Characteristics, sources, reactivity, and priority control of atmospheric VOCs in a national economic development zone in southern Jiangsu, China

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Abstract. This study examined the pollution characteristics, sources, and reactivity of VOCs in a national economic and technological development zone in southern Jiangsu, using hourly online observations from June 2023 to May 2024. The average TVOC concentration was 57.93±45.98 μg/m³, with alkanes and aromatics as the dominant components. VOCs exhibited distinct seasonal variations, peaking in winter and bottoming in summer, along with a multi-peak diurnal pattern. Positive matrix factorization (PMF) identified five major sources: industrial emissions (39.53%), solvent use (21.24%), oil and gas volatilization (20.76%), traffic emissions (16.20%), and combustion sources (2.27%). Potential source contribution function (PSCF) analysis revealed that local and short-range transport dominated in spring and summer, while long-range transport from northern and northwestern areas contributed more in autumn and winter. A comprehensive priority-control assessment, considering mass concentration, OFP, SOAFP, and toxicity, identified aromatic hydrocarbons as the top priority species, followed by certain alkanes and alkenes. These findings support refined VOC management and coordinated control of ozone and SOA in industrial development zones.

1 Introduction

In recent years, ozone (O_3) pollution has become a major challenge in atmospheric environmental management. Volatile organic compounds (VOCs), as key precursors of O_3 and secondary organic aerosol (SOA), play a critical role in atmospheric oxidation, haze formation and human health risks[1]. Extensive studies have investigated VOC characteristics and sources in key urban agglomerations in China, such as the Yangtze River Delta, Pearl River Delta, Beijing–Tianjin–Hebei region and Sichuan–Chongqing area[2]. However, limited research has focused on national economic and technological development zones (ETDZs), where industrial emissions, solvent usage and oil–gas volatilization are highly complex. This study focuses on a typical national ETDZ in southern Jiangsu, Yangtze River Delta. Based on one-year online observation data, we analyzed VOC concentration levels and temporal variations, quantified sources using PMF, identified regional transport via backward trajectories and PSCF, and estimated OFP and SOAFP contributions. The findings provide a scientific basis for targeted VOC control and coordinated O_3 mitigation in industrial zones[3].

2 Materials and Methods

2.1 Observation site

The observation site shown in Figure 1 was located at a regional environmental monitoring center within a national ETDZ in southern Jiangsu. The surrounding area is characterized by intensive industrial activities, factory buildings, and nearby major transportation corridors. The monitoring campaign lasted from 00:00 on 1 June 2023 to 23:00 on 1 June 2024, and ambient VOCs were measured at an hourly resolution[4]. After removing invalid records caused by instrument malfunction, power outage, and other abnormal conditions, the overall valid data rate was 88.3%[5].

Figure 1. Geographical distribution of sampling sites.

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2.2 Data analysis methods

2.2.1 Positive matrix factorization (PMF) model

The PMF 5.0 model developed by the US Environmental Protection Agency (EPA) was used to quantify the contributions of different sources based on the measured VOC composition. PMF decomposes the observed concentration matrix into a source contribution matrix (G) and a source profile matrix (F) under non-negative constraints, thereby identifying both source types and their relative contributions[6]. The optimal solution is obtained by minimizing the objective function Q and comparing the calculated Q value with the theoretical expectation.

In this study, the PMF 5.0 model was applied to apportion VOC sources. Species selection followed strict criteria: only compounds with signal-to-noise ratio (S/N) ⩾1.0 were retained (species with S/N<0.5 were classified as bad, 0.5–1.0 as weak), and those with>60% of samples below detection limit or residual errors >3 was excluded from modeling. After screening, representative tracers were selected, and five distinct emission sources were ultimately resolved by evaluating Q values and local air quality conditions.

$$X_{ij} = \sum_{k=1}^{p} g_{ik} + f_{kj} + e_{ij} \quad (1)$$

where X_{ij} is the concentration of species j in sample i, g_{ik} is the contribution of source k to sample i, f_{kj} is the fraction of species j in source k, e_{ij} is the residual, and p is the number of factors.

$$Q = \sum_{i=1}^{n}\sum_{j=1}^{m}\left[\frac{x_{ij}-\sum_{k=1}^{p} g_{ik}+f_{kj}}{u_{ij}}\right]^2 \quad (2)$$

In PMF, the objective function is weighted by species-specific uncertainty, and both G and F are constrained to be non-negative. This framework is particularly suitable for ambient VOC studies because it can resolve mixed sources without requiring prior source profiles.

$$Unc = \sqrt{(EF \times C)^2 + (0.5 \times MDL)^2}(c > MDL) \quad (3)$$

$$Unc = \frac{5}{6} \times MDL(c < MDL) \quad (4)$$

Concentration and uncertainty matrices were prepared according to the PMF 5.0 User Guide. Species below the method detection limit (MDL) were treated following the recommended uncertainty scheme, and the optimal number of factors was selected by considering Q values, residual distributions, factor interpretability, and seasonal consistency of the resolved source profiles.

2.2.2 Potential source contribution function (PSCF) model

Air-mass back trajectories were computed using the Meteoinfo model. The PSCF, which is based on the Meteoinfo model, can be used to infer pollution source regions. In this study, the pollution value was set as the average value of the species. The cell grid had an array of 0.5° × 0.5°. To reduce the influence of small values, PSCF values are multiplied by a weighting coefficient and more details are described by Wang[7].

3 Results and Discussion

3.1 Temporal variation of VOCs

Figure 2 illustrates the temporal variations of TVOC and grouped VOCs from June 2023 to May 2024. TVOC fluctuated between 40–100 μg/m^3, with alkanes dominating both absolute concentrations (peaking >80 μg/m^3) and proportional contributions (>60%), closely tracking TVOC trends. Alkenes and alkynes showed lower baseline levels but distinct episodic peaks, suggesting specific emission or photochemical events, confirming alkanes as the primary VOC component in this industrial zone.

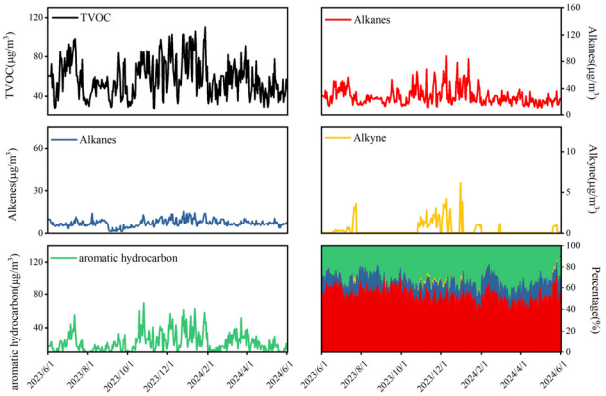

Figure 2. Time series of grouped VOC concentrations, TVOCs, and group contributions.

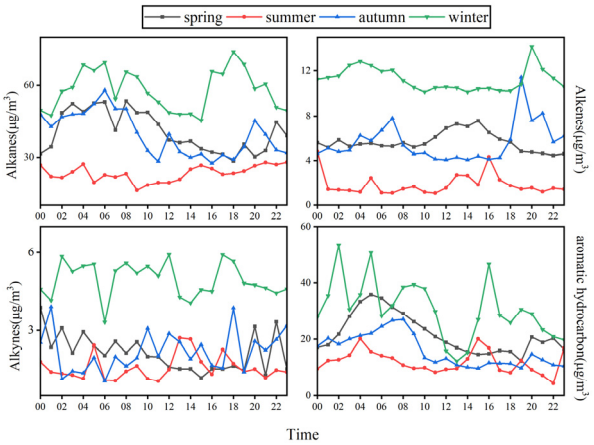

Figure 3. Seasonal diurnal variation of VOC groups.

3.2 Chemical composition of atmospheric VOCs

Figure 3 shows the diurnal and seasonal variations of VOCs. Alkanes and aromatics were dominant, with all groups peaking in winter and bottoming in summer. VOCs presented multi-peak diurnal patterns driven by

emissions, boundary layer, and photochemical loss. Winter elevated concentrations were caused by poor diffusion and weak photochemistry, while summer conditions reduced VOC levels[8]. Figure 4 illustrates seasonal group distributions. Alkanes were consistently high across seasons. Alkenes and acetylene were low w.th weak seasonal variation. Aromatics showed strong seasonality with higher levels in winter, likely due to accumulation and increased industrial and solvent emissions. These temporal features suggest that VOC pollution in the ETDZ was jointly influenced by emission intensity and meteorological conditions, especially boundary-layer evolution and short-term episodic release from local industrial activities.

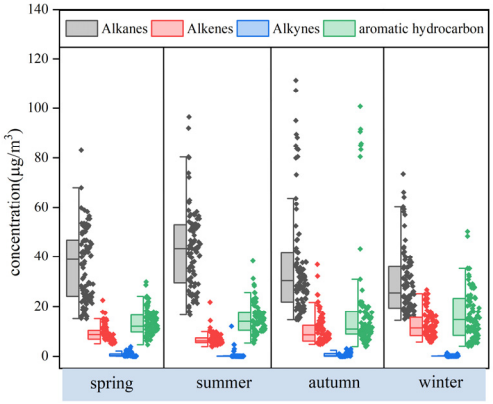

Figure 4. Seasonal distribution characteristics of VOC groups.

3.3 PMF source apportionment

Season-specific PMF analysis indicated a broadly consistent VOC source structure across the four seasons (Figure 5). Petroleum-related volatilization, industrial emissions, solvent use, and traffic-related emissions were identified in spring and summer, whereas an additional source factor became evident in the cold seasons. In autumn, gasoline volatilization characteristics were more pronounced, while in winter a distinct combustion factor was resolved. Factor identification was based on the dominant marker species in each profile together with their seasonal behavior, and the resolved factors were further grouped into five major source categories: industrial emissions, solvent use, oil and gas volatilization, transportation, and combustion. This source structure reflects the mixed industrial-functional characteristics of the ETDZ and indicates that local anthropogenic emissions were the primary driver of ambient VOC levels.

3.4 Potential source contribution function analysis

PMF results indicate that local industrial and traffic emissions are the dominant drivers of VOC pollution in the ETDZ, while regional transport also contributes to the observed concentration levels.

Figure 6 shows seasonal variations in potential source areas from PSCF analysis. In spring, high-value regions were located in the Yangtze River Delta urban clusters, dominated by local emissions and short-range transport. In summer, source areas shifted northward under monsoon circulation. In autumn, high values concentrated over the North China Plain, indicating stronger regional transport. In winter, main sources appeared over the southern Yangtze River Delta and eastern Jiangxi due to transport and accumulation under stable weather. VOC pollution in the ETDZ was jointly affected by local emissions and seasonal regional transport.

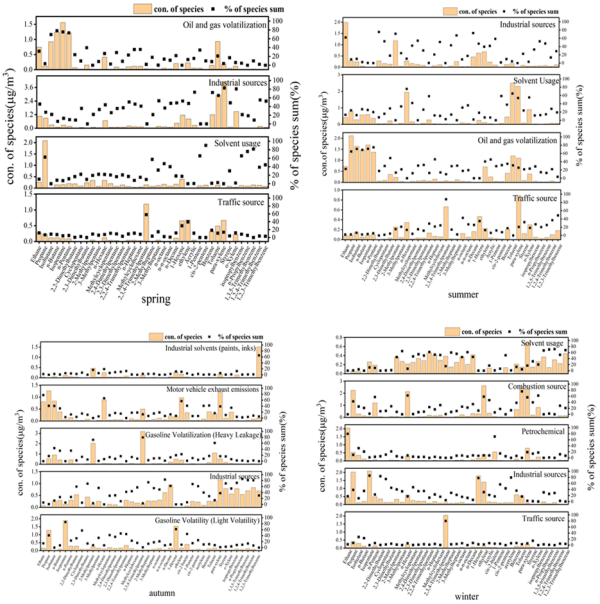

Figure 5. Seasonal PMF source profiles and source contributions: (a) spring; (b) summer; (c) autumn; (d) winter.

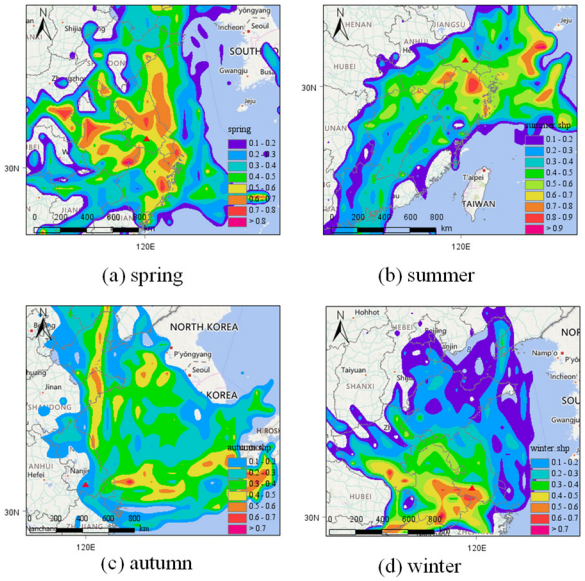

Figure 6. Distribution of potential TVOC source areas in the ETDZ in different seasons.

3.5 Reactivity analysis

This study integrated four indicators to identify priority VOCs: mass concentration, OFP (MIR), SOAFP (FAC), and toxicity (US EPA RfC). Due to missing toxicological and SOA parameters for some species, the ranking is a relative screening result rather than a full health-risk

assessment. The Classification criteria for VOC priority control indices as show in Table 1. Indicator weights were determined by the information entropy method after normalization.

Entropy-weighting analysis was performed on 50 effectively detected VOC species (excluding those with low detection frequencies) after normalizing mass concentration, OFP, SOAFP, and toxicity. The top-ranked species were mainly aromatics (xylenes, toluene, benzene), along with some reactive alkenes and light alkanes, classified as Level I (19 species), Level II (23), and Level III (8). This indicates that solvent-related and petrochemical/industrial emissions are key targets for refined VOC control in the ETDZ. Notably, the species with the highest control priority were not necessarily those with the highest mass concentrations, highlighting the importance of combining concentration, reactivity, SOA formation potential, and toxicity in VOC management.

Table 1. Classification criteria for VOC priority control indices.

Normalized Weight Range	Classification Criteria
$0.10 \leq W_i \leq 1.00$	I
$0.01 \leq W_i \leq 0.10$	II
$0.00 \leq W_i \leq 0.01$	III

3.6 Discussion

The present results show that the dominant VOC species in terms of concentration were not fully consistent with those contributing most to OFP, SOAFP, and priority control. In particular, aromatic hydrocarbons played a more important role in secondary pollution formation than suggested by their mass fraction alone. This highlights the need for VOC control strategies based on both concentration and atmospheric reactivity.

The combined source apportionment and transport analysis indicates that local industrial activities, solvent use, and oil-gas volatilization were the main contributors, while regional transport further enhanced VOC pollution in autumn and winter. Therefore, both local emission reduction and seasonal regional coordination are necessary. Some uncertainty remains due to the single-site observation and model-based source interpretation, and future work should include multi-site observations and more detailed emission information.

4 Conclusions

(1) Ambient VOC pollution in the ETDZ was at a moderate level, with an average TVOC concentration of 57.93 ± 45.98 μg/m^3. Alkanes and aromatics were the dominant components, and VOC concentrations were higher in winter than in summer.

(2) Industrial emissions were the dominant VOC source in the ETDZ, followed by solvent use, oil and gas volatilization, and transportation. VOC pollution was influenced by both local emissions and regional transport, with stronger long-range transport in autumn and winter.

(3) Aromatic hydrocarbons were the main contributors to secondary pollution and should be prioritized for control. Key reactive species included m/p-xylene, o-xylene, toluene, benzene, and ethylene due to their high contributions to OFP and SOAFP.

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