International Journal for Research in Environment
Published by: **Green Publications**
Article Type: **Research**
DOI:**10.53555/env.v1i1.2574**
Volume 01 Issue 01 March 2026

Deciphering Air Quality Patterns Through Multi-Pollutant Assessment

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Received:- 05/02/2026, Revised:- 06/03/2026, Accepted:- 13/03/2026, Published:- 20/03/2026

ABSTRACT

Air quality conditions arise from the interactions among particulate and gaseous pollutants, but many of the assessments still focus on the individual pollutants. Thus, the need for integrated analysis for the detection of common patterns as well as different pollutant behavior and recurring air quality profiles. This study aimed to decipher air quality patterns through a multi-pollutant assessment of PM2.5, CO_2, NO_2, SO_2, and O_3. A quantitative cross-sectional analysis was conducted using 5,999 complete observations. Descriptive statistics and distribution plots were used to characterize pollutant concentrations. Pearson correlation analysis assessed inter-pollutant relationships, principal component analysis reduced dimensionality, and K-means clustering identified distinct multi-pollutant profiles. CO_2, NO_2, and SO_2 showed the greatest relative variability, whereas O_3 was comparatively more stable. Moderate positive correlations were observed among CO_2, NO_2, and SO_2, while O_3 showed only weak associations with the remaining pollutants. The first two principal components explained 64.11% of the total variance, and the first three explained 79.18%. PM2.5, CO_2, NO_2, and SO_2 loaded mainly on the first component, whereas O_3 dominated the second. Three clusters were identified: two high-pollution profiles differentiated primarily by O_3 concentration and one lower-pollution profile containing 47.14% of observations. The results show that understanding air quality is best captured from air quality patterns rather than individual measurements. The integrated analytical framework offers a practical foundation for the classification, monitoring and management of pollutants in the environment.

Key words: air pollution, multi-pollutant assessment, principal component analysis, K-means clustering, air quality profiles

1. Introduction

Air pollution is one of the greatest environmental problems in the world due to the effects it has on ecosystems, climate and human health. The concentrations of particles and gaseous pollutants in the atmosphere have significantly risen due to rapid urbanization, industrialization, transport and combustion of fossil fuels, leading to a reduction in air quality in developed and developing areas. Air Quality monitoring is a high priority for environmental and public health monitoring because exposure to polluted air has been linked to increased mortality, chronic diseases and reduced quality of life around the world (Manisalidis et al., 2020). Air pollution is also a significant driver of disease burden, shown to be a significant risk factor for respiratory illness, cardiovascular diseases and early death in a variety of populations (Landrigan, 2017). The impact of poor air quality goes beyond human health, and is increasingly affecting socioeconomic development and environmental sustainability. Economically disadvantaged populations are also more likely to be exposed to high levels of pollutants compared to others, exacerbating pre-existing health inequalities and reducing the opportunities for sustainable development (Rentschler & Leonova, 2023). At the same time, the pollutants present in the atmosphere closely interact with climatic processes, and integrating environmental management strategies that also tackle climate change mitigation is essential (Pinho-Gomes et al., 2023). Recent evaluations also make clear that the high burden of global pollution remains despite better environmental regulation and monitoring, highlighting the need for improved evidence-based air quality management (Fuller et al., 2022).

Some of the pollutants that are monitored regularly can be considered as indicators of ambient air quality, including particulate matter, CO_2, NO_2, SO_2, and O_3. Fine particulate matter is well known to have detrimental cardiovascular effects, including oxidative stress and systemic inflammation (Hamanaka & Mutlu, 2018). Traffic-related air pollution has also been associated with neurological impairment, indicating that prolonged exposure to air pollutants is associated with multiple physiological systems other than the respiratory system (Costa et al., 2017). Likewise, cardiovascular effects of ambient air pollution have been well studied, and it is well established that exposure to a mixture of pollutants carries a higher burden than exposure to any individual pollutant (Bourdrel et al., 2017). In recent years, research has focused on the impacts of multiple atmospheric contaminants rather than on individual contaminants. The main findings of multi-pollutant exposure on respiratory health indicators highlight the relevance of integrated pollutant assessment for the understanding of overall air quality conditions (Meo et al., 2024a). The environmental monitoring technologies were further developed, which increased the accuracy and efficiency of ambient air quality measurements and made it possible to collect a more comprehensive data set for environmental assessment and decision-making (Kulykivskyi & Ponomarenko, 2025). These findings also confirm that the combination of multiple pollutants, rather than individual ones, is a better way to assess respiratory function because simultaneous changes in multiple pollutants have been demonstrated to have a more potent impact on respiratory function than changes in a single pollutant (Lee et al., 2024). A growing amount of monitoring data contains multiple variables and has become useful for analysing the data and explaining the monitoring results at an increasing level of complexity. Multivariate statistical methods have proven useful for analysing monitoring data and explaining monitoring results on an increasing level of complexity. Abundant environmental data can be analyzed and interpreted by reducing the dimensionality using principal component analysis (PCA), and finding the dominant pollution sources and underlying relations among several atmospheric pollutants successfully (Abdullah et al., 2018). More recently, integrated analytical frameworks accounting for multiple pollutants and advanced computational approaches have shown better potential to capture spatial and environmental air quality patterns, highlighting the increased relevance of multi-pollutant assessment in today's environmental studies (Davtalab et al., 2025).

While some studies have significantly contributed to the knowledge on the environmental and health impacts of air pollution, a large number of studies still target single pollutants or certain health effects. Researchers who have used integrated analytical techniques have focused more on predictive modeling or source attribution, and relatively few have integrated descriptive statistics, correlation analysis, dimensionality reduction and clustering into a single framework to describe the overall pollutant behavior. In this sense, the inter-relationships between the main pollutants as well as the identification of the different air quality profiles are not sufficiently explored by extensive statistical exploratory analysis. This is particularly helpful in the understanding of pollutant interactions and may help to better represent the air quality patterns that can be used for future environmental monitoring and management.

To address this, the current study was designed to elucidate air quality trends using a multi-pollutant assessment. The study analyses the distribution of PM2.5, CO_2, NO_2, SO_2 and O_3 levels, investigates the interdependencies between pollutants by correlation, presents principal components that explain the variations of pollutants through principal component analysis and finally groups the observations into air quality profiles using K-means clustering. The combination of descriptive and multivariate approaches allows a systematic interpretation of atmospheric pollutant behavior, which helps to find a more complete description of the multi-pollutant air quality patterns.

2. Methodology

2.1 Research Design

The research design of this study was quantitative and cross-sectional which aimed to study the pattern of air quality by analyzing the quality of air by integrating various air pollutants. A descriptive and multivariate statistical analysis was used to explain pollutant distributions, to explore relationships between pollutants, to reduce data dimensionality and to classify air quality profiles. The methodology was chosen to be able to provide a thorough analysis of pollutant behaviour while keeping the analysis of the air quality patterns as the study goal, being the deciphering of multi-pollutant air quality patterns.

2.2 Data Source

This study has employed the dataset available in a publicly available repository for environmental monitoring built by Trisna and Islam (2025). It included 5,999 complete observations of five major atmospheric pollutants: PM2.5, CO_2, NO_2, SO_2 and O_3; pollutant concentration measurements appropriate for exploratory environmental assessment. The dataset was chosen since it was complete and had no missing data, for the purpose of conducting multi-pollutant statistical analyses (Trisna & Islam, 2025).

2.3 Data Preparation

The quality of the data was determined by the type of data, the size of the data sets, missing data, duplicate data, and descriptive statistics. All variable names were uniformized in order to be consistent throughout the analysis and the numerical formats were checked before the statistical processing. No data were identified as being missing or duplicated and no data imputation or data removal processes were necessary and all observations were retained for subsequent analyses.

2.4 Statistical Analysis

Descriptive statistics are first computed to describe the spread and central tendency of the pollutants by means of the minimum concentration observed, maximum concentration observed, median, quartiles, standard deviation and coefficient of variation. Further insights into the distributional characteristics were obtained from histograms with kernel density estimates and standardized boxplots, assessing the distributional pattern and relative variation of pollutants. Pearson correlation analysis was then carried out to measure the magnitude and direction of linear associations between pairs of pollutants and to determine if there was multicollinearity.

2.5 Multivariate Analysis

To simplify the analysis of data and to identify the main sources of variability of the measured pollutants, principal component analysis (PCA) was performed on the standardized pollutant concentrations. To see how much variance is explained by each principal component, the proportion of variance explained for each component was considered, along with the loading matrix, which details the contribution of individual pollutants to the extracted component. The standardized data set was then used to create an air quality profile by applying K-means clustering. The elbow method for finding the optimal number of clusters was applied to the within-cluster sum of squares and finally a multi-pollutant classification model was used to classify the observations into multi-pollutant clusters. The composition of each air quality cluster and average concentrations of pollutants was then compared to characterize the characteristics of each air quality profile.

3. Results

3.1 Descriptive Characteristics of Air Pollutants

There were 5,999 observations included in the analysis, in which complete measurements were available for all five air pollutants. The ranges of concentrations of PM2.5, CO_2, NO_2, SO_2 and O_3 were very large. CO_2 showed the highest mean concentration (2330.33), followed by SO_2

(132.49), O_3 (124.65), NO_2 (101.00), and PM2.5 (20.61). The highest relative variability was observed for SO_2 (CV = 90.98%), CO_2 (89.80%) and NO_2 (89.08%), while the lowest variability was found for O_3 (CV = 47.37%). The results showed a high level of variability in the levels of pollutants, which has been used as a suitable basis for further multivariate analyses. Table 1 shows the descriptive statistics of the measured air pollutants.

Table 1. Descriptive Statistics of Air Pollutant Concentrations

Pollutant	**N**	**Mean**	**SD**	**Minimum**	**Q1**	**Median**	**Q3**	**Maximum**	**CV (%)**
PM2.5	5999	20.61	11.99	3	11.0	18.0	28.0	48	58.14
CO_2	5999	2330.33	2092.69	40	624.5	1183.0	4092.5	6999	89.80
NO_2	5999	101.00	89.96	5	27.0	48.0	174.0	300	89.08
SO_2	5999	132.49	120.54	1	35.0	59.0	229.0	400	90.98
O_3	5999	124.65	59.05	10	77.0	123.0	167.0	250	47.37

Note: SD, standard deviation; Q1, first quartile; Q3, third quartile; CV, coefficient of variation.

3.2 Distribution of Air Pollutant Concentrations

This was reflected in the differences in pollutant concentration patterns as shown in the frequency distributions. The distribution of PM2.5 was relatively broad with moderate dispersion, while the distributions of CO_2, NO_2 and SO_2 were positively skewed with a high number of lower concentration values and few of high concentration values. Comparatively, O_3 was found to have a more balanced distribution with low variability. These distributional characteristics suggest that each specific pollutant has a unique concentration distribution. The frequency distributions and kernel density estimates of the air pollutants measured are shown in Figure 1A. The standardized variability of pollutant concentrations for each variable is also compared in Figure 1B, which shows that CO_2, NO_2, and SO_2 have larger spreads compared to PM2.5 and O_3 after standardization.

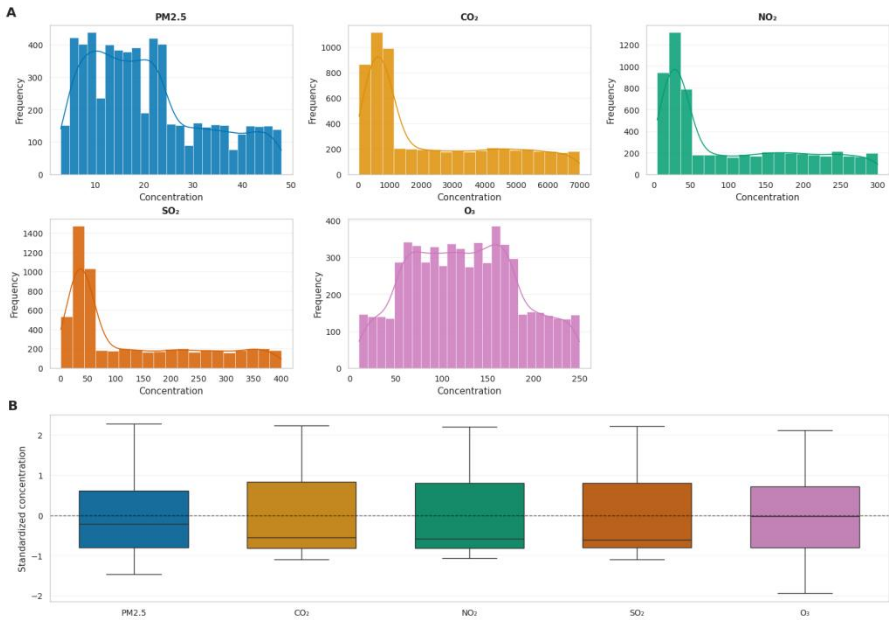

Figure 1. Distribution and Standardized Variability of Air Pollutants. (A) Frequency distributions and kernel density estimate of PM2.5, CO_2, NO_2, SO_2, and O_3 concentrations. (B) Standardized boxplots comparing the variability of pollutant concentrations across all observations.

3.3 Correlation Among Air Pollutants

All measured pollutants were positively correlated with each other, and the magnitude of the correlation varied widely; Pearson correlation analysis showed this. The strongest relationship was observed between CO_2 and NO_2 ($r = 0.489$), followed by NO_2 and SO_2 ($r = 0.475$), and CO_2 and SO_2 ($r = 0.473$). PM2.5 showed weak-to-moderate positive correlations with CO_2 ($r = 0.322$), NO_2 ($r = 0.314$), and SO_2 ($r = 0.307$). However, the correlations between O_3 and the other pollutants were only weak and positive ($r = 0.065$-0.092), indicating a relatively independent behaviour in the data set. Limited multicollinearity exists among the variables as there are no strong correlations above 0.70. The Pearson correlation coefficients are shown in Table 2.

Table 2. Pearson Correlation Coefficients Among Air Pollutants

	PM2.5	**CO_2**	**NO_2**	**SO_2**	**O_3**
PM2.5	1.000	0.322	0.314	0.307	0.070
CO_2	0.322	1.000	0.489	0.473	0.065
NO_2	0.314	0.489	1.000	0.475	0.082
SO_2	0.307	0.473	0.475	1.000	0.092
O_3	0.070	0.065	0.082	0.092	1.000

The correlation among pollutants is summarized visually in Figure 2, showing moderate positive correlations among PM2.5, CO_2, NO_2 and SO_2 and the relatively low correlations with O_3. Lower triangular heatmap showing pairwise Pearson correlation coefficients between PM2.5, CO_2, NO_2, SO_2 and O_3.

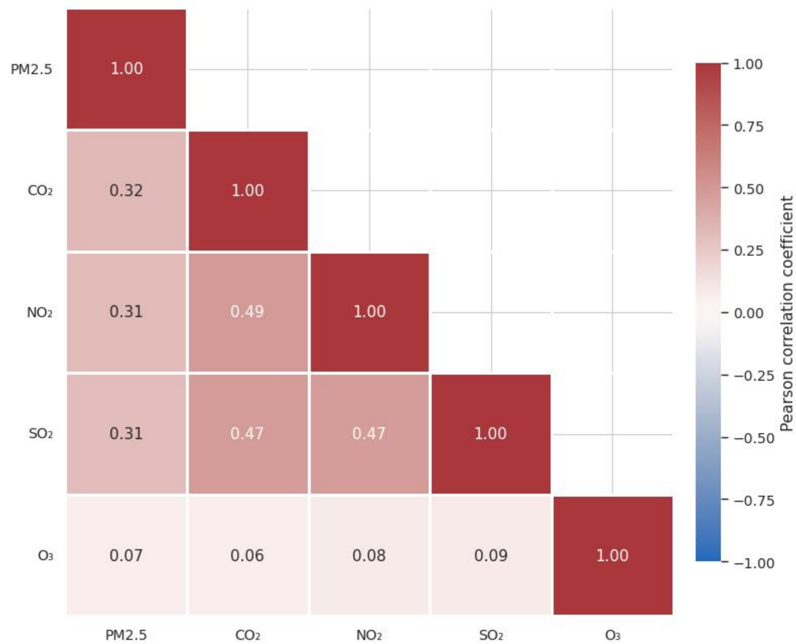

Figure 2. Pearson Correlation Matrix of Air Pollutants.

3.4 Principal Component Analysis

The first principal component accounted for 44.47% of the total variance, followed by 19.63% of the total variance by the second principal component, giving a total cumulative variance of 64.11%. These three first principal components explained 79.18% of the overall variability of the data set, suggesting that the multidimensional information about pollutants could be summarized by a few latent variables. The loading structure indicated that PM2.5, CO_2, NO_2 and SO_2 were mainly associated with the first principal component, while O_3 was mainly associated with the second principal component, indicating a comparatively independent variation of O_3. Figure 3A shows the results of this projection, with the samples spread out in the reduced-dimensional space before the patterns are interpreted.

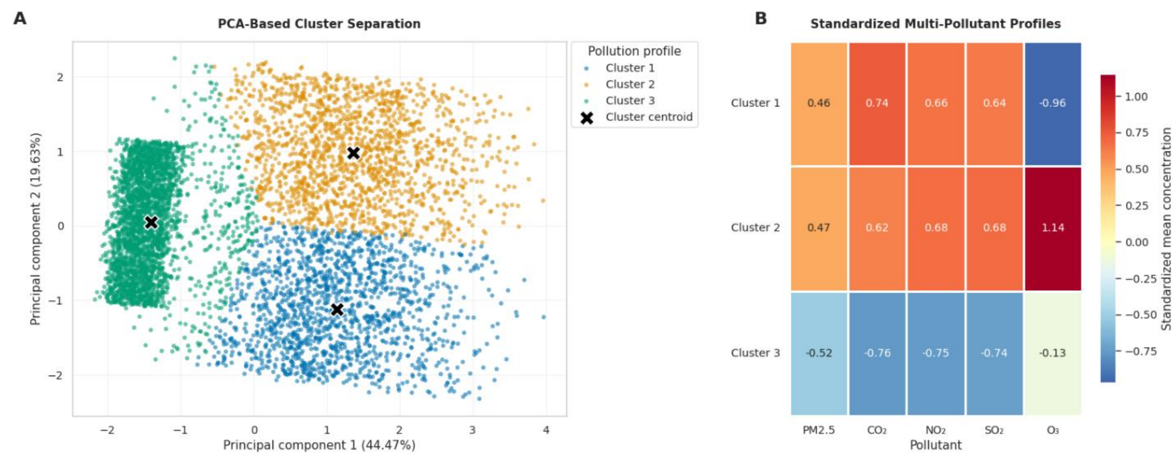

Figure 3. Multi-Pollutant Air Quality Profiles Identified Through Clustering. (A) Projection of observations onto the first two principal components, colored according to cluster membership, with black crosses representing cluster centroids. (B) Heatmap of standardized mean pollutant concentrations for each cluster.

3.5 Multi-Pollutant Cluster Profiles

The dataset was clustered into three pollutant profiles using K-means. Cluster 1 was a group of 1551 observations (25.85%) with high concentrations of PM2.5, CO_2, NO_2 and SO_2 and low concentrations of O_3. The cluster with 1620 observations accounted for 27.00% and had the same high concentrations of PM2.5, CO_2, NO_2 and SO_2 as Cluster 1, while having the highest concentrations of O_3 of the three clusters. Cluster 3 (2828 observations, 47.14%) exhibited significantly lower levels of PM2.5, CO_2, NO_2 and SO_2, but intermediate levels of O_3. The results suggest that there are different “multi-pollutant” air quality profiles. The composition of the clusters and mean concentration of pollutants are summarized in Table 3. The standardized mean pollutant concentrations for each cluster are shown in Figure 3B, which contrasts the different pollution profiles detected by the clustering algorithm.

Table 3. Cluster Size and Mean Multi-Pollutant Concentration Profiles

Cluster	**N**	**Percentage (%)**	**PM2.5**	**CO_2**	**NO_2**	**SO_2**	**O_3**
1	1551	25.85	26.14	3885.89	160.78	209.48	67.69
2	1620	27.00	26.22	3618.37	162.06	214.82	192.18
3	2828	47.14	14.37	739.36	33.23	43.11	117.20

4. Discussion

Substantial variation was found in the concentrations of the pollutants in PM2.5, CO_2, NO_2, SO_2, and O_3 among the 5,999 observations during the multi-pollutant assessment. Note that the CO_2, NO_2 and SO_2 had higher coefficients of variation, which suggests that these pollutants were more variable under the conditions measured and that O_3 was more stable. The distributions of CO_2, NO_2 and SO_2 are positively skewed, indicating that the lower concentrations happened more often with a smaller number of observations at higher levels of pollution. The dispersion of PM2.5 was moderate and this was a different pattern of concentration than the primary pollutants, O_3 was more balanced. The correlation is further evidence of the coordinated behavior of CO_2, NO_2, SO_2 and PM2.5. The moderate positive correlations between CO_2, NO_2 and SO_2 suggest that these pollutants may be emitted in similar amounts. Their relationships with PM2.5 were less pronounced but were positive, indicating some overlap in their concentrations. The weak correlation of O_3 with the other pollutants is related to the different behavior of O_3 in the atmosphere. O_3 is usually generated as a secondary photochemical product, and the concentration can therefore vary from the one related to the emissions of the pollutants that generate it to the one related to the environmental conditions. These relationships were subsequently illustrated by Principal component analysis, which distinguished between two main dimensions of pollutants. This was primarily the result of CO_2, NO_2, SO_2, and PM2.5, which indicate a common gradient of pollution caused by primary pollutants. The second component was almost exclusively correlated with O_3, indicating the presence of an independent dimension in the overall air quality pattern, independent of O_3. The first two components captured 64.11% of the total variance, and the first three captured 79.18%, indicating that the five-pollutant structure could be captured with a smaller number of latent dimensions. This cluster analysis determined three meaningful air quality clusters. The elevated levels of PM2.5, CO_2, NO_2 and SO_2 were found in both clusters with significantly different concentrations of O_3. Cluster 1 was a high primary pollutant profile and a low ozone profile, while Cluster 2 was a high primary pollutant profile with a high ozone profile. Most of the observations (nearly 50%) were in Cluster 3, where the PM2.5, CO_2, NO_2, and SO_2 were relatively low, whereas O_3 was relatively high. The profiles illustrated here show that the air quality is not well represented by a single pollutant but is rather a representation of different combinations of primary and secondary pollutants.

The different variations found in pollutants is consistent with the findings from Chengdu that showed that the temporal and spatial characteristics of PM2.5, SO_2, NO_2, O_3 and CO were not the same (Xiao et al., 2018). There is also evidence of variability in pollutants across Indian metros, with seasonality and urban location having a significant impact on pollutant concentrations (Sharma et al., 2025a). The positive correlation between PM2.5 and other combustion-related pollutants, i.e., NO_2 and SO_2, is also found to be consistent with the study done in Gazipur, where gaseous pollutants and particulates showed a similar seasonal trend under the influence of industry and urbanization (Mukta et al., 2020). Similar data from Tehran revealed that PM concentration and SO_2 concentration were correlated under the varying atmospheric and emission conditions, further highlighting the importance of jointly analyzing pollutants (Ahmadian et al., 2025). The results of the PCA are in agreement with other previous applications of multivariate source-oriented analysis. Delhi-based research showed that using PCA techniques, one could be able to identify major sources of PM2.5 and could summarise the complicated relationships between them in an urban setting (Jain et al., 2017). A similar study in the city of Mosul also revealed that principal component analysis could identify the main sources of air pollution and explain the temporal variations in air quality (Shihab, 2022).

The unique role of O_3 in the second PC is related to the studies that have found that ozone can react differently from other directly emitted pollutants. Temporal modelling in Delhi has shown that the trends of pollutants need to be considered separately, as primary pollutants and O_3 have different responses to emissions and atmospheric processes (Alawi et al., 2024). The integrated exposure modeling in urban areas with high density has also highlighted that multi-pollutant assessment is essential due to the differences in contribution to the combined exposure pattern from individual pollutants (Li et al., 2024). The three-cluster solution is also in line with previous classification studies. The successful clustering of recurrent PM2.5 composition patterns in Seoul by k-means clustering demonstrates the potential of cluster analysis to identify meaningful temporal pollution regimes (Choi et al., 2024). The use of multivariate classification with mobile sensor data has also been able to differentiate urban air pollution profiles that could not be observed from single-variable analysis (De Oliveira et al., 2019). These profiles are relevant to health because there is evidence that exposure to multiple pollutants (PM2.5, NO_2, SO_2, CO, and O_3) can interact to have a stronger impact on lung function than exposure to individual pollutants alone (Meo et al., 2024b). Furthermore, the analytical frameworks that could describe the PM2.5

dynamics, with a nonlinear and multi-scale variation, have proved to be beneficial in the context of the complex pollution behavior, as predicted by research by Sharma et al. (2025b).

The results confirm the need for multi-pollutant approaches to air quality assessment. Pollutant monitoring programs may miss combinations of pollutants, especially when high levels of primary pollutants are accompanied by either low or high O_3 levels. Clusters identified can assist with the classification of pollution events, prioritization of monitoring actions, and development of profile-specific control actions. PCA is also a very useful tool to reduce the complicated monitoring information to understandable dimensions without losing most of the variance.

A few limitations should be considered. There was no temporal, spatial, meteorological or source-specific information in the dataset, which limited the interpretation of seasonal variation, spatial distribution and emission origin. The pollutant concentrations were then assessed as a composite monitoring record, instead of in specific environmental conditions. Future studies should include the inclusion of timestamps, monitoring location, temperature, humidity, wind conditions and land-use characteristics. Longitudinal modelling, source apportionment and external validation of the identified air quality profiles to multiple cities would further improve the generalizability and environmental interpretation of profiles.

5. Conclusion

The multi-pollutant assessment demonstrated that PM2.5, CO_2, NO_2, SO_2 and O3 exhibited different behaviour and variability from one another and between the pollutants and time. CO_2, NO_2 and SO_2 were the most variable relative and were the most correlated with the other pollution components (PM2.5), whereas O_3 was more independent. The five-pollutant data were reduced to a smaller set of interpretable dimensions using principal component analysis, which accounted for 79.18% of the total variation in the first three components. Three air quality profiles were further distinguished using k-means clustering, consisting of two clusters with high pollution levels, clearly separated by the O_3 concentration and one cluster with lower pollution levels, where the PM2.5, CO_2, NO_2 and SO_2 concentrations were reduced. The results of this study indicate that the combined pattern of pollutants can provide a better understanding than individual measurements of air quality. The integrated approach of descriptive statistics, correlation analysis, principal component analysis, and clustering is used for a practical approach to dominant pollutant relationships and the classification of contrasting air quality conditions.

These profiles can help to more precisely monitor, understand and manage pollution episodes. Assessments that integrate temporal, spatial, meteorological and source data in the future would give a more descriptive account of the mechanisms of the development and change of these multi-pollutant patterns.

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