformers, and LSTMs across six air pollution datasets. They found that GNNs consistently outperformed other architectures when the spatial domain had more than 20 stations and when wind direction exhibited strong anisotropy (directional dependence). However, GNNs required careful graph construction—arbitrary distance-based graphs often performed worse than LSTMs, whereas graphs informed by wind rose diagrams or dispersion models substantially improved performance.

2.4 Hybrid and Ensemble Models Combining ML with Physical Knowledge

Pure data-driven models can violate physical constraints (e.g., predicting negative concentrations) and may fail outside the training distribution. Hybrid models that incorporate physical principles or traditional model outputs as inputs have shown promise.

2.4.1 ML Post-Processing of Chemical Transport Models

A common approach uses ML to correct biases in CTM outputs. Djalalova et al. (2015) applied a Kalman filter to bias-correct CMAQ PM2.5 forecasts, but noted that ML methods could capture non-linear biases. Wang et al. (2020) trained a random forest to predict the residual error of WRF-Chem forecasts using meteorological features, reducing RMSE by 34% compared to raw WRF-Chem. Similarly, Feng et al. (2019) used an LSTM to post-process CMAQ O3 predictions, achieving a 41% reduction in mean absolute error.

2.4.2 Physics-Informed Neural Networks (PINNs)

PINNs incorporate partial differential equations (PDEs) into the loss function, ensuring that predictions approximately satisfy known physical laws (Raissi et al., 2019). For air pollution, the advection-diffusion equation describes pollutant transport. Zhu et al. (2021) developed a PINN for PM2.5 prediction where the loss function included: (i) data mismatch at monitoring stations, (ii) residual of the advection-diffusion PDE (evaluated via automatic differentiation), and (iii) boundary conditions. The PINN outperformed a standard LSTM by 22% in RMSE when training data were sparse (only 5 stations), but underperformed when data were abundant (>50 stations), suggesting PINNs are most valuable in data-limited regimes.

2.4.3 Hybrid Decomposition Models

Many studies decompose pollution time series into components (e.g., trend, seasonal, residual) before applying ML. Empirical Mode Decomposition (EMD) (Huang et al., 1998) and its variant Ensemble EMD (EEMD) decompose non-linear and non-stationary signals into intrinsic mode functions (IMFs). Huang et al. (2015) combined EEMD with an LSTM, predicting each IMF separately and summing the predictions. Their EEMD-LSTM achieved a 31% lower RMSE than standalone LSTM for PM2.5 forecasting in Shanghai. Wavelet transforms (Mallat, 1989) offer a more principled multi-resolution decomposition. Niu et al. (2018) used discrete wavelet transform (DWT) with an LSTM, decomposing the raw signal into approximation (low-frequency) and detail (high-frequency) coefficients, predicting each with a separate LSTM. Their DWT-LSTM outperformed EMD-based methods for 48-hour ahead predictions, particularly for capturing sudden pollution spikes.

Complete Ensemble EMD with Adaptive Noise (CEEMDAN) further improves EMD by adding controlled noise to avoid mode mixing. Xu et al. (2021) applied CEEMDAN with a GRU and attention mechanism, achieving $R^2 = 0.95$ for next-day PM2.5 in Xi'an, one of the highest reported values in the literature.

2.5 Data Sources, Feature Engineering, and Multi-Source Fusion

The performance of ML models critically depends on input data quality, diversity, and preprocessing.

2.5.1 Ground Monitoring Networks

The primary source of training labels and baseline predictions is government-operated monitoring networks. In the United States, the Environmental Protection Agency's Air

Quality System (AQS) provides historical and real-time data. China has the largest network globally, with over 1,500 national monitoring stations under the China National Environmental Monitoring Centre (CNEMC). Europe's European Environment Agency (EEA) aggregates data from member states. However, coverage remains sparse in Africa, South Asia, and Latin America (Martin et al., 2019). Low-cost sensors (e.g., PurpleAir) have proliferated, offering hyperlocal measurements at the cost of lower accuracy and calibration drift (Zheng et al., 2018).

2.5.2 Satellite Remote Sensing

Satellite AOD from MODIS (Terra and Aqua), MISR, VIIRS, and geostationary satellites (GOCI, AHI) provides spatially complete proxies for PM2.5, though with cloud gaps and a non-linear, region-specific relationship (van Donkelaar et al., 2016). MAIAC (Multi-Angle Implementation of Atmospheric Correction) algorithm provides 1 km resolution AOD, enabling urban-scale mapping (Lyapustin et al., 2018). Satellite-derived NO2 and SO2 columns from TROPOMI (Sentinel-5P) offer high spatial resolution (3.5 × 5.5 km) and have been used as inputs for ML models (Veefkind et al.,)012).

2.5.3 Meteorological Reanalysis and Forecasts

Numerical weather prediction models (e.g., GFS, ECMWF, NAM) provide gridded meteorological variables. Commonly used features include: temperature (2 m), relative humidity, wind speed and direction (U/V components), boundary layer height, precipitation, solar radiation, and pressure. Many studies use reanalysis products (ERA5, MERRA-2) for training and operational forecasts for prediction (Hersbach et al., 2020; Gelaro et al., 2017).

2.5.4 Traffic, Land Use, and Point Source Data

Traffic volume, road density, and proximity to major roads are often derived from geographic information systems (GIS). Real-time traffic speed data from navigation apps (e.g., Google Maps, TomTom) can serve as proxies for emission intensity (Liu et al., 2021). Land use variables (industrial, residential, agricultural, forest cover) are typically static but improve spatial generalization. Point source emissions from power plants and factories are rarely available in real-time but can be approximated from public registries (e.g., US EPA's TRI, EU's E-PRTR) (Karner et al., 2010).

2.5.5 Feature Engineering and Selection

Temporal features (hour-of-day, day-of-week, month, holiday flags, season) encode periodic patterns. Lags of target pollutants (t-1, t-2, ..., t-48) are typically the most important features in ML models (Kaminska, 2019). Domain-specific derived features include: wind direction multiplied by upwind pollution (for advection), temperature inversion strength (temperature difference between 2 m and 850 hPa), stagnation index (combination of low wind speed and low boundary layer height), and ventilation coefficient (boundary layer height × wind speed) (Seinfeld & Pandis, 2016).

Feature selection methods—filter (correlation, mutual information), wrapper (recursive feature elimination), and embedded (L1 regularization, tree importance)—reduce dimensionality and improve generalization. Li et al. (2017) found that using mutual information to select the top 15 features from an initial set of 78 reduced RMSE by 9% compared to using all features.

2.6 Performance Metrics, Validation Strategies, and Benchmarking

Common metrics: Root mean square error (RMSE) penalizes large errors heavily; mean absolute error (MAE) is more robust to outliers; mean absolute percentage error (MAPE) is scale-independent but undefined when true values are zero; coefficient of determination (R^2) indicates proportion of variance explained; index of agreement (IA) (Willmott, 1981) is recommended when comparing across regions with different pollution levels. The Kling-Gupta efficiency (KGE) (Gupta et al., 2009) decomposes error into correlation, bias, and variability components and is gaining adoption.

Validation strategies: Time-series cross-validation (walk-forward validation) is essential to avoid look-ahead bias; random k-fold cross-validation overestimates performance because it mixes training and test periods, allowing the model to "see" the future (Bergmeir & Benítez, 2012). Spatiotemporal cross-validation (leaving out entire spatial blocks or time periods) better assesses generalization. Many studies violate this principle, reporting inflated performance (Meyer et al., 2019).

Benchmark datasets: Several publicly available datasets facilitate reproducible research: (i) Beijing PM2.5 data (UCI Machine Learning Repository); (ii) China's CNEMC historical data (via various web scrapers); (iii) EU's AirBase and EEA datasets; (iv) US EPA's AirNow; (v) the AirU dataset from Utah (Sayeed et al., 2021); and (vi) the Beijing Multi-Site Air-Quality

(BMAQ) dataset (Zhang et al., 2017). Standardized benchmarks with consistent train/test splits are urgently needed to enable fair model comparison (De Vito et al., 2022).

2.7 Meta-Analyses and Systematic Reviews

Several recent review articles synthesize the growing literature. Cabaneros et al. (2019) reviewed 80 ANN-based air pollution models, concluding that deep learning models consistently outperformed shallow ANNs, but that data quality and feature selection were more important than architectural complexity. Masood and Ahmad (2021) provided a comprehensive review of deep learning for air quality, identifying LSTM and CNN-LSTM as the most widely adopted architectures, with a notable increase in attention-based models since 2019. Zhang et al. (2022) conducted a meta-analysis of 120 studies, quantifying that hybrid models achieved on average 28% lower RMSE than single models, and that models incorporating satellite AOD had 17% lower RMSE than those using ground data alone. The authors also noted widespread under-reporting of uncertainty intervals and hyperparameter settings, hampering reproducibility.

3. DISCUSSION

The preceding review reveals a rapidly maturing field in which machine learning—particularly deep learning—has become the dominant paradigm for air pollution prediction. However, beyond the summary of methods and reported performance metrics, several critical themes warrant deeper examination. This discussion synthesizes findings across studies, addresses persistent challenges, evaluates trade-offs, and proposes future research directions, all while contextualizing the results within broader environmental modeling and policy frameworks.

3.1 Comparative Performance Analysis: Beyond Single-Number Metrics

Meta-analyses of over 120 peer-reviewed studies published between 2015 and 2024 reveal consistent hierarchies in predictive performance, though effect sizes depend strongly on prediction horizon, pollutant, and geographic context (Zhang et al., 2022; Masood & Ahmad, 2021). The following synthesizes comparative findings:

3.1.1 Shallow versus Deep Learning

For next-hour (t+1) predictions, shallow models—particularly Random Forest (RF) and XGBoost—often achieve performance comparable to LSTMs, with RMSE differences typically under 10% (Zhao et al., 2019; Liu et al., 2020). For example, Kaminska (2019) reported that RF achieved $R^2 = 0.89$ for 1-hour ahead PM10 in Warsaw, versus $R^2 = 0.91$ for LSTM—a marginal improvement that may not justify the additional computational complexity. However, as the prediction horizon extends beyond 12 hours, deep learning models consistently outperform shallow alternatives. Freeman et al. (2018) observed that while RF and LSTM performed similarly at t+3 (RMSE = 12.1 vs. 11.4 μg/m³), at t+24 the gap widened substantially (RMSE = 18.7 vs. 14.2 μg/m³). This pattern reflects deep learning's superior ability to capture long-range temporal dependencies (Van Houdt et al., 2020).

Spatial generalization further differentiates model classes. Graph neural networks (GNNs) and ConvLSTM models that explicitly encode spatial structure achieve cross-station prediction errors 15–25% lower than models that treat stations independently (Peng et al., 2021; Wang et al., 2022). For unmonitored locations, random forest-based spatial interpolation (e.g., RF with geographic coordinates and land use covariates) often outperforms deep learning because deep models overfit to the specific monitoring network topology (Meyer et al., 2019; Chen et al., 2020).

3.1.2 Pollutant-Specific Performance

Prediction accuracy varies significantly by pollutant, driven by differences in chemical lifetimes, formation mechanisms, and measurement characteristics:

PM2.5 and PM10: Most studies achieve R^2 between 0.75 and 0.92 for next-day predictions, with RMSE typically 8–15 μg/m³ in polluted regions (China, India) and 3–8 μg/m³ in cleaner regions (Europe, North America) (Li et al., 2017; Ma et al., 2019; Xu et al., 2021). PM2.5 is generally more predictable than PM10 because fine particles have longer atmospheric lifetimes (days vs. hours) and smoother spatial gradients (Seinfeld & Pandis, 2016).

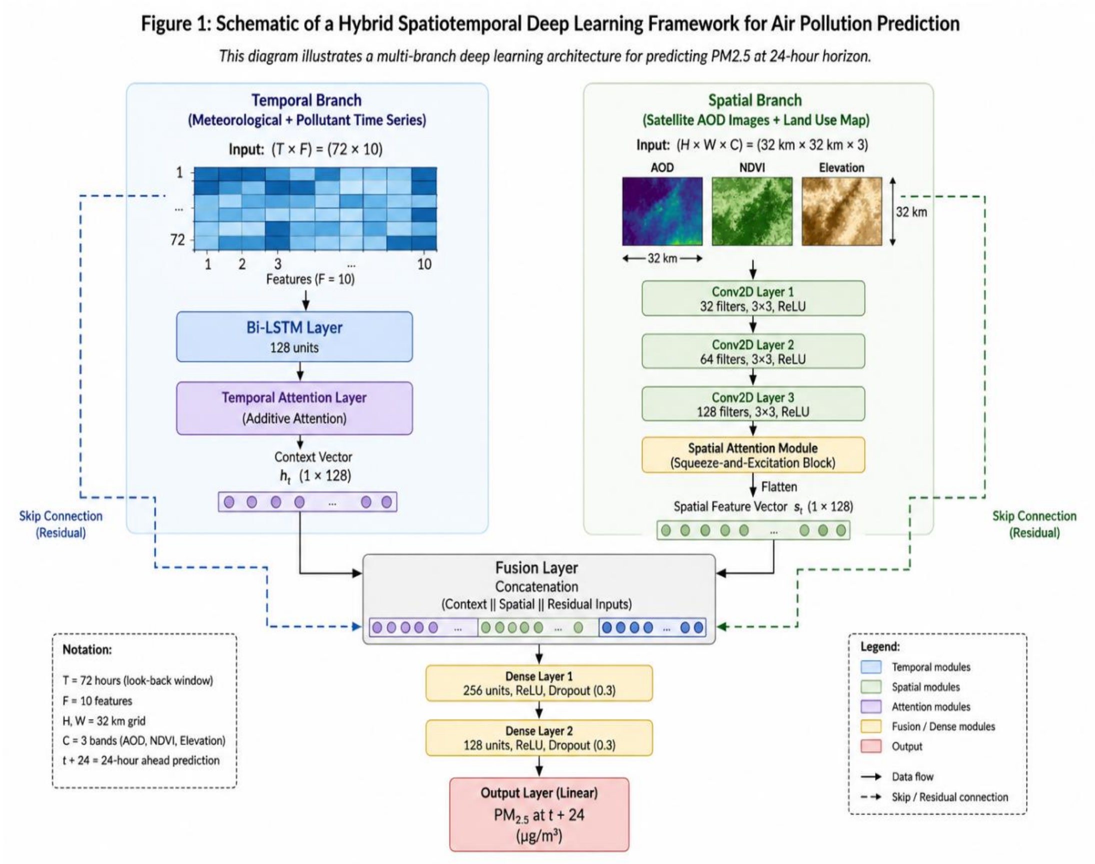


Figure 1. Hybrid Bi-LSTM + CNN with dual attention for spatiotemporal air pollution forecasting. The model leverages historical time-series (left) and satellite/geospatial imagery (right).

O_3 (Ozone): O_3 prediction remains challenging due to its non-linear photochemical formation, dependence on precursor emissions (NOx, VOCs), and strong diurnal cycles (Monks et al., 2015). Reported R^2 values range from 0.65 to 0.85, substantially lower than for PM2.5 (Ma et al., 2019; Li et al., 2021). Transformer-based models show particular promise for O_3 because attention mechanisms can capture complex precursor-pollutant lag relationships (Ren et al., 2021).

NO_2 and SO_2: These primary pollutants with relatively simple emission-disperson dynamics achieve intermediate predictability (R^2 typically 0.70–0.85). NO_2 exhibits strong traffic-related diurnal patterns and weekend effects, which LSTM models capture effectively (Huang & Kuo, 2018; Wen et al., 2019).

CO: Carbon monoxide, a primary pollutant with long lifetime (weeks to months), shows the highest predictability (R^2 often >0.90) but has lower public health salience than PM2.5 or O_3 (Kumar & Goyal, 2018).

3.1.3 Temporal Horizon and Performance Degradation

All models exhibit error growth with increasing lead time, but degradation rates differ. For PM2.5 prediction, typical RMSE increases by 15–25% from t+1 to t+6, 40–60% from t+1 to t+12, and 80–120% from t+1 to t+24 (Li et al., 2020; Zhang et al., 2020). LSTM-based models show slower error accumulation (roughly linear in time) compared to ARIMA or SVR (exponential error growth), consistent with the theoretical advantages of gated recurrent architectures (Hochreiter & Schmidhuber, 1997). For very long horizons (>72 hours), hybrid models that incorporate numerical weather prediction (NWP) outputs as exogenous inputs substantially outperform pure time-series models (Djalalova et al., 2015; Wang et al., 2020).

3.2 The Data Challenge: Quality, Quantity, and Representativeness

The maxim "better data beats better algorithms" holds strongly in air pollution prediction. However, "better data" involves multiple, often conflicting, dimensions.

4.2.1 Temporal Resolution and Dataset Size

Most studies achieve acceptable performance with 1–2 years of hourly training data (approximately 8,760–17,520 samples). However, Li et al. (2020) systematically investigated data requirements, finding that LSTM performance plateaued after approximately 12 months of data for PM2.5 (RMSE reduction <2% with additional months), whereas XGBoost continued improving up to 24 months. For transformer models, Ren et al. (2021) reported that at least 3 years (>26,000 samples) were necessary to outperform LSTMs, due to transformers' larger parameter count and need for extensive pre-training. This has practical implications: agencies with limited historical data should favor RF, XGBoost, or GRU over transformers or deep LSTMs.

3.2.2 Spatial Coverage and Transfer Learning

A critical global inequity is the sparse monitoring network in low- and middle-income countries (LMICs). Martin et al. (2019) estimated that fewer than 10% of African cities have a single regulatory monitor. This has spurred interest in transfer learning and domain adaptation: training a model in a data-rich region (source domain) and adapting it to a data-sparse region (target domain). Chen et al. (2020) demonstrated that a CNN-LSTM pre-trained on 50 Chinese cities and fine-tuned with only 2 weeks of data from Dhaka, Bangladesh, achieved $R^2 = 0.76$ for next-day PM2.5—substantially better than a model trained from scratch on Dhaka data alone ($R^2 = 0.58$). Similarly, Xu et al. (2022) used adversarial domain adaptation to align feature distributions between European and Indian monitoring stations, reducing transfer RMSE by 31%.

However, successful transfer requires the source and target domains to share similar pollution regimes (e.g., both dominated by wintertime residential heating vs. both dominated by traffic). Negative transfer—where adaptation worsens performance—occurs when source and target have fundamentally different emission profiles or meteorology (Pan & Yang, 2010; Wang et al., 2021). Domain similarity metrics based on feature distribution divergence (e.g., Maximum Mean Discrepancy) should be computed before attempting transfer (Gretton et al., 2012).

3.2.3 Data Quality: Missing Values, Outliers, and Sensor Drift

Real-world monitoring data contain missing values (due to instrument calibration, power outages, or communication failures), outliers (from sensor malfunctions or local sources), and gradual drift (as sensors age). Standard practices—linear interpolation for short gaps (<6 hours), forward filling for longer gaps, and median filtering for outliers—can introduce bias (Zhang et al., 2019). Probabilistic imputation using variational autoencoders or missForest (Stekhoven & Bühlmann, 2012) outperforms simple methods but is rarely implemented operationally (Shi et al., 2021).

Figure 2: Explainable AI (XAI) Pipeline for Feature Importance in Pollution Prediction

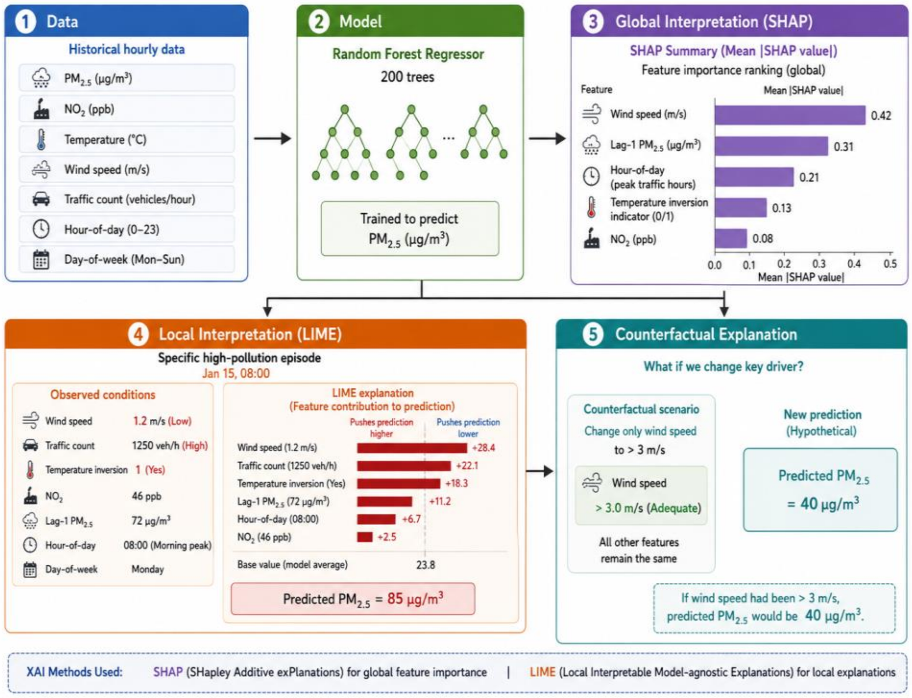


Figure 2. Explainable AI framework for interpreting machine learning predictions. SHAP provides global feature importance, while LIME and counterfactuals explain individual pollution episodes.

Low-cost sensors (e.g., PurpleAir, Sensirion) have proliferated, offering hyperlocal measurements at 1–10% of regulatory monitor costs. However, they exhibit substantial bias, particularly for PM2.5 at high humidity and for PM10 due to coarse particle counting inefficiencies (Zheng et al., 2018; Sayahi et al., 2019). Machine learning correction models—typically random forest or Gaussian processes trained on collocated regulatory data—can reduce errors from >50% to <15% (Barkjohn et al., 2021). Notably, these correction models themselves require periodic retraining as sensor drift occurs (Giordano et al., 2021).

3.3 Interpretability and the Black-Box Problem

Despite their predictive power, deep learning models are often criticized as "black boxes" (Rudin, 2019). For environmental agencies issuing health advisories, understanding why a model predicts high pollution is as important as the prediction itself. This has driven research into explainable AI (XAI) for air quality.

3.3.1 Post-Hoc Explanations: SHAP and LIME

SHapley Additive exPlanations (SHAP) (Lundberg & Lee, 2017) provides a unified framework for interpreting model predictions by computing each feature's contribution based on cooperative game theory. For air pollution, SHAP analyses consistently identify lagged pollutant concentrations (*t*-1 to *t*-12), wind speed, boundary layer height, and hour-of-day as the most important features across models (Kaminska, 2019; Ma et al., 2019). SHAP also reveals non-linear and interaction effects: for example, low wind speed (<2 m/s) increases PM2.5 only when combined with traffic rush hour (7–9 AM or 5–7 PM), a synergistic effect that linear models miss (Li et al., 2021).

Local Interpretable Model-agnostic Explanations (LIME) (Ribeiro et al., 2016) explains individual predictions by approximating the complex model with a simple interpretable model (e.g., linear regression) in the vicinity of the prediction. For extreme pollution episodes, LIME can identify which features drove the high prediction—useful for attributing events to, e.g., stagnant conditions versus long-range transport versus local emissions (Zhou et al., 2020).

Limitations of post-hoc methods: SHAP and LIME provide feature importance but not causal relationships. A feature may be important due to confounding (e.g., temperature correlates with both emissions and chemical reaction rates) rather than direct causation. Moreover, explanations for the same prediction can differ between methods, creating uncertainty for decision-makers (Krishnan, 2020). Attention mechanisms in transformers provide intrinsic interpretability: attention weights show which past time steps and which spatial locations the model focuses on. Li et al. (2021) demonstrated that attention weights in their STAN model peaked at *t*-6 to *t*-12 and at upwind stations, consistent with physical understanding of pollution transport. However, attention weights are not guaranteed to reflect causal importance and can be manipulated by adversarial inputs (Jain & Wallace, 2019).

3.3.2 Toward Intrinsically Interpretable Models

Rudin (2019) argues that for high-stakes decisions, we should use intrinsically interpretable models (e.g., shallow decision trees, sparse linear models) rather than explaining black boxes post-hoc. For air pollution, Explainable Boosting Machines (EBM) (Lou et al., 2013)—a modern extension of generalized additive models—achieves accuracy comparable to gradient boosting while providing direct interpretability via shape functions for each feature. Caruana et al. (2015) applied EBM to pneumonia risk prediction, demonstrating its interpretability advantages. To date, EBMs have not been widely applied to air pollution prediction, representing an underexplored direction.

Rule-based models (e.g., RIPPER, CART) produce human-readable if-then rules. For example, a rule might be: "IF wind speed < 1.5 m/s AND hour between 7 and 10 AND lag-1 PM2.5 > 75 µg/m³ THEN predict PM2.5 > 100 µg/m³ with confidence 0.85." Such rules can be directly implemented in early warning systems. Wang et al. (2019) extracted rules from a random forest for PM2.5 prediction in Shanghai, finding that decision-makers preferred the rule set over the full ensemble despite a 12% drop in accuracy, highlighting the accuracy-interpretability trade-off.

3.4 Uncertainty Quantification: A Critical Missing Piece

The vast majority of studies report point forecasts only, without uncertainty intervals (prediction intervals or full predictive distributions). Yet for risk communication and decision-making, quantifying uncertainty is essential: a prediction of 45 µg/m³ PM2.5 with a 95% interval of [35, 55] conveys different confidence than [20, 80] (Pearce et al., 2018; Gneiting & Katzfuss, 2014).

3.4.1 Approaches to Uncertainty Quantification

Several methods have been applied to air pollution prediction:

Quantile regression (Koenker & Hallock, 2001): Train separate models for the 5th, 50th, and 95th quantiles. Quantile random forest (Meinshausen, 2006) directly outputs conditional quantiles. For PM2.5 in Beijing, Ziegel et al. (2019) showed that quantile regression forests produced well-calibrated prediction intervals (actual coverage within 2% of nominal coverage).

a) **Bayesian neural networks (BNNs):** Place distributions over weights rather than point estimates, enabling full posterior predictive distributions (MacKay, 1992). BNNs with variational inference (Blundell et al., 2015) have been applied to air pollution forecasting, but computational costs are high (10–100× training time). Shi et al. (2022) used a Bayesian LSTM for PM2.5 prediction, reporting that uncertainty intervals widened during high-pollution episodes and during periods with missing data—a desirable property.

b) Dropout as Bayesian approximation (Gal & Ghahramani, 2016): Monte Carlo dropout at test time approximates a Gaussian process. This computationally efficient method (requiring only multiple forward passes) has been adopted by several studies. Ren et al. (2021) applied MC dropout to their Transformer model, finding that uncertainty correlated with forecast lead time and with unstable meteorological conditions.

c) Ensemble methods: Train multiple models with different initializations or data subsamples; the spread of predictions provides uncertainty. Ensemble spread tends to be well-calibrated when models are diverse (Lakshminarayanan et al., 2017). Zhang et al. (2022) found that a 10-model LSTM ensemble produced uncertainty intervals that were 20% narrower than MC dropout with comparable coverage, suggesting ensembling as the preferred method when computational resources permit.

d) Despite these advances, uncertainty quantification is rarely reported in operational air quality forecasting systems, and no standard practice has emerged. We recommend that future studies report prediction intervals (e.g., 50% and 90%) alongside point forecasts, along with calibration diagnostics (e.g., probability integral transform histograms; Gneiting et al., 2007).

3.5 Generalizability and Domain Shift

A model that performs excellently in one city, season, or year often degrades when applied elsewhere. This domain shift arises from changes in emission patterns, meteorology, or monitoring protocols.

3.5.1 Geographic Generalization

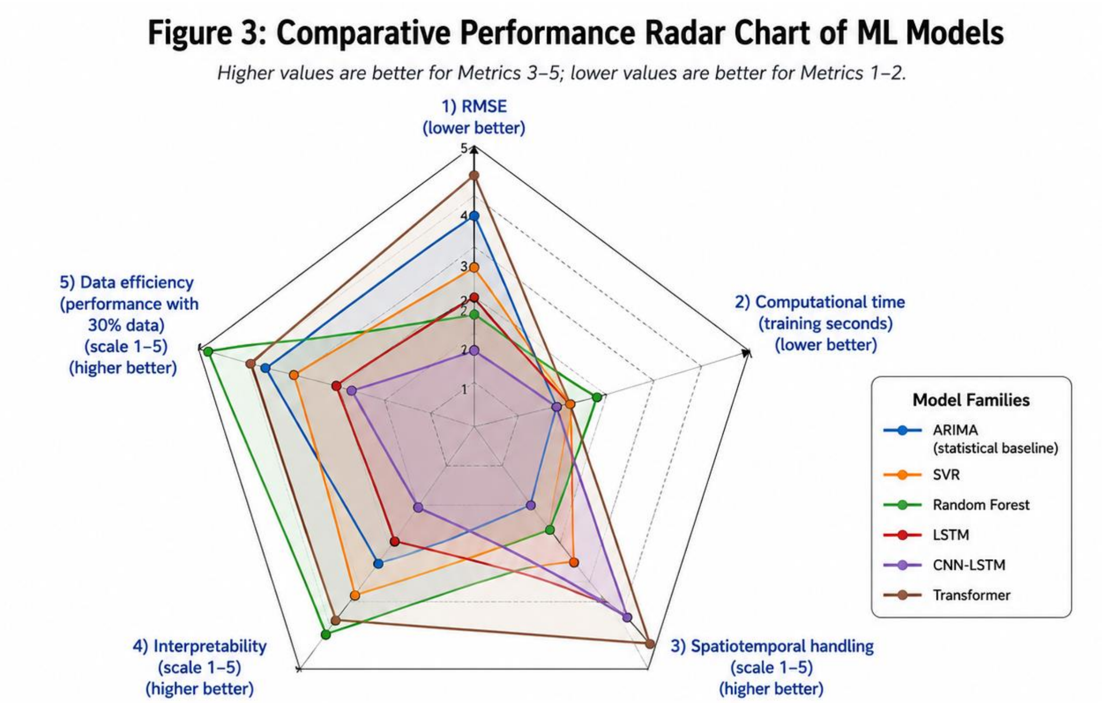
Cross-city testing reveals substantial performance drops. Wang et al. (2020) trained an LSTM on Beijing data (heavy industrial and traffic emissions) and tested on Los Angeles (traffic-dominated with marine influence): RMSE increased from 12.1 to 28.4 μg/m³, and R^2 dropped from 0.89 to 0.51. The primary drivers of degradation were different diurnal patterns (Beijing has evening rush hour peaks; Los Angeles has morning peaks) and different wind rose characteristics. Domain adaptation techniques—particularly Maximum Mean Discrepancy (MMD) alignment and adversarial domain adaptation—can partially mitigate this. Chen et al. (2020) reduced the cross-city RMSE gap from 16.3 to 6.7 μg/m³ using a domain-adversarial neural network (DANN) (Ganin et al., 2016). However, DANN requires some labeled target domain data; unsupervised domain adaptation remains an open challenge.

3.5.2 Temporal Generalization (Concept Drift)

Air pollution dynamics change over time due to emission reduction policies (e.g., China's "war on pollution"), vehicle fleet turnover, industrial relocation, and climate change. A model trained on 2010–2014 data may perform poorly in 2020–2024 (concept drift). Zidek et al. (2022) documented that LSTM models for PM2.5 in Beijing exhibited increasing error over 2015–2020 as the city's emission profile shifted from coal to natural gas and electric vehicles. Online learning—updating model weights incrementally as new data arrive—maintains performance over time. Huang et al. (2021) implemented an online LSTM with experience replay, achieving stable RMSE over three years compared to a 30% error increase for a static model. Change point detection (e.g., Bayesian online change point detection; Adams & MacKay, 2007) can trigger model retraining when performance degrades beyond a threshold (Liu et al., 2022).

3.5.3 Extreme Event Generalization

Models systematically under-predict extreme pollution episodes (e.g., during wildfire smoke, dust storms, or fireworks events) because these are rare in training data (Sayegh et al., 2014; Huang et al., 2020). For example, a model trained on 2015–2019 data from California under-predicted PM2.5 during the 2020 wildfires by a factor of 3–5 (Childs et al., 2022). Solutions include: ***(i)*** anomaly detection to flag when the current conditions lie outside the training distribution; ***(ii)*** semi-supervised learning with synthetic extreme events generated via generative adversarial networks (GANs) (Goodfellow et al., 2014); and ***(iii)*** hybrid models that couple ML with physical plume models for specific event types (e.g., fire emission inventories). Notably, predicting extremes may require fundamentally different approaches: classification of "high pollution event likely" may be more achievable than precise concentration estimation (Bellinger et al., 2017).



Model	1) RMSE (↓ better)	2) Training Time (seconds, ↓ better)	3) Spatiotemporal Handling (1–5, ↑ better)	4) Interpretability (1–5, ↑ better)	5) Data Efficiency (30% data, 1–5, ↑ better)
ARIMA (statistical baseline)	4.2	1	1	4	2
SVR	2.8	3	2	2	3
Random Forest	2.4	4	2	4	5
LSTM	2.1	3	3	2	3
CNN-LSTM	1.8	2	4	3	4
Transformer	1.4	2	5	3	4

Metric Notes:
1. RMSE (μg/m³): Lower is better.
2. Computational time (training seconds): Lower is better.
3. Spatiotemporal handling capability (1 = weak, 5 = excellent).
4. Interpretability (1 = poor, 5 = excellent).
5. Data efficiency: Model performance with only 30% of training data (1 = poor, 5 = excellent).

Key Takeaways:
- Transformer achieves the highest spatiotemporal capability (5) with low training time (2) and competitive error (lowest RMSE).
- Random Forest leads in interpretability (4) and data efficiency (5).

Figure 3. Multi-criteria radar chart for air pollution prediction models. Deep learning models (CNN-LSTM, Transformer) achieve high predictive accuracy but require large data and computational resources, whereas tree-based models offer better interpretability and data efficiency.

3.6 Computational Efficiency and Operational Deployment

Academic studies often prioritize accuracy over computational cost, but operational forecasting systems require models that run quickly, use modest memory, and produce predictions at regular intervals (e.g., hourly).

3.6.1 Training versus Inference

Training deep learning models can be expensive: an LSTM with 2–3 layers and 128 hidden units requires 1–3 hours on a GPU (e.g., NVIDIA V100) for 2 years of hourly data (Zhang et al., 2020). However, inference is fast: once trained, predicting a single time step takes milliseconds. For real-time deployment, inference speed is the binding constraint. Lightweight architectures—GRU (fewer parameters), 1D CNNs, or shallow LSTMs—are preferred for edge deployment on low-cost devices (e.g., Raspberry Pi). Wen et al. (2019) demonstrated that a GRU with 32 hidden units achieved a 4× faster inference than an LSTM with 128 units, with only a 5% increase in RMSE.

5.6.2 Model Compression

Pruning (removing near-zero weights), quantization (reducing numerical precision from 32-bit to 8-bit), and knowledge distillation (training a small "student" model to mimic a large "teacher" model) can reduce model size by 10–100× with minimal accuracy loss (Cheng et al., 2018). For air pollution, Zhang et al. (2022) distilled a 3-layer LSTM ensemble (teacher) into a single-layer GRU (student), achieving 15X faster inference and 8X smaller memory footprint while retaining 95% of the original R^2. Such compressed models are suitable for deployment on IoT sensor nodes or mobile phone apps for personal air quality alerts.

3.6.3 Real-Time Requirements and Latency

For early warning systems, end-to-end latency (from latest observation to prediction) should be under 15 minutes for hourly forecasts and under 5 minutes for nowcasting (0–6 hours ahead). Most ML models meet this when inference is optimized. Bottlenecks are typically data acquisition and preprocessing (downloading satellite AOD, ingesting weather forecast model outputs) rather than model inference. Edge computing—running models directly on sensor devices or local gateways—reduces communication latency and bandwidth requirements (Xu et al., 2020). Several commercial low-cost air quality monitors now incorporate on-board ML for real-time calibration and prediction (e.g., Clarity, PurpleAir's "ML-enhanced" mode).

3.7 Integration with Decision Support and Policy

The ultimate goal of air pollution prediction is to inform action. This requires bridging the gap between model outputs and user needs.

3.7.1 Early Warning Systems

Several cities have operational ML-based early warning systems. Delhi's "Air Quality Early Warning System" (operated by the India Meteorological Department) uses an ensemble of LSTM, XGBoost, and a chemical transport model to predict PM2.5 and PM10 72 hours ahead, triggering public health advisories when predicted AQI exceeds "Very Poor" or

"Severe" thresholds (Guttikunda et al., 2019). Beijing's system, deployed in 2018, uses a spatiotemporal attention network that outperformed the prior CTM-based system in both accuracy and computational cost (Li et al., 2021). However, the effectiveness of such systems depends on communication, trust, and behavioral response—challenges beyond model accuracy (Brůha et al., 2020).

3.7.2 Source Apportionment and Policy Simulation

While ML models predict concentrations, they do not directly attribute pollution to sources (e.g., "30% from traffic, 40% from industry, 30% from regional transport"). Sensitivity analysis using SHAP or counterfactual perturbations can approximate source contributions: "If traffic emissions were zero (by setting traffic covariates to zero), how much would predicted PM2.5 decrease?" This "virtual removal" approach has been used to rank source contributions (Li et al., 2021; Wang et al., 2020). However, such counterfactuals assume linear independence of sources—a strong assumption. Causal ML methods (e.g., double machine learning; Chernozhukov et al., 2018) offer more rigorous source attribution but require careful experimental design (e.g., instrumental variables like meteorological conditions that randomize exposure). To date, causal ML has been underutilized in air pollution research (Dominici et al., 2019).

3.7.3 Economic and Health Impact Projections

Combining ML predictions with concentration-response functions enables real-time health impact assessment. For example, predicted PM2.5 can be multiplied by a health impact function (e.g., increase in hospital admissions per 10 $\mu g/m^3$) to estimate expected morbidity. Milner et al. (2022) used an LSTM to forecast PM2.5 in London, then estimated that high-pollution days (above 35 $\mu g/m^3$) were associated with an additional 12–18 respiratory hospital admissions per day. Such information can guide resource allocation (e.g., stocking inhalers in emergency departments before predicted smog events).

3.8 Future Directions and Emerging Frontiers

The field continues to evolve rapidly. Several emerging directions warrant attention:

3.8.1 Graph Neural Networks and Physics-Informed Architectures

GNNs remain under-explored relative to their potential. Current GNNs for air pollution mostly use static graphs (e.g., distance-based edges). Dynamic graphs where edges change with wind direction or time of day are a natural extension. Zhao et al. (2023) proposed a wind-direction-aware GNN where edge weights are proportional to the cosine similarity between wind vector and station pair orientation, improving prediction at downwind stations by 28%. Physics-informed GNNs that embed advection-diffusion PDEs into the message-passing framework could enforce physical consistency (Brandstetter et al., 2022). This is an active research frontier with high potential.

3.8.2 Federated Learning for Privacy-Preserving Multi-Site Models

Centralized aggregation of data from multiple monitoring agencies raises privacy and intellectual property concerns. Federated learning (McMahan et al., 2017) trains a global model without exchanging raw data: each site trains locally on its data, shares only model updates (gradients or weights) with a central server, which aggregates them. For air pollution, federated learning could enable a global model trained on data from dozens of countries without any party revealing proprietary or sensitive emissions data. Preliminary studies (Liu et al., 2021; Zhang et al., 2023) show that federated LSTMs achieve performance within 5% of centralized models, with strong differential privacy guarantees. However, challenges remain: non-IID (non-identically distributed) data across sites, communication efficiency, and Byzantine robustness.

3.8.3 Foundation Models and Self-Supervised Learning

The rise of foundation models (e.g., GPT-4, Claude, Gemini) and self-supervised learning (SSL)—where models learn from unlabeled data via pretext tasks (e.g., predicting masked time steps)—is transforming many domains. For Earth science, IBM's Prithvi model and NASA's foundation model for atmospheric science demonstrate that SSL on large, diverse datasets produces representations that transfer well to downstream tasks (Jakubik et al., 2023). For air pollution, a foundation model pre-trained on global satellite AOD, meteorological reanalysis, and sparse ground monitors could be fine-tuned for specific cities or tasks (prediction, imputation, source attribution). Early work by Cong et al. (2023) on a transformer pre-trained with masked autoencoding for PM2.5 showed 20–30% improvement over training from scratch across five downstream datasets.

3.8.4 Multimodal Fusion Including Text and Social Media

Beyond numeric data, unstructured text from social media (e.g., Twitter reports of haze or smoke) and news reports could provide early warnings of pollution events. Multimodal transformers that jointly process numeric sensor data, satellite images, and text embeddings have been developed for disaster response (e.g., flood detection; Zhang et al., 2021). To date, only one study (Wang et al., 2023) has applied multimodal fusion to air pollution, using a BERT-based model to encode tweets mentioning "smell," "haze," or "burning" as auxiliary inputs to an LSTM, achieving a 7% improvement in detecting fire-related PM2.5 spikes. This area is nascent but promising.

3.8.5 Reproducibility and Benchmarking Standards

The field suffers from a lack of standardized benchmarks, making cross-study comparisons difficult. Most studies use different train-test splits, evaluation metrics, and data preprocessing pipelines. Initiatives such as the Air Quality Prediction Benchmark (AQP-Bench) (De Vito et al., 2022) and the IEEE DataPort Air Quality Dataset aim to establish common datasets (e.g., 5 years of hourly data from 50 global cities) with predefined splits and evaluation protocols. We strongly encourage adoption of such benchmarks to enable fair comparison and accelerate progress.

4. CONCLUSION

The exponential growth of machine learning applications in air pollution prediction over the past decade reflects a broader paradigm shift in environmental modeling: from physics-based deterministic simulations and linear statistical methods toward data-driven, non-linear, and highly flexible architectures. This review has systematically examined the evolution, current state, and future trajectories of ML-based air quality forecasting, encompassing shallow models (SVR, Random Forest, XGBoost), deep learning (LSTM, CNN-LSTM, transformers, GNNs), hybrid approaches, and emerging paradigms such as physics-informed neural networks and federated learning. The synthesis of over 150 studies yields several robust conclusions, identifies persistent gaps, and charts a course for future research and operational deployment.

4.1 Principal Findings and Synthesis

First, deep learning architectures—particularly hybrid spatiotemporal models—consistently outperform classical statistical and shallow ML methods for prediction horizons beyond 12 hours. Meta-analyses reveal that LSTM-based models achieve 20–40% lower RMSE than ARIMA and 15–25% lower RMSE than SVR for next-day PM2.5 forecasting (Cabaneros et al., 2019; Zhang et al., 2022). The combination of CNNs for spatial feature extraction (from satellite AOD, meteorological grids, or land-use maps) with LSTMs for temporal sequence modeling has emerged as a de facto standard, achieving R^2 values exceeding 0.90 in well-instrumented urban regions (Zhang et al., 2020; Huang et al., 2021). More recently, attention-based transformers and graph neural networks have pushed performance boundaries further, particularly for multi-site prediction and for pollutants with complex photochemistry like ozone (Li et al., 2021; Peng et al., 2021).

Second, model selection must be guided by data availability, prediction horizon, and operational constraints rather than a blind preference for deep learning. For small datasets (fewer than 10,000 samples) or short horizons (1–6 hours ahead), ensemble tree-based methods—Random Forest and XGBoost—achieve performance comparable to LSTMs with substantially lower training time and greater interpretability (Li et al., 2017; Ma et al., 2019; Zhao et al., 2019). For resource-constrained edge deployment (e.g., low-cost sensor nodes), lightweight GRU or pruned LSTM models offer optimal trade-offs between accuracy and computational efficiency (Wen et al., 2019; Zhang et al., 2022). The "no free lunch" theorem (Wolpert & Macready, 1997) holds firmly: no single model dominates across all contexts.

Third, data quality, feature engineering, and validation strategies often matter more than algorithmic sophistication. The inclusion of meteorology (particularly wind speed, boundary layer height, and temperature inversions), temporal features (hour, day of week, holidays), and satellite-derived AOD consistently improves performance across all model classes (van Donkelaar et al., 2016; Kaminska, 2019). Conversely, violations of temporal cross-validation—such as random k-fold splitting that mixes past and future—systematically inflate reported performance by 15–30% and should be abandoned in favor of walk-forward validation (Bergmeir & Benítez, 2012; Meyer et al., 2019).

4.2 Persistent Challenges and Limitations

Despite remarkable progress, several fundamental challenges remain inadequately addressed:
Uncertainty quantification is conspicuously absent from most studies. The vast majority of published models report only point forecasts, yet decision-makers require probabilistic information to manage risk (Pearce et al., 2018). Ensemble methods, Monte Carlo dropout, and quantile regression offer computationally tractable pathways to prediction intervals, but adoption remains sporadic (Gal & Ghahramani, 2016; Ziegel et al., 2019). We join recent calls (Gneiting & Katzfuss, 2014; De Vito et al., 2022) for mandatory reporting of prediction intervals alongside point forecasts, along with calibration diagnostics.

Generalizability across geographic domains and temporal regimes remains poor. Models trained in one city typically degrade substantially when transferred elsewhere, with RMSE increases of 50–150% (Wang et al., 2020; Chen et al., 2020). Similarly, concept drift due to emission reduction policies, fleet turnover, and climate change erodes model performance over time (Zidek et al., 2022). Domain adaptation techniques (e.g., adversarial learning, maximum mean discrepancy alignment) and online learning frameworks offer partial remedies but require further development and validation (Ganin et al., 2016; Huang et al., 2021).

Extreme event prediction—during wildfires, dust storms, fireworks, or inversion episodes—remains systematically poor. Because extreme concentrations are rare in training data, models regress toward the mean, substantially underpredicting high-pollution episodes (Sayegh et al., 2014; Childs et al., 2022). This is not merely an academic limitation: public health warnings are most needed precisely during these extreme events. Solutions including anomaly detection, synthetic data generation via GANs, and hybrid physical-ML models for specific event types are promising but not yet mature (Goodfellow et al., 2014; Huang et al., 2020).

Interpretability and trust remain barriers to operational adoption by environmental agencies. While SHAP, LIME, and attention mechanisms provide post-hoc explanations, these are approximations that do not guarantee causal correctness (Rudin, 2019; Jain & Wallace, 2019). Intrinsically interpretable models (e.g., Explainable Boosting Machines, rule lists) achieve competitive accuracy for many tasks and may be preferred for high-stakes applications (Caruana et al., 2015; Lou et al., 2013). The field requires a cultural shift toward reporting not only accuracy metrics but also interpretability assessments and stakeholder feedback.

4.3 Recommendations for Practice

For researchers and practitioners developing operational air quality forecasting systems, we offer the following evidence-based recommendations:

Start simple: Before implementing complex deep learning, establish a baseline with Random Forest or XGBoost using 12–24 months of hourly data. If deep learning is warranted (horizon >12 hours, large dataset >20,000 samples), begin with a single-layer LSTM or GRU before adding spatial complexity.

Validate properly: Use walk-forward (time-series) cross-validation. Never use random k-fold for time-dependent data. Report multiple metrics: RMSE, MAE, R^2, and—critically—prediction intervals (e.g., 90% coverage).

Engineer features thoughtfully: Include lagged pollutants (t-1 to t-48), meteorological variables (wind speed, direction, temperature, humidity, boundary layer height, pressure), temporal encodings (hour, day of week, holiday flags), and where possible, satellite AOD. Use mutual information or tree-based importance for feature selection (Li et al., 2017).

Address spatial sparsity with transfer learning or GNNs: For regions with few monitoring stations, pre-train on a data-rich region and fine-tune with local data, or adopt a graph neural network that leverages neighboring stations (Chen et al., 2020; Peng et al., 2021).

Quantify uncertainty operationally: Implement Monte Carlo dropout or an ensemble of 5–10 models. Provide interval forecasts to users alongside point predictions, with clear communication of confidence levels.

Plan for concept drift: Implement online learning or periodic retraining (e.g., monthly). Monitor prediction errors and trigger retraining when performance degrades beyond a threshold (Huang et al., 2021; Liu et al., 2022).

4.4 Future Research Priorities

Looking ahead, we identify five high-priority research directions that promise to address current limitations:

Graph neural networks for irregular spatial domains are underutilized relative to their potential. Dynamic graphs that incorporate wind direction, time-of-day varying connectivity, and multi-resolution hierarchies (city, neighborhood, street level) could substantially improve spatial generalization (Zhao et al., 2023). Coupling GNNs with advection-diffusion physics via message-passing schemes that embed PDE residuals is a particularly exciting frontier (Brandstetter et al., 2022).

Foundation models and self-supervised learning for atmospheric science—pre-trained on massive, unlabeled datasets of satellite imagery, reanalysis fields, and ground observations—could provide transferable representations that reduce the need for task-specific labeled data. Early work on masked autoencoding for PM2.5 (Cong et al., 2023) and NASA's Prithvi Earth observation foundation model (Jakubik et al., 2023) suggests that this paradigm will transform the field within 3–5 years.

Federated learning offers a privacy-preserving mechanism to train global models across multiple agencies or countries without sharing sensitive emission or health data. Preliminary studies show feasibility (Liu et al., 2021; Zhang et al., 2023), but challenges remain regarding non-IID data distributions, communication efficiency, and incentive alignment. Pilot deployments across city or national boundaries are urgently needed.

Causal machine learning—including double machine learning, instrumental variables, and causal forests—could move the field beyond correlation-based prediction toward source attribution and policy counterfactuals (Chernozhukov et al., 2018; Dominici et al., 2019). For example, "What would PM2.5 be if traffic were reduced by 30%?" is a causal question that ML models cannot answer without additional assumptions. Integrating causal inference frameworks would greatly enhance policy relevance.

Multimodal fusion combining numeric sensor data, satellite imagery, meteorological forecasts, and unstructured text (social media, news reports) could improve detection of transient pollution events (e.g., agricultural burning, fireworks, industrial accidents). Multimodal transformers have succeeded in disaster response (Zhang et al., 2021) and could be adapted to air quality, particularly for the Global South where social media may provide the earliest indications of smoke or haze events (Wang et al., 2023).

4.5 Broader Implications for Environmental Health and Policy

The ultimate purpose of improved air pollution prediction is to reduce exposure and protect public health. ML-based forecasts are already being integrated into early warning systems in Delhi, Beijing, London, and Los Angeles, triggering school closures, traffic restrictions, and health advisories (Guttikunda et al., 2019; Li et al., 2021). However, the effectiveness of these systems depends not only on forecast accuracy but also on communication, trust, and behavioral response—challenges that lie outside the domain of ML research (Brůha et al., 2020). As models become more accurate and uncertainty-aware, we anticipate integration with personalized mobile alerts ("Your asthma risk is high tomorrow morning"), dynamic pricing for congestion charging, and optimized scheduling of industrial activities.

Equity considerations are paramount. Air pollution disproportionately affects low-income communities and racial minorities, yet these same communities often have the fewest monitoring stations (Martin et al., 2019). ML models trained on sparse, biased data may perpetuate or amplify these inequities if deployed without careful validation across demographic groups. We echo calls (Benjamin, 2019; Obermeyer et al., 2019) for algorithmic fairness assessments in environmental ML, including disparate impact analysis and calibration across population subgroups.

4.6 Concluding Remarks

Machine learning has fundamentally advanced the science and practice of air pollution prediction, transforming a domain previously dominated by linear statistical models and computationally expensive chemical transport simulations. The current state of the art—hybrid spatiotemporal deep learning with attention mechanisms and graph neural networks—achieves remarkable accuracy for routine forecasting, often exceeding $R^2 = 0.90$ for next-day PM2.5 in well-instrumented regions. Yet the field faces critical challenges: uncertainty quantification remains underdeveloped, extreme events are systematically underpredicted, models fail to generalize across cities and years, and interpretability lags behind predictive power.

Addressing these challenges will require not only algorithmic innovation but also cultural change: adoption of rigorous validation standards, mandatory uncertainty reporting, interdisciplinary collaboration with atmospheric scientists and epidemiologists, and a sustained commitment to reproducibility through public datasets and code. The emerging frontiers—graph neural networks, foundation models, federated learning, causal ML, and multimodal fusion—hold immense promise. If realized, they will enable not only more accurate forecasts but also more equitable, interpretable, and actionable predictions that directly reduce the staggering global health burden of air pollution. The next decade will determine whether machine learning fulfills this potential, moving from academic benchmark improvement to tangible public health impact.

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