

Diurnal, Seasonal and Spatial Patterns of Weather Influences on PM_{2.5} Concentrations in Poland: An Explainable Machine Learning Approach

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INTRODUCTION

- The relationship between meteorological conditions and PM_{2.5} concentrations is complex, involving nonlinear interactions and seasonal variability. Traditional statistical methods often fail to capture these dynamics fully.
- Recent advances in explainable machine learning, particularly the SHAP (SHapley Additive exPlanations) framework, offer a novel pathway to interpret model predictions and disentangle variable importance in environmental systems (Lundberg & Lee, 2017; Molnar, 2022).
- In this study, we analyze a decade of hourly PM_{2.5} and meteorological data (2014–2023) from 11 cities across Poland, applying SHAP to reveal **how weather features modulate air pollution under varying temporal and spatial contexts**. The objective is to move beyond simple correlation, and instead quantify **how, when, and where** different meteorological drivers affect PM_{2.5} formation and dispersion.
- This approach allows us to identify both consistent physical relationships and emergent, context-specific behaviors consistent with atmospheric chemistry and boundary-layer dynamics (Petäjä et al. 2016).

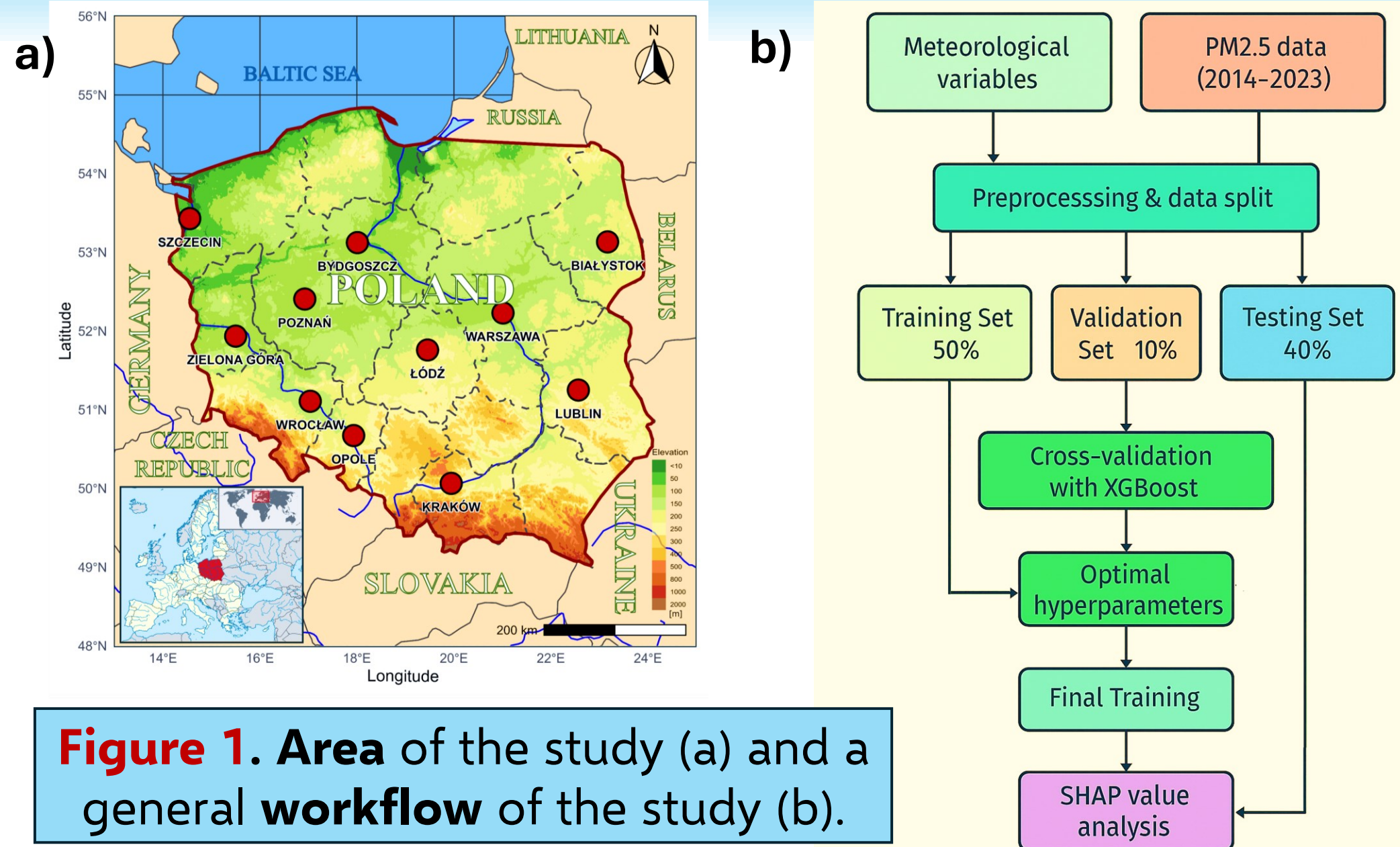


Figure 1. Area of the study (a) and a general workflow of the study (b).

DATA & METHODS

- ✓ We trained a gradient boosting model (XGBoost) to predict **hourly PM_{2.5} concentrations** based on meteorological inputs from the WRF (Weather Research and Forecasting) model.
- ✓ For each forecast hour, the model used both **instantaneous values** and **24-hour rolling means** of: precipitation, 2-m temperature, shortwave radiation, wind speed, wind direction, planetary boundary layer height, relative humidity, sea-level pressure as predictors.
- ✓ **Hourly PM_{2.5} data (2014–2023)** used as the dependent variable came from CEIP (Chief Inspectorate of Environmental Protection, Poland) at 11 cities (Fig. 1, a). Each location included 1–5 stations; data were spatially averaged per city.
- ✓ **10% of data** were used for **temporal cross-validation** to tune six hyperparameters: *max_depth*, *sample_size*, *Mtry*, *min_N*, *learn_rate*, *Ntree*. **50% of data** were used for training, **40%** – for testing. The full workflow summary is shown in Fig 1, b.
- ✓ The final model achieved mean absolute error (MAE) of **5.35 µg·m⁻³** and **R² of 0.79**.
- ✓ Using the *caret* package in R, we applied SHAP (SHapley Additive exPlanations) to the test predictions. SHAP values decompose each prediction into **individual variable contributions**. This method calculates feature importance by comparing model predictions with and without each feature across **all possible subsets of features**. For each subset *S*, two models are trained: one including the feature *i* and one excluding it. **The prediction difference shows the feature's impact**, and averaging these differences over all subsets gives the Shapley value as the final feature attribution.

➤ Positive SHAP → variable increases PM_{2.5}

➤ Negative SHAP → variable reduces PM_{2.5}

RESULTS & DISCUSSION

DECADAL TRENDS

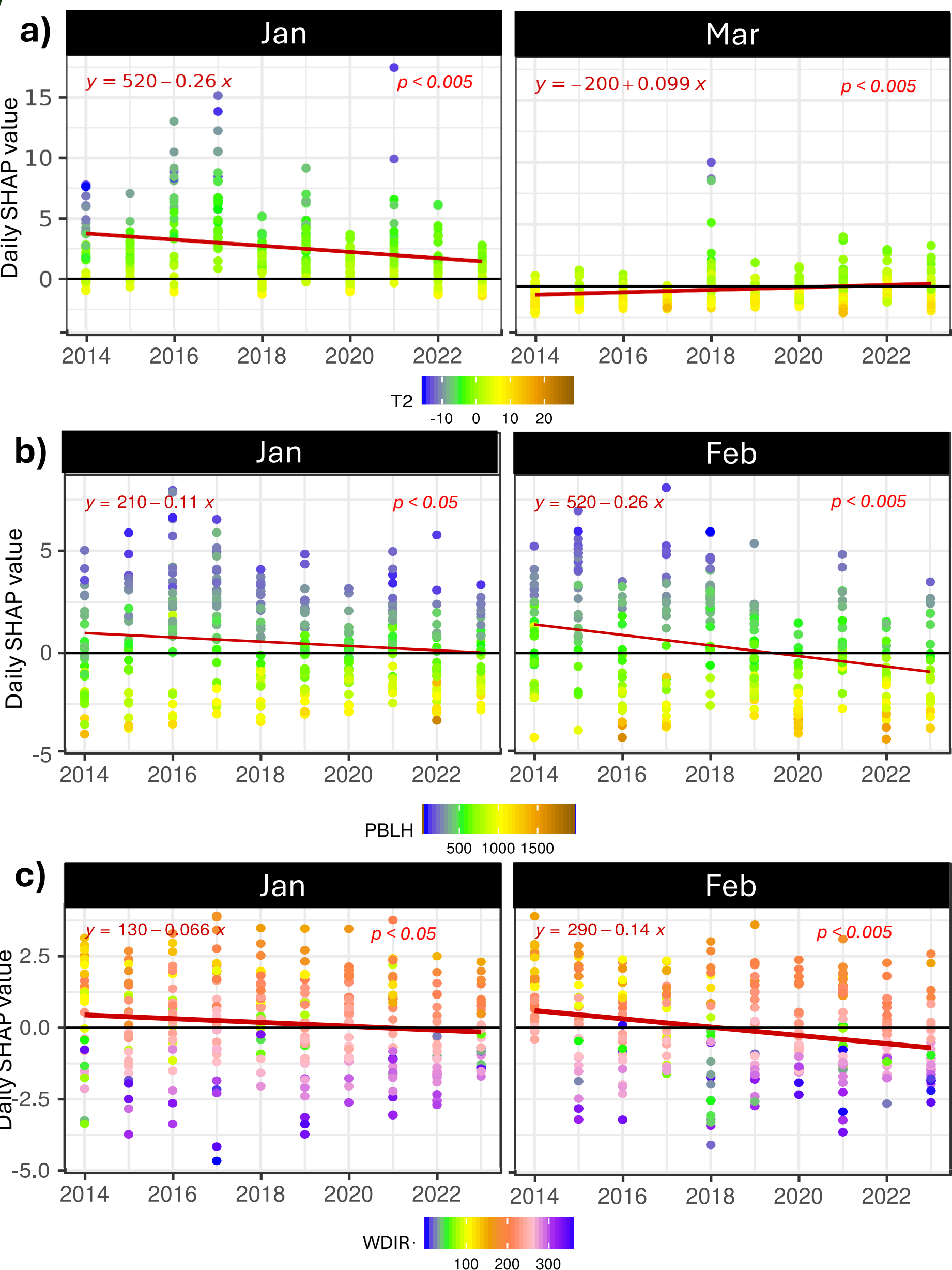


Figure 2. Decadal trends of temperature (a), PBLH (b), and wind direction (c) influences on PM_{2.5}

- ☑ **Temperature influence in Jan** has significantly declined over the decade, suggesting that warmer conditions are reducing cold-related PM_{2.5} build-up. For months from **Mar to Aug**, significant **positive trends** were found instead, indicating the increasing positive temperature impact during spring and summer.
- ☑ **PBLH influence in Jan and Feb** shows a declining or negative trend, indicating a growing role of atmospheric mixing and more variable synoptic conditions in mid-winter. Similar significant trends were found for **Oct and Nov**.
- ☑ **Wind direction influence in Jan and Feb** is shifting toward cleaner patterns. Negative trend in wind direction implies more frequent NW/W/SW ventilation events, replacing stagnant continental easterly patterns.

DIURNAL AND SEASONAL PATTERNS

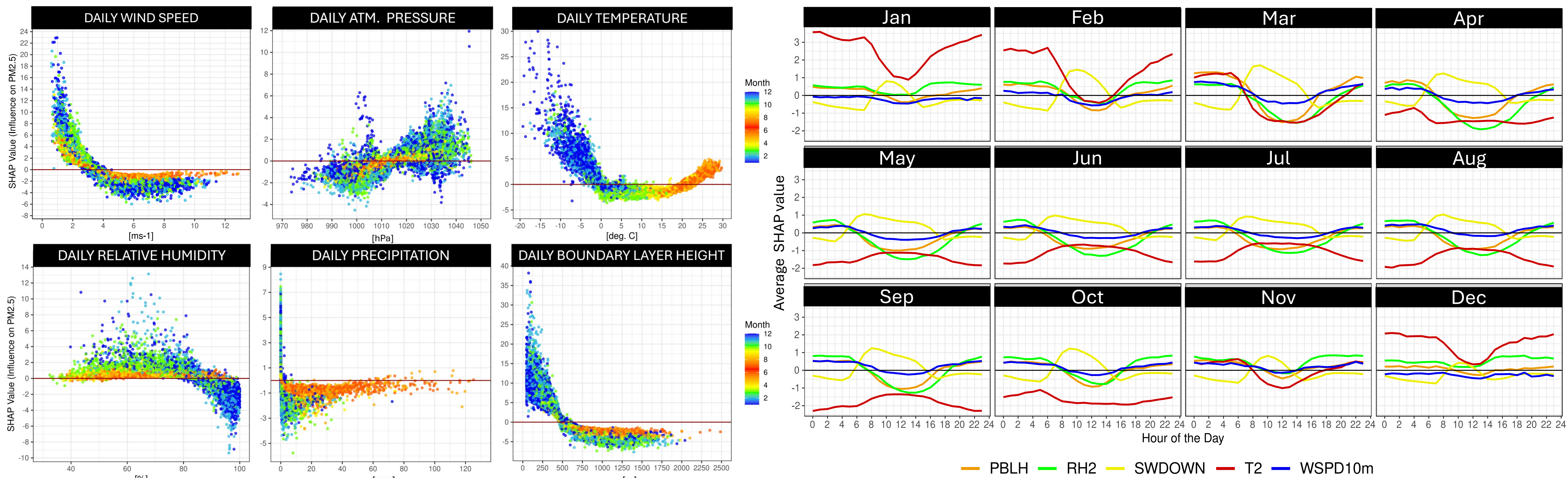


Figure 3. Seasonal patterns of daily wind speed, relative humidity, atmospheric pressure, precipitation, temperature and boundary layer height (PBLH) influence on PM_{2.5}.

Figure 4. Diurnal patterns of PBLH, relative humidity (RH2), shortwave radiation (SWDOWN), temperature (T2) and wind speed (WSPD10m) influence on PM_{2.5} by month

Figure 5. Spatial patterns of PBLH influence on PM_{2.5} shown by month

Wind Speed

- The strongest positive effect on PM_{2.5} occurs at wind speeds < 3 m/s across all seasons. At wind speeds > 4 m/s, the impact becomes negative. Effects are more pronounced in colder seasons, and weaker in summer, even at higher speeds.

Relative Humidity

- Daily RH shows peak influence on PM_{2.5} (positive SHAP) at mid-range (55–70%) in transitional seasons. Very high daily RH (>90%) in cold seasons flips SHAP negative.

Atmospheric Pressure

- High pressure (>1020 hPa) aligns with higher PM_{2.5} under stagnant anticyclonic conditions; low pressure is associated with lower PM_{2.5}, especially in transitional months.

Precipitation

- In cold seasons, even moderate rain reduces PM_{2.5} (negative SHAP). In summer, this effect weakens—possibly due to much shorter but more intensive precipitation events and already low pollution.

Temperature

- SHAP values rise sharply below 0°C (suggesting heating & inversions) in winter. In the 0°C – 20°C range, the effect on PM_{2.5} is predominantly negative. SHAP turns positive again in summer months—when daily temperature exceeds ~20°C.

Boundary Layer Height (PBLH)

- PBLH below 500 m is linked to strong positive SHAP. Higher PBL flattens SHAP and turns it negative, showing cleaning effects of convective mixing, most pronounced in transitional months.

Wind Direction

- N/NW/W winds show mostly negative SHAP, suggesting cleaning effects of polar and marine air masses. E–SE–S winds show mostly positive influence on PM_{2.5}. SW/NE show both positive and negative contributions. The influence is most pronounced in winter months and the weakest in summer.

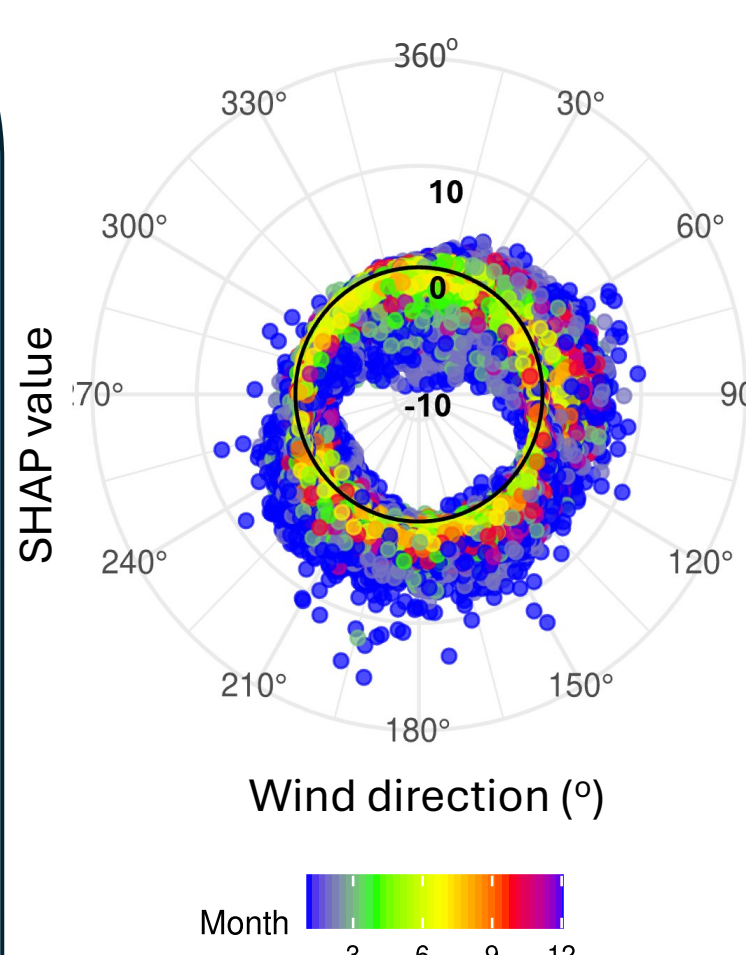


Figure 6. Seasonal patterns of wind direction influence on PM_{2.5}.

Boundary Layer Height (PBLH)

- SHAP values are negative during the daytime—indicating that solar-driven PBLH rise reduces PM_{2.5} by enhancing dispersion. The effect is most evident in early spring, associated with sharp daytime increases in PBLH. SHAP turns positive in early morning and evening hours, correlating with persistently shallow boundary layers. In winter, the diurnal variation of PBLH influence becomes less pronounced.

Relative Humidity (RH2)

- Generally positive SHAP values overnight and in the early morning, especially during cooler months. These turn more neutral or negative by midday, with the strongest variation seen in spring. The overall pattern resembles that of PBLH.

Shortwave Radiation (SWDOWN)

- Positive SHAP influence during the day, peaking from Feb to Apr—possibly indicating sunlight enhances photochemical PM_{2.5} formation (e.g., secondary aerosols). Nighttime influence is minimal, consistent with the lack of direct radiative effects.

Temperature (T2)

- The diurnal pattern forms an upward parabola from Nov to Mar, with lower or negative SHAP values during the day and high positive values at night—suggesting winter nights are linked to stable, polluted conditions (thermal inversions + combustion emissions). In summer, the trend reverses into a downward parabola: daytime may coincide with increased emissions, secondary aerosol formation, and resuspension, while nighttime tends to show reduced emissions.

Wind Speed (WSPD10m)

- Slightly negative SHAP values in the afternoon, especially in spring and autumn, indicating modest dispersion effects. Mostly positive overnight and in early morning hours—a pattern similar to PBLH and RH.

REFERENCES

Lundberg, S. M., & Lee, S.-I. (2017). A Unified Approach to Interpreting Model Predictions. *Advances in Neural Information Processing Systems*, 30. Molnar, C. (2022). *Interpretable Machine Learning*. Leanpub. Petäjä, T., et al. (2016). Enhanced air pollution via aerosol-boundary-layer feedback in China. *Scientific Reports*, 6, 16996.

CONCLUSIONS

- ✓ Explainable machine learning reveals **consistent physical rules** in how weather influences PM_{2.5}, highlighting the method's strength for interpreting air quality models.
- ✓ PM_{2.5} responses to meteorology are **highly scale- and context-dependent**, with clear seasonal, diurnal, and spatial modulations.
- ✓ SHAP analysis captured **both expected patterns and subtle regime shifts**, such as later onset of dispersion effects in some cities or temperature-related PM_{2.5} rise in warm conditions.
- ✓ Observed decadal trends suggested **evolving pollutant sensitivity**, likely linked to **changing emissions and climate factors**.
- ✓ Overall, the approach offers a **valuable framework to track, explain, and anticipate air quality dynamics** in a changing environment.

ACKNOWLEDGMENTS

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