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Machine Learning for Air Quality Forecasting and Prediction- A Review of Explainable AI Methods for Enhanced Interpretability and Transparency

[1] Suraj Mohite, [2] Gauri Chavan
[1] Student, Guru Nanak Khalsa College, Mumbai, India
[2] Assistant Professor, Guru Nanak Khalsa College, Mumbai & Research Scholar, PAHER University, Udaipur, Rajasthan, India
Corresponding Author's Email: [1]g24.suraj.mohite@gnkhalsa.edu.in

Abstract— Air-quality forecasting is essential for public health and urban planning because pollutants such as PM2.5 and ozone have major adverse effects. Recent progress in machine learning and deep learning has substantially enhanced the precision of air-quality predictions, but their complexity often hides how predictions are formed. This review surveys peer-reviewed and preprint work published between 2019 and 2025, retrieved from open access repositories and publisher platforms, and focuses on methods that improve model interpretability. From an initial pool of records we screened, 52 studies met predefined inclusion criteria and were analysed in detail. Tree ensembles (for example Random Forest and gradient-boosted models) and deep networks (including LSTM and CNN variants) dominate forecasting experiments; alongside these, post-hoc explainability tools such as SHAP and LIME are increasingly applied to expose driver variables. We summarize the main strengths and limitations of current XAI practices in air-quality forecasting and outline priorities for method validation, reporting standards, and operational deployment.

Keywords— Air Quality Forecasting, Explainable Artificial Intelligence, Machine Learning, Model Interpretability, Pollution Prediction

1. INTRODUCTION

Air pollution remains a major global concern and one of the leading environmental threats to public health (WHO, 2023). Fine particles such as $PM_{2.5}$ and PM_{10} can reach deep lung tissues and enter the bloodstream, contributing to respiratory and cardiovascular disorders. Gaseous pollutants—including ozone (O_3), nitrogen dioxide (NO_2), sulfur dioxide (SO_2), and carbon monoxide (CO)—are associated with reduced lung capacity, cognitive decline, and increased hospital admissions (Cohen et al., 2017). Beyond human health, pollution intensifies climate change, harms ecosystems, and causes significant economic losses through healthcare expenses and productivity reduction (UNEP, 2021). Developing predictive systems that are both accurate and interpretable is therefore essential for informed environmental policy and community well-being.

Earlier approaches such as linear regression and generalized additive models were valued for their simplicity and interpretability but struggled to represent nonlinear and spatiotemporal dependencies in air-quality data. Modern data-driven techniques—Random Forest, Gradient Boosting, Support Vector Machines, and deep learning architectures like LSTM, CNN, and Transformer networks—achieve far better accuracy by modeling complex relationships across diverse datasets.

Yet, these sophisticated models often behave as "black boxes," offering limited insight into how specific inputs influence outputs. This opacity restricts their use by policymakers who require transparent reasoning behind predictions. Explainable AI (XAI) methods aim to address this gap by clarifying the contribution of each input feature. Model-agnostic tools such as SHAP, LIME, and Partial Dependence Plots, together with model-specific approaches including Layer-wise Relevance Propagation and Guided Backpropagation, are increasingly applied to enhance interpretability (Adadi & Berrada, 2018; Samek et al., 2017; Lundberg & Lee, 2017).

Nevertheless, uncertainty persists regarding which explanation methods are most effective for air-quality applications, how they treat correlated variables, and how their visualizations can best support environmental decisions. Accordingly, this review:

1. Summarizes major model families and interpretability approaches used in recent air-quality research;
2. Examines situations where each method yields the most informative insights; and
3. Highlights current challenges and future directions for transparent forecasting systems that assist policymakers and local communities.

2. METHODOLOGY

2.1 Information Sources

Relevant studies were collected from ResearchGate, MDPI, ScienceDirect, arXiv, and Google Scholar — databases known for covering environmental and AI research extensively. Most papers were open-access, allowing transparent assessment and easy verification.

2.2 Search Strategy

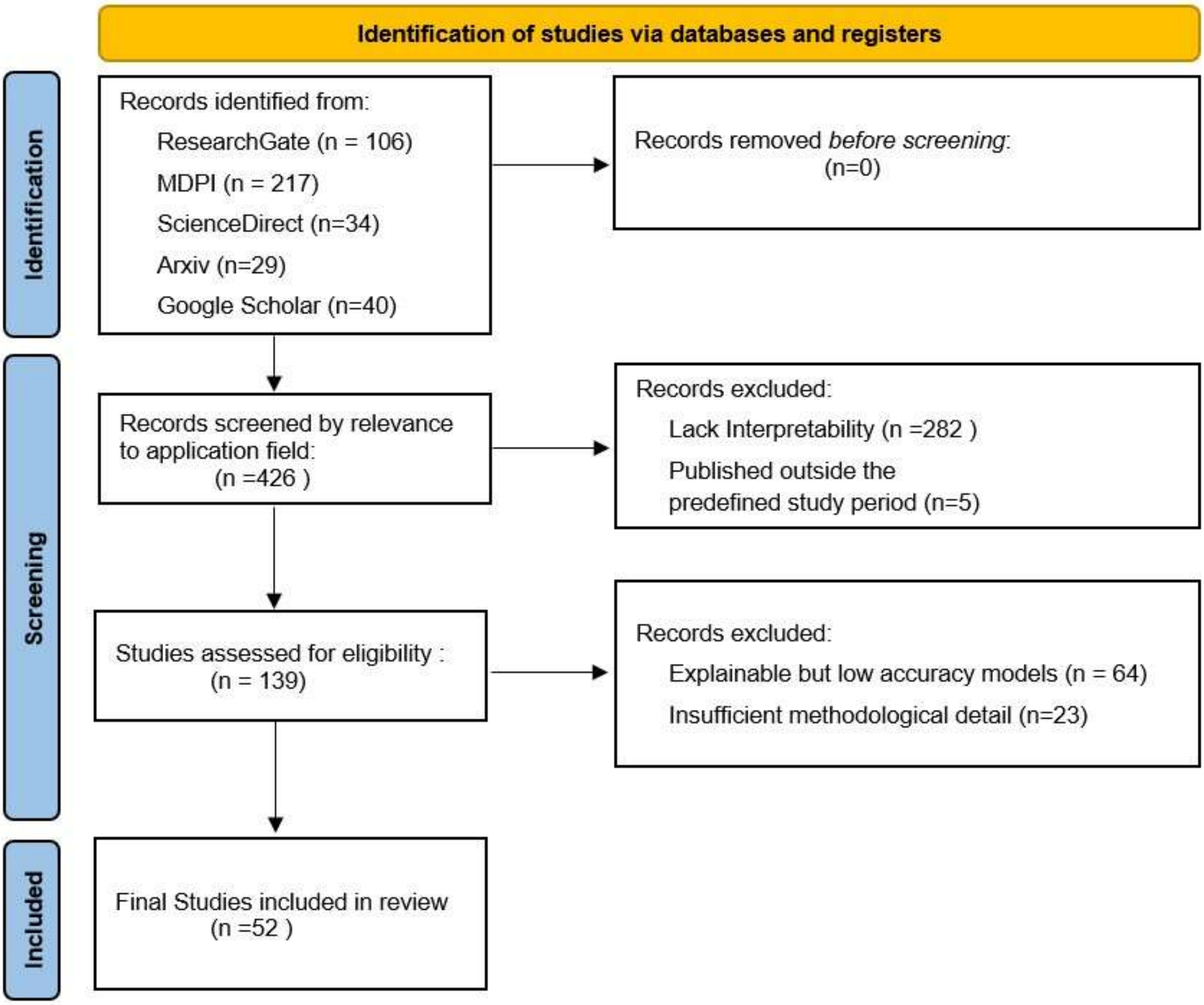
The search combined four main topics: air pollution, ozone, machine learning, and interpretability/explainability, along with their related terms. The keywords were applied to titles, abstracts, and keywords of studies published in English between 2019 and 2025. This period was chosen to reflect the latest developments in interpretable ML applied to environmental systems. No subject filters were used, but the results naturally included environmental science, engineering, computer science, and atmospheric studies.

2.3 Inclusion and Exclusion criteria

A paper was included if it used ML or DL to forecast or classify air quality indicators and incorporated interpretability or explainability methods. Studies related to pollutant forecasting, spatiotemporal mapping, and air quality assessment with an explainability component were all considered. Papers were excluded if they lacked sufficient methodological details, had poor accuracy, or mentioned interpretability without actually applying it.

3.2 Characteristics of the Reviewed Studies

Most studies came from China (38.5%), followed by India (11.5%) and Germany (5.8%). A few others originated from Europe, North America, and global datasets. PM2.5 was the most studied pollutant (30 papers), followed by ozone (18) and NO_2 (12). The dominance of PM2.5 and ozone reflects their serious health and environmental effects. The geographic distribution shows that East and South Asia are the most active regions in explainable air quality research.



3. RESULTS

3.1 Study Selection

Out of 426 papers identified, 282 were removed for lacking interpretability and 5 were outside the time window. After reviewing 139 full texts, 64 were excluded for low accuracy and 23 for insufficient details. The final review included 52 studies that met all selection criteria.

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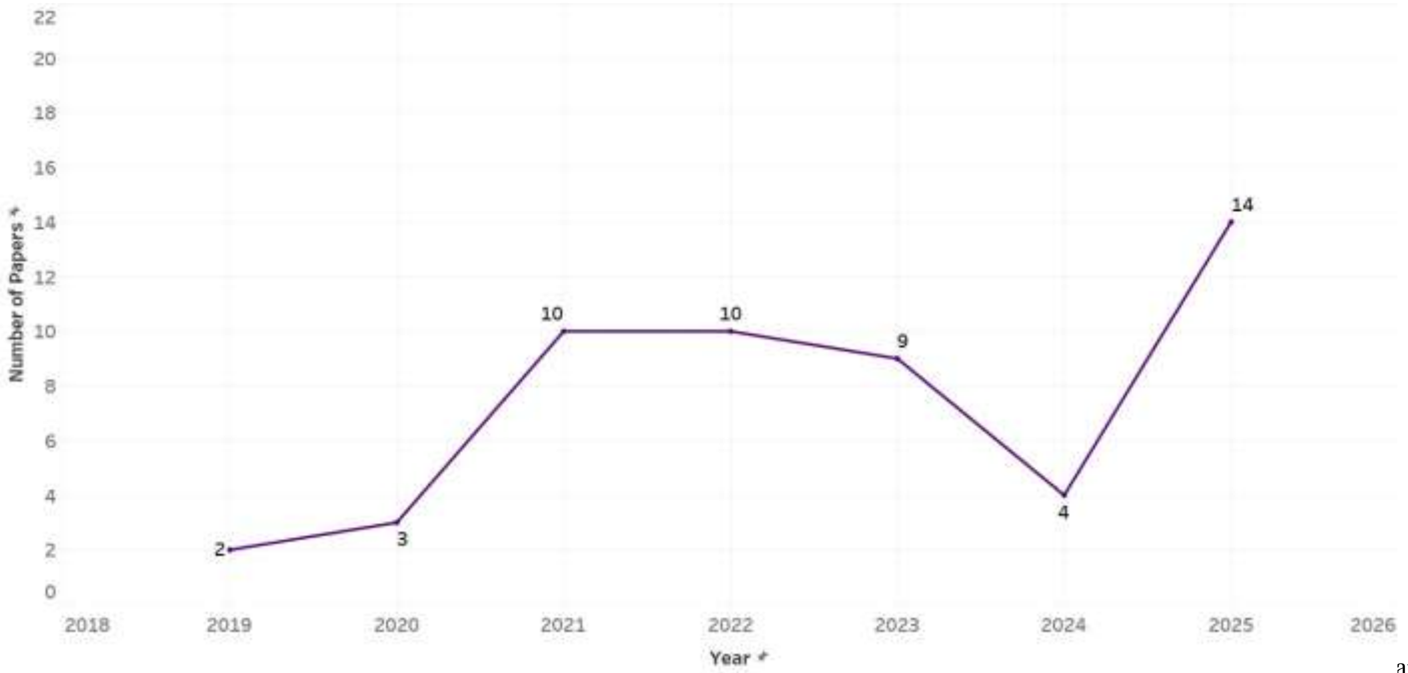

3.3 Interpretable Machine Learning

Machine-learning methods for predicting air quality can be broadly classified as white-box models, which are simple and interpretable but sometimes less accurate, and black-box models, which achieve high predictive skill but offer little transparency (Molnar, 2022). Interpretable machine learning provides tools that clarify how complex algorithms make decisions. These tools fall into two categories: model-agnostic, which analyze inputs and outputs independently of model architecture, and model-specific, which rely on the internal structure of neural or ensemble systems (Ribeiro et al., 2016; Bach et al., 2015).

Across the 52 studies reviewed, several trends emerged. SHAP was the most frequently adopted technique, appearing in 61.5 percent of papers, while LIME appeared in roughly 13.5 percent. LRP, used mainly in deep learning settings, accounted for about 9.6 percent. Only a few studies employed Partial Dependence Plots (PDPs) or Grad-CAM (≈ 3.8 percent each). A smaller group explored new interpretable designs such as graph attention networks, symbolic regression, and hybrid deep-learning frameworks that embed transparency within the model itself.

3.3.1 Model-Agnostic Methods

These methods explain a model's predictions by examining input–output behaviour rather than its internal structure. Their flexibility makes them suitable for tree ensembles, regression models, and neural networks alike.

Shapley Additive Explanations (SHAP)

SHAP, derived from cooperative game theory (Shapley, 1953), distributes a model's prediction among its input variables according to their contribution. It can provide both global feature rankings and local case-level explanations (Lundberg & Lee, 2017).

Several studies demonstrated its value. Gao et al. (2023) applied SHAP to a hybrid Graph Neural Network– Temporal Convolutional Network model for multi-horizon $PM_{2.5}$ forecasting in eastern China. Their system improved root-

and revealed that lagged $PM_{2.5}$, humidity, and wind speed were the main temporal drivers of pollution dynamics.

Yenkikar et al. (2025) combined Random Forest regression with ARIMA for urban air-quality prediction across several Indian cities. SHAP analysis highlighted particulate matter ($PM_{2.5}$ and PM_{10}) and traffic indices as the most influential variables, linking statistical and machine-learning approaches in one interpretable framework. Similarly, Dimitriou & Kassomenos (2022) used SHAP with LSTM, GRU, and CNN networks to study PM_{10} behaviour in Athens. Their best LSTM model achieved $R^2 > 0.85$, and SHAP confirmed that meaningful meteorological variables—wind speed and temperature—rather than mere persistence, explained its performance.

Local Interpretable Model-Agnostic Explanations (LIME)

LIME (Ribeiro et al., 2016) builds locally perturbed samples around a prediction and fits a simple surrogate, often a linear model, to approximate the complex model's behaviour near that point. It is designed for local interpretability, showing why a specific prediction was produced.

Chakraborty et al. (2024) paired LIME with SHAP to interpret AQI predictions from Random Forest, KNN, and XGBoost models across Indian cities. SHAP identified $PM_{2.5}$ and PM_{10} as global drivers, while LIME exposed local meteorological influences—mainly wind and temperature—that differed by region. Nabavi et al. (2021) used LIME to interpret ozone (O_3) forecasting models and showed that short-term variations in solar radiation and temperature were key to episodic O_3 peaks. Their model reached $R^2 > 0.80$, and LIME explanations verified that accuracy stemmed from realistic atmospheric factors.

Partial Dependence Plots (PDPS)

Introduced by Friedman (2001), PDPs visualize how one or two features affect predicted outputs while averaging others. In air-quality applications, they help reveal nonlinear or monotonic pollutant–predictor relations. Dimitriou & Kassomenos (2022) used PDPs alongside SHAP to confirm that wind speed and temperature show nonlinear effects on PM_{10} levels, validating the physical realism of their deep-learning models.

Bootstrapping (BS)

Bootstrapping (Efron, 1979) repeatedly resamples data to evaluate the stability of model interpretations. Kleinert et al. (2021) used a bootstrapped deep-learning framework for O_3 forecasting. By perturbing inputs and recalculating feature importance, they confirmed that temperature and wind speed remained robust drivers across resampled sets, increasing trust in their model's explanations.

3.3.2 Model-Specific Methods

Model-specific techniques use internal computations of algorithms to attribute predictions to features, offering fine-grained but architecture-dependent insights.

Layer-wise Relevance Propagation (LRP)

LRP (Bach et al., 2015; Montavon et al., 2019) back-propagates a prediction through neural layers to assign "relevance scores" to input variables. Mirzavand Borujeni et al. (2023) applied LRP to a GRU encoder–decoder model for ozone forecasting, identifying temporal lags as dominant contributors and enabling pruning without accuracy loss. Park et al. (2019) used LRP in CNNs for $PM_{2.5}$ mapping, locating monitoring stations that produced high-error events. Kim et al. (2022) separated meteorological influences from autoregressive ones in pollutant forecasts using LRP, and Chen et al. (2025) used it at continental scale to validate seasonal patterns within a physics-informed deep-learning setup.

Guided Backpropagation (GB)

Guided Backpropagation (Springenberg et al., 2014) filters gradients so that only positive contributions are propagated backward, creating sharper saliency maps. Song et al. (2023) applied it within their MCST-Tree ensemble to reconstruct fine-scale $PM_{2.5}$ maps in Chengdu, China. Their model combined gradient-boosted trees with calibration layers and achieved $R^2 \approx 0.94$ and RMSE ≈ 4.04 µg/m³. GB visualizations showed that traffic density and road networks were dominant local drivers, while meteorological factors provided background influence.

Gradient-Weighted Class Activation Mapping (GRAD-CAM)

Grad-CAM (Selvaraju et al., 2017) produces spatial heatmaps from CNNs to highlight regions most responsible for outputs. Saxena et al. (2025) integrated Grad-CAM, SHAP, and LIME within a ConvLSTM–XGBoost pipeline to forecast $PM_{2.5}$ and NO_2 across 15 megacities. Their saliency maps confirmed that industrial and traffic-dense zones drove predicted hotspots ($R^2 \approx 0.92$). Alauddin et al. (2025) employed Grad-CAM on a CNN-based AQI classifier using street-level photos in Indonesia, linking visible haze and traffic directly to model decisions.

3.3.3 Emerging and Divergent Approaches

Beyond standard tools, newer studies embed interpretability within model architecture.

Graph-Attention Spatio-Temporal Models

Graph-convolution and attention hybrids, such as the Graph-LSTM + GCN + multi-head attention model (Wang et al., 2024), explicitly encode station connectivity and temporal relations. Using a Qinghai Province dataset (2019–2021), this model achieved lower MAE and RMSE than VAR, LSTM, GRU, and CNN-LSTM baselines. Attention maps revealed which stations and time lags most affected predictions, offering interpretable, time resolved insights.

Satellite-Driven Interpretable Retrievals

Remote-sensing models such as EntityDenseNet and SIDLM (Yan et al., 2020; 2021) integrate CNN/DenseNet structures with interpretability features. EntityDenseNet, trained on Himawari-8 imagery, achieved province level RMSE improvements over tree baselines and visualized which spectral or spatial patterns informed $PM_{2.5}$ retrievals. SIDLM separated linear seasonal effects from nonlinear spatial ones, enabling clearer explanation of physical drivers in satellite-based $PM_{2.5}$ estimation.

Traffic-Centric Interpretable Models

Lešnik et al. (2019) developed GA-based multivariate regression with traffic telemetry for PM_{10} prediction, comparing it with ANN, SVM, and ensemble methods. Retaining explicit regression coefficients allowed direct interpretation of which lagged traffic volumes most influenced morning peaks—providing actionable insights for urban planners.

Symbolic And Causal Models

Symbolic regression and fuzzy cognitive maps (FCMs) offer human-readable expressions or causal graphs. Lucena-Sánchez et al. (2021) presented a symbolic regression pipeline for air-quality time series that yielded closed-form equations competitive with neural networks. Peng et al. (2022) used FCMs to link energy use and air-quality variables, highlighting causal-like influence patterns that can be easily communicated to policymakers.

Hybrid Interpretable Architectures

Hybrid models combine the strengths of deep learning and interpretable modules. Gu et al. (2022) proposed HIP-ML, merging a deep neural network with a nonlinear ARMA component and feature-selection stage to output horizon-specific importance values. Chen et al. (2021) built a Self-Adaptive Deep Neural Network (SADNN) with embedded attention layers, generating daily predictor-importance maps. These hybrids preserved accuracy while producing time-resolved explanations directly from within the model.

Variational Bayes and Information-Filtering Frameworks

Jin et al. (2023) introduced a Variational Bayesian Network with a mutual-information-based filtering stage to retain only the most informative inputs for $PM_{2.5}$ forecasting in Beijing. The approach slightly improved accuracy over deterministic baselines and enhanced interpretability by identifying key conditional dependencies among variables.

Multi-Target / Multi-Horizon Explainable Forecasting

Jiménez-Navarro et al. (2024) designed multi-target architectures with built-in explanation modules that separate drivers for each pollutant and forecast horizon. This approach helps reveal how control actions may affect several pollutants differently, supporting coordinated air-quality management.

4. DISCUSSION

4.1 Dominance of SHAP & LIME

Across recent literature, SHAP and LIME dominate as interpretability tools. SHAP, rooted in game theory, assigns fair importance to each variable and supports both global and local explanations. It helps link general pollutant patterns with case-specific variations, though it can overweight correlated inputs

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and sometimes shows contribution differences rather than direct prediction changes.

LIME is simpler and easy to interpret, using small local surrogates around individual cases—ideal for short term events such as pollution spikes. Its main weakness is sensitivity to neighborhood settings, which can affect consistency. Many studies combined both: SHAP for broad global insight, LIME for localized clarity. Together they balanced transparency and detail, explaining their widespread adoption in explainable-AI air quality research.

4.2 Limited Use of Other Methods

Methods like PDPs, Grad-CAM, and LRP appeared in few papers despite their value. PDPs reveal nonlinear pollutant–meteorology links (Friedman, 2001); Grad-CAM visualizes spatial regions driving CNN forecasts (Selvaraju et al., 2017); and LRP traces feature relevance through deep layers (Bach et al., 2015). Their rarity likely stems from limited generalizability and interpretive complexity. A smaller group built interpretability into model design—using hybrid neural networks with attention layers, symbolic-regression pipelines, or Bayesian variable-filtering frameworks. These show a shift toward models that are transparent by construction rather than explained afterward.

Overall, interpretability serves three roles: validating models against atmospheric science, converting forecasts into policy-relevant insights, and building public trust. SHAP remains the most versatile, LIME offers accessible local detail, and newer hybrid approaches point toward inherently interpretable forecasting systems. Regional context also matters: large Asian datasets favour robust general tools, whereas European and North-American work often experiments with new techniques.

5. LIMITATIONS AND FUTURE DIRECTIONS

This review systematically summarized how interpretability is applied in air-quality forecasting, revealing clear trends across 52 studies. By emphasizing interpretability over accuracy alone, it shows how SHAP and LIME help confirm whether models align with atmospheric knowledge. Yet, several limits remain: most work centers on a few pollutants and regions; SHAP dominates, with little exploration of alternatives such as Grad-CAM, LRP, or symbolic approaches; and inconsistent reporting on preprocessing or correlation handling restricts cross-comparison.

Future studies should expand interpretability techniques and improve methodological transparency. The next step is real-time interpretable systems that process live pollution and meteorological data and present outputs through user-friendly dashboards highlighting key drivers and uncertainties. Turning prototypes into operational tools would make interpretability a direct resource for health and environmental agencies.

6. CONCLUSION

Explainable AI is now vital for ensuring that complex forecasting models remain transparent and trustworthy. Among 52 studies, SHAP and LIME emerged as the leading methods, combining global understanding with local explanation. Their popularity reflects the need for tools that validate model logic and convey results clearly to policymakers and the public.

Less common methods—Grad-CAM, LRP, symbolic or Bayesian frameworks—show promise but need broader application. Overall, interpretability in this field is still uneven, concentrated in limited pollutants and regions. The future lies in real-time, user-oriented forecasting systems that merge strong predictive accuracy with clear reasoning interfaces, turning explainable AI from an academic goal into a practical instrument for environmental decision-making.

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