

Article

Variation and Transport Characteristics of Atmospheric SF₆ Column Concentrations over Hefei Retrieved from Ground-Based Remote Sensing Observations

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Highlights

What are the main findings?

- Atmospheric SF₆ column concentrations over Hefei during 2023–2025 were successfully retrieved using ground-based high-resolution FTIR observations with a total retrieval uncertainty of 5.70%.
- SF₆ concentrations showed clear seasonal variations, with higher values in summer and lower values in winter, while the annual growth rate of X_{SF6} reached 0.88 ppt yr^{−1}.

What are the implications of the main findings?

- High-SF₆ events over Hefei were mainly influenced by regional transport from eastern and southern China, particularly during summer.
- The results provide observational evidence for understanding the long-term variation characteristics and regional transport influences of atmospheric SF₆ over eastern China.

Abstract

Sulfur hexafluoride (SF₆) is a typical long-lived greenhouse gas that has attracted considerable attention due to its extremely long atmospheric lifetime and high global warming potential. In this study, atmospheric SF₆ column concentrations from 2023 to 2025 were retrieved using ground-based high-resolution Fourier transform infrared (FTIR) remote sensing observations at the Hefei site, China. The seasonal variation and annual trends of SF₆ were analyzed, and the potential influencing regions and transport characteristics of high-value events were investigated by combining wind direction statistics with backward trajectory clustering analysis. The results show that high SF₆ column concentrations over Hefei mainly occurred in summer, while relatively low concentrations appeared in winter during the observation period from 2023 to 2025. The average total column concentration of SF₆ is 2.80×10^{14} molec·cm^{−2}, the average dry-air column-averaged mole fraction is 13.06 ppt, and the annual growth rate is 0.88 ppt yr^{−1}. The high-value events of SF₆ at the Hefei site are mainly concentrated in summer, and the wind direction mainly corresponds to the northeast and the southeast wind. The air masses with high concentrations of SF₆ mainly originated from the transportation path in the nearby southern regions of the station. During summer, the season with relatively higher SF₆ concentrations, the air masses were mainly southerly and easterly winds. The results of this study provide observational evidence and scientific support for understanding the characteristics of variation in atmo-



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spheric SF₆ column concentrations over Hefei and the influence of regional transport on high SF₆ values.

Keywords: sulfur hexafluoride; column concentration; Fourier transform infrared spectroscopy; variation characteristics; backward trajectory analysis

1. Introduction

Sulfur hexafluoride (SF₆) is a typical long-lived greenhouse gas with an extremely high global warming potential (GWP), and has been listed as one of the six major greenhouse gases in the Kyoto Protocol. According to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change (IPCC), the 100-year global warming potential of SF₆ is 24,300, meaning that the emission of 1 kg SF₆ has a climate impact equivalent to approximately 24.3 t CO₂ over a 100-year time horizon [1]. SF₆ emissions are almost entirely anthropogenic, mainly originating from industrial activities such as electrical power equipment, semiconductor manufacturing, and metal smelting. During production and use, some gases are leaked and released into nature. Top-down estimates based on AGAGE observations showed that global SF₆ emissions increased from 7.3 ± 0.6 Gg yr⁻¹ in 2008 to 9.04 ± 0.35 Gg yr⁻¹ in 2018 [2]. In recent years, with the development of industry and the increase in power demand, the global atmospheric concentration of SF₆ has continued to rise. Due to its strong infrared absorption capacity, the continuous increase in SF₆ concentrations can enhance the absorption of terrestrial longwave radiation, thereby increasing atmospheric radiative forcing and making a sustained contribution to global warming. IPCC AR6 reported that the effective radiative forcing (ERF) of SF₆ was $5.6 \text{ mW} \cdot \text{m}^{-2}$ in 2019 [3]. Although the current contribution of SF₆ to total radiative forcing is smaller than that of major greenhouse gases such as CO₂, SF₆ has an extremely long atmospheric lifetime, with the most widely estimated value reaching up to 3200 years; SF₆ easily accumulates in the atmosphere over long periods [4,5]. Consequently, if emissions continue to increase, the long-term greenhouse effect of SF₆ may be further amplified. In addition, because SF₆ is chemically stable and shows almost no chemical transformation in the atmosphere, it is removed only slowly through photolysis in the stratosphere. Therefore, it has also been widely used as an important tracer in studies of atmospheric background variations and the influence of anthropogenic emissions.

Due to its extremely high global warming potential and exceptionally long atmospheric lifetime, its potential impact on global climate change has attracted widespread attention. Observations of atmospheric SF₆ can be traced back to the 1970s. Lovelock et al. conducted early measurements in Ireland using gas chromatography and reported atmospheric mixing ratios of only 0.03–0.12 ppt, indicating that SF₆ concentrations were extremely low at that time [6]. With the development of observational techniques, SF₆ measurements gradually evolved into long-term continuous observations globally. Among them, the Global Greenhouse Gas Reference Network (GGGRN) established by the National Oceanic and Atmospheric Administration (NOAA) has carried out long-term monitoring of multiple greenhouse gases, including SF₆, using methods such as flask air sampling since 1997 [7]. According to NOAA marine background station data, the global atmospheric SF₆ concentration increased from 4.11 ppt in January 1998 to 12.03 ppt in January 2025, with the annual growth rate reaching 0.47 ppt yr⁻¹ in 2025, indicating an accelerated increase over the past decade [7]. Based on model predictions, Tuğba Önder et al. found that without further worldwide emission reduction measures, the atmospheric SF₆ concentration could reach approximately 21–23 ppt by 2050, representing an increase of 87–96% compared with

2023 [8]. In addition, other observational approaches have also been applied to monitoring the global variation of long-lived halogenated gases. De Longueville et al. used long-term observations from the Infrared Atmospheric Sounding Interferometer (IASI) satellite during 2008–2021 to retrieve concentration variations of several long-lived halogenated gases, including SF₆. The results show a continuous global increase in SF₆, with the global mean atmospheric mixing ratio reaching approximately 11 ppt in 2021 and an annual growth rate of about 0.34 ± 0.03 ppt yr^{−1}, which is in good agreement with observations from the Advanced Global Atmospheric Gases Experiment (AGAGE) and NOAA ground-based monitoring networks [9].

China has conducted long-term SF₆ observations at the Waliguan station in Qinghai since 1996 and has subsequently established additional regional background stations, such as Shangdianzi in Beijing [10,11]. Later, several regional atmospheric background stations were established at Longfengshan in Heilongjiang, Lin'an in Zhejiang, Shangri-La in Yunnan, Jinsha in Hubei, and Akedala in Xinjiang, gradually forming an atmospheric background observation network that covers different regional types across China [12,13]. According to the observational results reported in the China Greenhouse Gas Bulletin 2024 issued by the China Meteorological Administration, atmospheric SF₆ concentrations in China have shown a persistent long-term increase. In 2024, the annual average concentration at the Waliguan and Shangdianzi stations reached the highest value since the start of observations, about 12.08 ppt [14]. An et al. reported, based on long-term atmospheric inversion studies, that China has become one of the major contributors to global SF₆ emissions. From 2011 to 2021, China's SF₆ emissions increased from approximately 2.6 Gg yr^{−1} to 5.1 Gg yr^{−1}, mainly associated with the use and leakage of gas-insulated equipment in power systems, with emission growth exceeding the increase in global total emissions during the same period [13].

In addition to anthropogenic emission strength, regional variations in SF₆ concentration can also be modulated by atmospheric transport conditions. Patra et al. used an atmospheric general circulation model (AGCM)-based chemistry transport model and continuous observations from multiple sites to systematically investigate the transport mechanisms responsible for synoptic, seasonal, and interannual variations in SF₆. Their results indicated that SF₆ variability is closely related to atmospheric circulation, advection, convective transport, and vertical diffusion [15]. Zhao et al. investigated the changes in concentrations and potential source regions of greenhouse gases at the Akedala background station in Central Asia from 2009 to 2019 and found that SF₆ concentrations showed a significant increasing trend. Their backward trajectory analysis showed that Akedala was strongly influenced by northwesterly airflows in all seasons, while the contribution of air masses from southern Russia increased in summer, which may affect greenhouse gas concentrations at the station [12].

At present, atmospheric SF₆ observations in China are mainly based on in situ measurements at background stations, while studies on SF₆ remote sensing observations and column concentration variation characteristics remain limited, especially in regions outside atmospheric background stations. The remote sensing measurements provide total column concentrations integrated from the surface to the top of the atmosphere, and are less influenced by local emissions and boundary layer height variations. Therefore, they can better reflect large-scale spatial distribution characteristics and are more suitable for studies of regional greenhouse gas variability and long-term trends. Among ground-based remote sensing techniques, high-resolution Fourier transform infrared (FTIR) spectroscopy retrieves atmospheric trace gas column concentrations by measuring solar mid-infrared spectra, enabling investigations of long-term SF₆ column variations and providing a new observational approach for SF₆ concentration monitoring. Krieg et al. conducted SF₆

column retrievals using ground-based FTIR spectroscopy at several sites, including Ny-Ålesund (79°N), Jungfraujoch (47°N), and Kitt Peak (32°N). The results showed a continuous increase in tropospheric mean SF₆ concentrations and have good agreement with simultaneous surface observations [16]. Zhou et al. measured the column concentration of SF₆ on Reunion Island in the Indian Ocean based on ground-based FTIR spectroscopy. The growth rate of SF₆ from 2004 to 2016 was about 0.265 ± 0.013 ppt yr⁻¹, which was consistent with ground in situ and MIPAS, ACE-FTS satellite observations, indicating that FTIR observations can stably characterize the long-term trend in SF₆ [17]. Atmospheric SF₆ is mainly distributed near the surface and within the troposphere, but its concentration is very low, with maximum levels of only several to a dozen ppt. The spectral absorption characteristics are very weak, and the absorption bands are affected by multiple interfering gases, making accurate retrieval of SF₆ column concentrations challenging.

Although previous studies have reported long-term increases in atmospheric SF₆ concentrations and emissions in China, the seasonal variability and high-SF₆ events over eastern China remain insufficiently characterized, particularly in terms of their association with regional anthropogenic emissions and atmospheric transport. Hefei is located in the Yangtze River Delta (YRD) region of eastern China, one of the most economically developed regions in China. Rapid expansion of industrial activities and electricity infrastructure has increased anthropogenic SF₆ emissions, making this region highly susceptible to the combined influence of regional emissions and atmospheric transport. Therefore, analyzing the temporal variations of SF₆ column concentrations over Hefei based on ground-based FTIR observations, together with wind statistics, backward trajectories, and emission inventories, is important for discussing the potential influence regions and transport characteristics of high-SF₆ events and for improving our understanding of SF₆ variations and their regional influencing factors over eastern China.

To investigate the recent temporal variations and transport characteristics of atmospheric SF₆ over this region, this study focuses on FTIR observations during 2023–2025. The solar absorption spectra collected by ground-based high-resolution FTIR spectroscopy were used to retrieve atmospheric SF₆ column concentrations over Hefei, and their temporal variation characteristics were analyzed. Furthermore, wind statistics, HYSPLIT backward trajectory analysis, the EDGAR emission inventory, and emission inversion studies based on atmospheric observations were combined to discuss the potential influence regions associated with elevated SF₆ concentrations and to evaluate the possible impacts of regional anthropogenic emissions and atmospheric transport on high-SF₆ events. Section 2 describes the Hefei ground-based FTIR observation system and the SF₆ spectral retrieval method. Section 3 analyzes the temporal variation characteristics of SF₆ column concentrations during 2023–2025. Section 4 focuses on the potential influence regions and transport characteristics associated with different seasons and high-value events. Finally, Section 5 presents the conclusions of this study.

2. Materials and Methods

2.1. Observation Site and Instrumentation

The observation is conducted at the Atmospheric Environment Observation Station of the Anhui Institute of Optics and Fine Mechanics, Hefei, China (117.17°E, 31.91°N, 34.5 m above sea level). The ground-based FTIR observation system includes a Bruker IFS 125HR spectrometer, an A547N solar tracker (Bruker Optics GmbH, Ettlingen, Germany), and a Zeno meteorological station (Coastal Environmental Systems, Seattle, WA, USA). Solar absorption spectra in the 700–1350 cm⁻¹ range were recorded with 0.005 cm⁻¹ spectral resolution and 180 cm optical path difference. During clear sky daytime conditions, the rooftop solar tracker precisely tracks the sun, receives solar radiation, and directs it

into the indoor spectrometer. Simultaneously with spectral measurements, the rooftop meteorological station continuously records meteorological parameters. Site operation procedures, data acquisition, and data recording follow the data quality requirements of the Network for the Detection of Atmospheric Composition Change (NDACC) [18]. At present, the observation site has been officially incorporated into the standard observation network of the NDACC Infrared Working Group (NDACC-IRWG).

2.2. Retrieval Method and Strategy

SF₆ column concentrations were obtained using SFIT4 (v0.9.4.4) with an optimal estimation approach that links observed spectra to atmospheric state parameters [19]. The forward model can be expressed as follows:

$$y = \mathbf{F}(x, b) + \varepsilon \quad (1)$$

where y represents the measured spectrum, $\mathbf{F}(x, b)$ is the forward model, x is the state vector, b denotes the model parameters, and ε represents the measurement error. During the retrieval process, the forward model is linearized, and the Jacobian matrix describing the sensitivity of the measured spectrum to the state vector can be written as follows:

$$\mathbf{K} = \frac{\partial \mathbf{F}(x, b)}{\partial x} \quad (2)$$

where $\mathbf{K}$ characterizes the sensitivity of the observed spectrum to changes in atmospheric state parameters at different altitudes. The OEM iteratively minimizes the residual between the measured and simulated spectra. The corresponding cost function is given by the following:

$$\chi^2 = \sum_{i=1}^M \frac{(Y_i^{Mea} - Y_i^{Cal})^2}{\sigma_i^2} \quad (3)$$

where Y_i^{Mea} and Y_i^{Cal} represent the measured and simulated spectra, and σ_i denotes the measurement error variance.

The a priori atmospheric state parameters required for the retrieval, including temperature, pressure, and H₂O profiles, were obtained from the National Centers for Environmental Prediction (NCEP) reanalysis data [20]. The a priori profiles of SF₆ and interfering gases were taken from the Whole Atmosphere Community Climate Model (WACCM) v7. Spectral line parameters for SF₆ were obtained from the empirical pseudo-line lists (PLL) molecular database developed at NASA Jet Propulsion Laboratory (JPL) based on laboratory transmission spectra, while the spectral line parameters of all other gases were adopted from the HITRAN 2020 database [21]. Because trace gas absorption in the infrared spectral region can be significantly affected by strong absorption gas such as H₂O and CO₂, an appropriate retrieval window must be selected to ensure a distinct SF₆ absorption signature. The spectral region around 947.9 cm^{−1} (946.5–949.0 cm^{−1}) was chosen for the retrieval. To reduce errors caused by spectral line overlap, interfering gases including H₂O, CO₂, C₂H₄, and O₃ were simultaneously fitted during the retrieval.

Due to the weak absorption signal and limited information content of SF₆, direct retrieval of the vertical profile can easily lead to unrealistic oscillations. In order to improve the stability of the retrieval results, the Tikhonov L1 regularization method was applied to provide a smoothing constraint on the state vector [22,23]. The selection of the regularization parameter α has a significant influence on the retrieval. In this study, the optimal regularization strength was determined by minimizing the error test, and a regularization parameter of $\alpha = 20$ was selected to ensure the stability of the retrieval results.

A typical spectrum was selected to evaluate the retrieval strategy. As shown in Figure 1, for the selected spectrum acquired on 18 February 2025 at 03:52:04 UTC, the root mean square (RMS) residual between the measured and fitted spectra was 0.297%, indicating a good spectral fitting result within the selected retrieval window. Figure 2 presents the retrieved SF₆ profiles after introducing Tikhonov regularization. When using the OEM retrieval, the retrieved profile exhibited obvious oscillations and unrealistically enhanced concentrations within the troposphere and lower stratosphere. The SF₆ absorption signal is weak and the vertical information is limited, so the retrieval results are easily affected by measurement noise. After applying Tikhonov regularization, the retrieved profile became more stable and unrealistic oscillations were significantly reduced, improving the stability of the retrieval results. Figure 3 shows the SF₆ averaging kernel matrix after applying Tikhonov regularization. The retrieval exhibits relatively high sensitivity mainly in the troposphere and lower stratosphere, particularly within the altitude range of about 5–12 km. Above 30 km, the sensitivity decreases rapidly, indicating a greater dependence on the a priori profile at higher altitudes. After applying Tikhonov regularization, the degree of freedom for the signal (DOFS) increased from 0.82 to 1.05. This result suggests limited vertical information content in the SF₆ retrieval, with the retrieved profiles primarily representing total column variations.

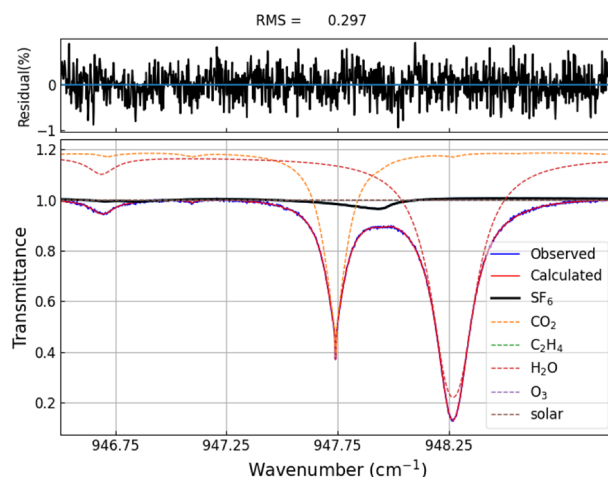


Figure 1. Spectral fitting of the SF₆ in the 946.5–949.0 cm^{−1} retrieval window, including the fitting residuals and interfering gases.

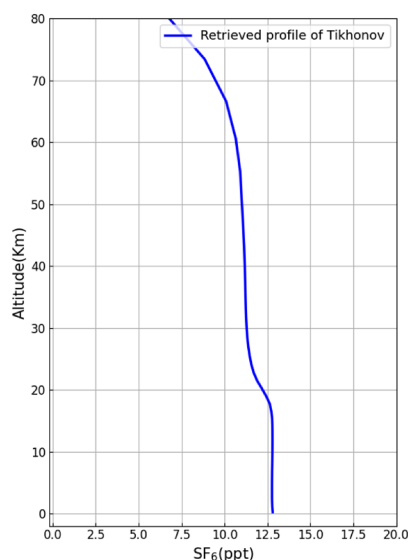


Figure 2. Retrieved SF₆ profile.

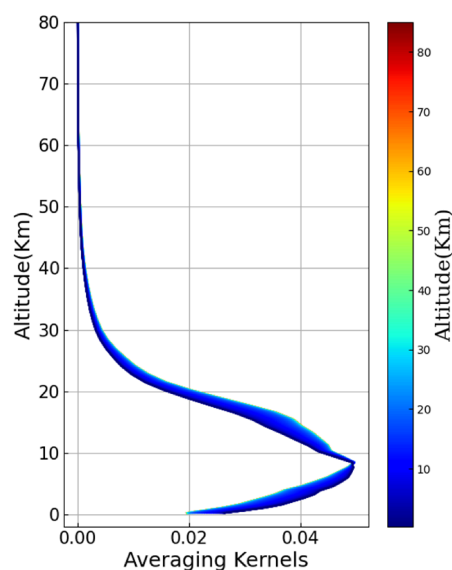


Figure 3. Averaging kernels for the SF₆ retrieval.

2.3. Uncertainty Analysis of Retrieval Results

Observation noise, spectroscopic parameter uncertainties, and the selection of the retrieval strategy all contribute to uncertainty in the SF₆ retrieval results. Therefore, uncertainty analysis is important for understanding the influence of different error sources and for evaluating the reliability and accuracy of the results. Based on Rodgers' posterior error estimation method [24], this study analyzes and evaluates the sources and impacts of retrieval uncertainties using results in 2025. During the retrieval process, a priori covariance matrices were constructed according to the uncertainties of the corresponding prior parameters. The temperature covariance matrix was obtained from the NCEP reanalysis data. The uncertainty of the SF₆ spectroscopic parameters was set to 2% based on the empirical pseudo-line list database. The systematic and random uncertainties of the solar zenith angle (SZA) were both set to 3%, while those of the instrumental line shape (ILS) parameters were both assumed to be 5%. The final posterior error estimation results are summarized in Table 1. The systematic uncertainty of the retrieved column was 2.97%. The smoothing error was the largest contributor, with a value of 2.53%. This indicates that limited vertical sensitivity and a priori constraints have a significant influence on the retrieved SF₆ columns. Other error sources, including uncertainties in the solar zenith angle, line intensity and instrumental line shape also contributed to the systematic uncertainty. The random uncertainty was 4.09%, mainly contributed by measurement noise and temperature uncertainty, with measurement error and random temperature error of 3.30% and 2.09%, respectively. The total retrieval uncertainty was estimated to be 5.70%. It can be seen that retrieved atmospheric SF₆ concentrations in this study have relatively low uncertainties, demonstrating that the adopted spectroscopic parameters and retrieval strategy are reliable.

Table 1. Error analysis results of SF₆ retrieval.

Parameter	Systematic (%)	Random (%)
Smoothing	2.53	-
Measurement	-	3.30
Retrieval parameters	0.11	-
Interfering species	0.39	-
Temperature	0.34	2.09
SZA	1.13	1.13

Table 1. Cont.

Parameter	Systematic (%)	Random (%)
Line intensity	0.77	-
Temperature dependence of line width	0.15	-
Air-broadening of line width	0.11	-
ILS	0.46	0.46
Total	2.97	4.09

2.4. Time Series Analysis Method

To characterize the seasonal variation and estimate the temporal trend of atmospheric SF₆ column concentrations, the observational time series was fitted using a Fourier series. The fitting function is expressed as follows:

$$F(t) = a + b \cdot t + \sum_{k=1}^3 (c_{2k-1} \cos(2\pi kt) + c_{2k} \sin(2\pi kt)) \quad (4)$$

where a is the intercept, b represents the annual trend term, and t is the fractional year. The coefficients c_1 to c_6 correspond to the cosine and sine harmonic terms of the Fourier series describing the seasonal cycle.

3. Results

The temporal variations of SF₆ column concentrations during 2023–2025 were analyzed using the fitting function described in Section 2.4. Figure 4 presents all individual SF₆ column measurements and the calculated daily mean values during 2023–2025. The black solid line represents the Fourier-fitted curve, while the red dashed line denotes the linear fitting trend. The total SF₆ column displays a clear seasonal pattern, with peak values in June and July and the lowest values in February. Furthermore, Figure 5 shows the monthly mean variations after removing the annual trend. The monthly values were obtained by subtracting the annual mean of each year from the corresponding monthly mean values, and the difference between the maximum and minimum monthly mean values reached 6.60×10^{13} molec·cm^{−2}. This variation may be related to differences in regional atmospheric background, seasonal atmospheric transport processes, and air mass source areas. The evident seasonal cycle indicates that, besides the long-term increase in atmospheric SF₆, seasonal atmospheric transport is also likely to influence the observed column concentrations over Hefei. P. K. Patra et al. compared global atmospheric transport model simulations with surface concentration observations and found that, because SF₆ is a long-lived greenhouse gas that shows almost no chemical reactions in the atmosphere, its seasonal concentration variations are mainly controlled by atmospheric circulation and regional transport processes [15]. To further investigate this issue, Section 4 will further discuss the high-value SF₆ event and seasonal transport characteristics in combination with wind direction statistics and HYSPLIT (Hybrid Single-Particle Lagrangian Integrated Trajectory) backward trajectory analysis.

In addition, the average atmospheric SF₆ total column observed at the Hefei site during 2023–2025 was 2.80×10^{14} molec·cm^{−2}, showing an overall increase from 2023 to 2025 with an average annual growth rate of $6.33 \pm 0.28\%$ yr^{−1}. In order to directly compare with results from different observation methods, the retrieved total columns were further converted into the dry-air column-averaged mole fraction X_{SF_6} . The calculated mean X_{SF_6} at the Hefei site during 2023–2025 was 13.06 ppt, which is close to the annual mean surface concentration of 12.08 ppt measured at the Waliguan and Shangdianzi stations in 2024 [14]. This agreement reflects the relatively uniform distribution of SF₆ among different regions as a long-lived greenhouse gas. Meanwhile, the average annual growth rate of X_{SF_6} at the

Hefei site during 2023–2025 was 0.88 ppt yr^{-1} , which is higher than the growth rate of $0.265 \text{ ppt yr}^{-1}$ reported by Zhou et al. at Réunion Island during 2004–2016 [17], the annual growth rate of 0.47 ppt yr^{-1} observed at NOAA marine background stations in 2025 [7], and the annual growth rates of $0.53\text{--}0.45 \text{ ppt yr}^{-1}$ reported at the Waliguan and Shangdianzi stations during 2023–2024 [14,25]. The relatively faster increase in SF_6 over the Hefei region may be associated with enhanced emissions caused by recent industrial development in the area. The SF_6 growth rate obtained in this study is higher than that reported at background stations and in previous studies, which may be related to the location of the observation site. Hefei is located in the Yangtze River Delta, where intensive industrial activities and extensive electricity infrastructure are associated with relatively high anthropogenic SF_6 emissions. Emission inversion studies based on atmospheric observations by Chen et al. also suggested substantial anthropogenic SF_6 emissions over southeastern China [26]. Therefore, regional anthropogenic emissions may have contributed to the increase in atmospheric SF_6 concentrations over Hefei.

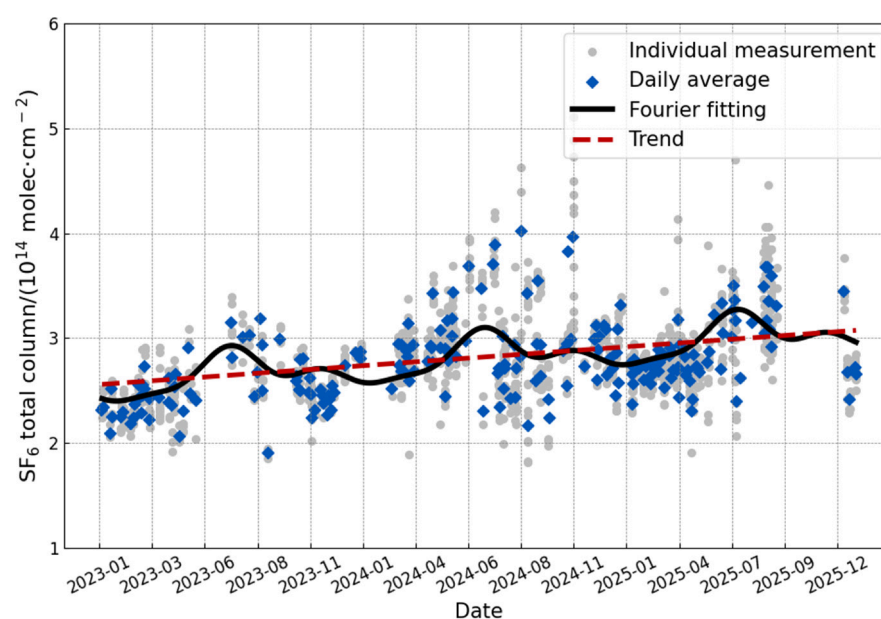


Figure 4. Time series of SF_6 column concentrations over Hefei.

Meanwhile, the WACCM simulations were used for comparison and analysis in this study. As a global climate chemical model designed to investigate atmospheric dynamics, radiation, and chemical processes, the WACCM can provide continuous distributions of atmospheric constituents and their long-term variation trends [27]. In this study, WACCM data were also used to provide the a priori profile information for the retrieval. The WACCM simulation data for the Hefei site consist of monthly vertical SF_6 concentration profiles from the surface up to 120 km altitude. The mean total SF_6 column simulated by WACCM during 2023–2025 was calculated to be $2.48 \times 10^{14} \text{ molec}\cdot\text{cm}^{-2}$, corresponding to the X_{SF_6} of 11.65 ppt and an annual growth rate of 0.36 ppt yr^{-1} . To further quantitatively evaluate the agreement between the WACCM simulations and FTIR observations, the FTIR retrievals were averaged to monthly means to match the temporal resolution of the WACCM data. The comparison resulted in a correlation coefficient (R) of 0.631, a mean bias (WACCM – FTIR) of -1.485 ppt , and an RMSE of 1.960 ppt . These results indicate that WACCM captures the temporal variability of atmospheric SF_6 over Hefei reasonably well but systematically underestimates the observed X_{SF_6} . These values are all lower than those observed at the Hefei FTIR site and at the background observations at the Waliguan

and Shangdianzi stations, indicating that the WACCM tends to underestimate both the background concentration and the growth rate of atmospheric SF₆.

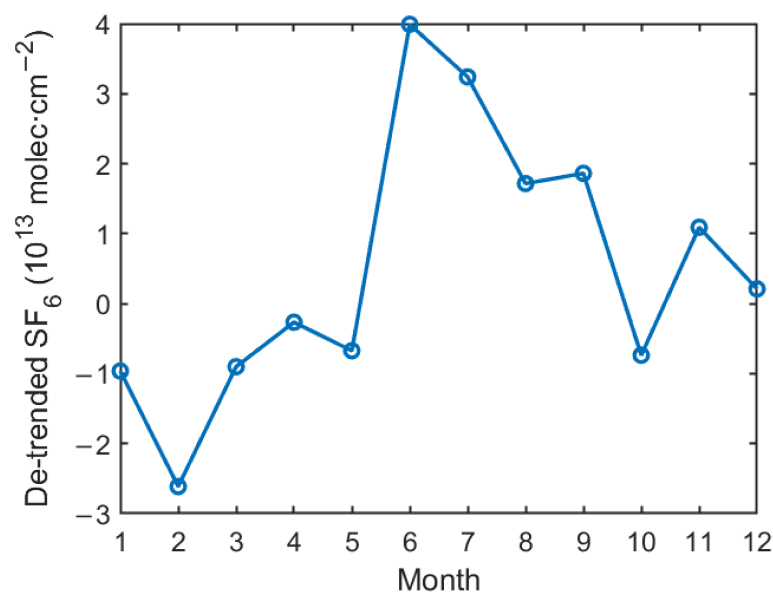


Figure 5. Monthly mean detrended SF₆ column concentrations over Hefei.

4. Discussion

4.1. Wind Field Characteristics

The Hefei ground-based remote sensing site is located in the northwestern suburb of Hefei, about 12 km from the city center. The site is surrounded by water on three sides, with nearby areas consist mainly of forest land, farmland, and grassland, with a relatively open and flat environment. Hefei is located in central Anhui Province and experiences a subtropical monsoon climate, with southeasterly winds prevailing in summer and north-easterly winds in winter. The region is highly industrialized and densely populated, with significant anthropogenic emissions and notable influence from regional atmospheric transport. To analyze the overall wind field characteristics during the SF₆ observation period, wind direction and speed distributions were plotted based on synchronous meteorological measurements from 2023 to 2025. In Figure 6, WF represents wind frequency, indicating the frequency ratio of each wind direction and the dominant wind direction, while WS represents wind speed, reflecting the average wind speed under different wind directions. The overall wind direction distribution shows that the wind frequency at the Hefei site is mainly in the direction from southeast (SE) to northeast (NE), with the highest frequency observed for southeast winds (SE). During the study period, the site was mainly influenced by air masses from the east and southeast. In contrast, westerly winds were less frequent, particularly from the northwest (NW) and north (N). Wind speed (WS) exhibits different characteristics, with stronger winds primarily from the west (W), while the winds from the east (E) and northeast (NE) are relatively weaker. Therefore, the wind field at the observation site is characterized by a high frequency of easterly winds and stronger westerly winds.

To investigate the wind field conditions associated with high-SF₆ events, high-concentration observations were screened in this study. Data points with SF₆ concentrations exceeding the mean value plus two standard deviations ($\mu + 2\sigma$) in the time series were defined as the high-value data. The wind direction, wind speed data and mean SF₆ column concentration were analyzed, as shown in Figure 7. The wind direction distribution during high SF₆ periods exhibits clear directional characteristics, with wind frequency (WF) mainly

concentrated in the easterly direction. Among these, east-northeast (ENE) and southeast (SE) winds show relatively high frequencies, while westerly winds did not appear, indicating that the high SF₆ concentration events were more likely to occur under easterly flow conditions. In addition, the wind speed (WS) distribution shows that relatively strong winds mainly occur from the south (S) and south-southeast (SSE), representing the dominant transport pathways associated with enhanced atmospheric transport, while wind speeds from other directions are comparatively weaker. From the relationship between SF₆ column concentration and wind speed, the mean SF₆ column concentration was relatively high under northerly (N) winds, but the corresponding wind speed was very low. This suggests that the high-SF₆ events under this direction may be related to SF₆ accumulation around the observation site caused by limited atmospheric dispersion under weak wind conditions. Relatively high SF₆ column concentrations were also observed under south-southeasterly (SSE) winds, where the mean wind speed was relatively high. This indicates that stronger transport conditions from the south-to-southeast sector may have facilitated the transport of regional air masses to the observation site, thereby contributing high-SF₆ events. Considering the spatial location of the observation site, the Hefei site is situated to the northwest of the urban area, while the densely populated urban region lies to the east and southeast of the site. Under easterly to southeasterly flow conditions, the potential influence of anthropogenic emissions from the urban area and its surrounding regions on the SF₆ column concentrations observed at the site may be enhanced. Overall, high-SF₆ events may be associated with both near-regional accumulation and regional transport processes.

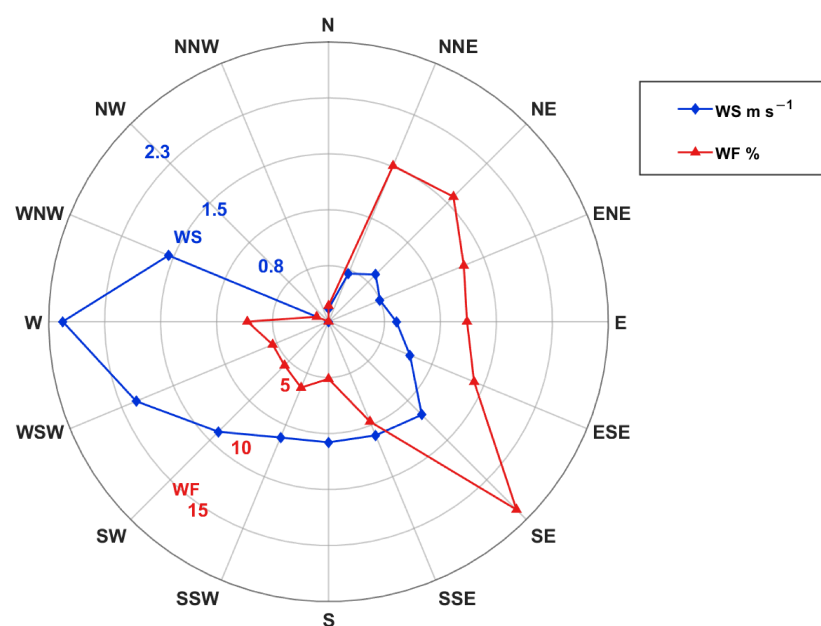


Figure 6. Wind characteristics during the SF₆ observation period at the Hefei site.

Furthermore, to identify the potential source areas of high SF₆ concentrations in different seasons, the high-value observations were analyzed seasonal wind field characteristics and SF₆ column concentrations were plotted, as shown in Figure 8. The number of high-value events varies among seasons, with the largest number occurring in summer, followed by autumn and spring, while no high-SF₆ events were observed during winter. Therefore, Figure 8 only shows the characteristics of high-value wind fields in spring, summer and autumn.

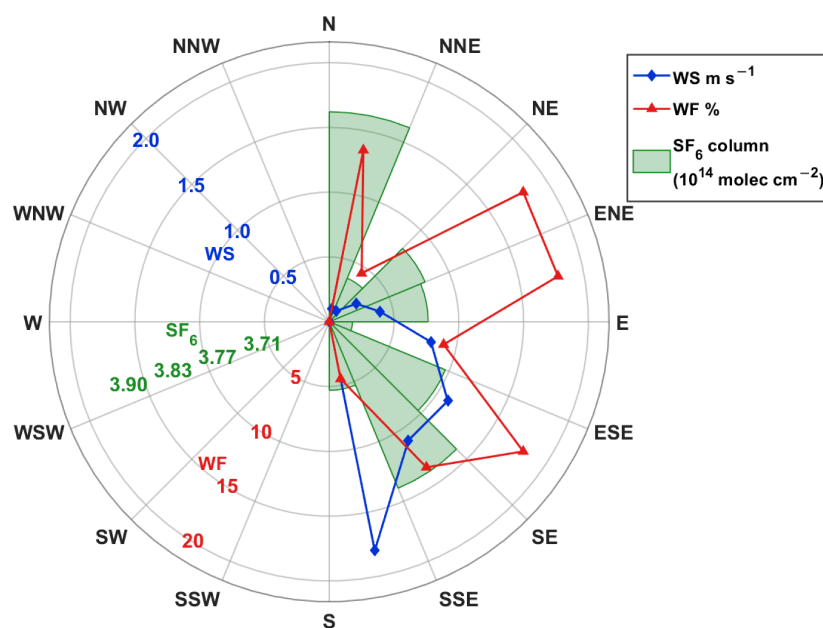


Figure 7. Wind characteristics and SF₆ column concentrations with high SF₆ at the Hefei site.

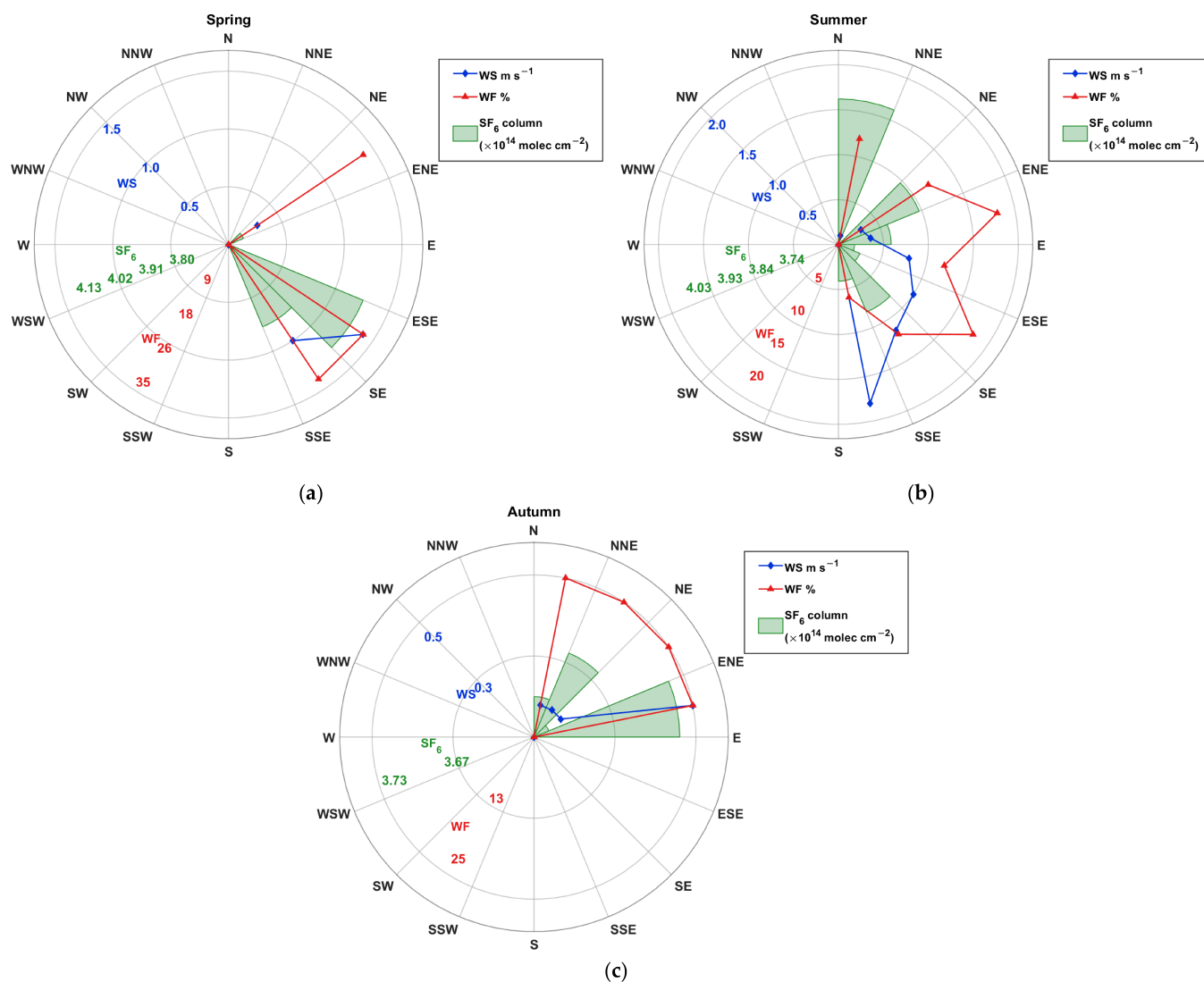


Figure 8. Seasonal wind field characteristics and SF₆ column concentrations with high SF₆ at the Hefei site: (a) spring; (b) summer; (c) autumn.

In spring, high-SF₆ events mainly occurred under southeasterly flow conditions. The ESE-to-SSE sector was characterized by relatively high wind frequency and relatively large wind speed. This indicates that spring high-SF₆ events were closely related to regional transport conditions from the southeasterly sector. In summer, the wind field and concentration characteristics associated with high-SF₆ events were more complex. On the one hand, the N and NNE directions corresponded to relatively high mean SF₆ column concentrations but low wind speeds, suggesting that these directions may be related to near-regional SF₆ accumulation under weak wind conditions. On the other hand, relatively high SF₆ column concentrations were also observed from the E-to-S sector, with relatively large mean wind speeds in the SSE and S directions. This suggests that stronger atmospheric transport conditions from the south-to-southeast sector may have facilitated the transport of regional air masses to the observation site. Therefore, summer high-SF₆ events may be influenced by both weak wind accumulation and regional transport processes. In autumn, high-SF₆ events were mainly concentrated under northeasterly flow conditions, with relatively high SF₆ column concentrations observed in the NE, ENE, and E directions. However, wind speeds in autumn were generally lower than in spring and summer, suggesting that the autumn high SF₆ may be related to relatively stable northeasterly flow conditions and weaker atmospheric dispersion.

4.2. Transport Pathways with High-SF₆ Events and in Different Seasons

In order to further identify potential source areas and transport pathways for typical high-SF₆ events, backward trajectory calculations were performed using the HYSPLIT model for all observation times associated with high SF₆ concentrations. In addition, to analyze seasonal differences in background transport conditions, backward trajectory analyses were conducted for observation days in different seasons. HYSPLIT (Hybrid Single-Particle Lagrangian Integrated Trajectory) is a hybrid Lagrangian trajectory model developed by the Air Resources Laboratory (ARL) of the NOAA. It has been widely used in studies of atmospheric transport and dispersion processes. The model can use a variety of meteorological reanalysis data to calculate the complex transmission, diffusion and conversion of atmospheric particles along forward or backward paths in the air, and to identify pollutant transmission paths and source areas, as well as to perform large-scale regional transport analysis [28,29]. In this study, the transport path of contaminated air mass is traced through backward trajectory simulation, and similar trajectories are combined for cluster analysis to identify the main potential influence regions and transport characteristics. The simulation starts from the Hefei site, and the initial altitude is set at 1 km. Meteorological fields were obtained from the Global Data Assimilation System (GDAS) provided by NCEP, with a spatial resolution of 1° × 1°. The backward simulation duration was set to 48 h. The calculated backward trajectories were further classified using the angle–distance clustering method implemented in HYSPLIT. This clustering approach groups trajectories with similar transport pathways, thereby simplifying the large number of trajectories and facilitating the identification of the dominant transport pathways and potential source regions. It should be noted that the vertical degrees of freedom of the FTIR SF₆ retrieval are limited, and the retrieval results mainly reflect variations in the total atmospheric column. However, since SF₆ primarily originates from anthropogenic surface emissions, lower tropospheric transport plays an important role in transporting surface emissions to the air column above the observation site. In this study, 1 km was selected as the representative starting height for the HYSPLIT backward trajectories to analyze lower tropospheric air mass transport pathways over the Hefei FTIR site.

For the seasonal transport analysis, the backward trajectories were initialized at 12:00 local time (04:00 UTC) on each observation day, corresponding to the main FTIR observation

period at the Hefei site. Figure 9 shows the clustering results for backward trajectories during SF₆ observations in different seasons. In spring (Figure 9a), air masses were mainly transported from the northeast near the site (47%), with additional contributions from long-distance transport originating in the northwest. During summer (Figure 9b), when SF₆ concentrations are relatively high, air masses mainly originated from nearby regions to the south of the site (59%), indicating that short-range transport and near-regional accumulation may have played an important role in the summer SF₆ enhancement. The far transportation in southern China (31%), as well as the transportation in some eastern coastal areas (10%), shows summer high SF₆ may have been jointly influenced by near-regional accumulation and southerly to easterly regional transport. In autumn (Figure 9c), the dominant transport pathways were from the eastern and northeastern coastal regions (53%), followed by nearby southern regional transport (25%) and long-range transport from the northwest (22%). During winter (Figure 9d), when SF₆ concentrations were relatively low, multiple transport pathways were distributed from the west, northwest, and northeast of the site, with similar contributions from each direction.

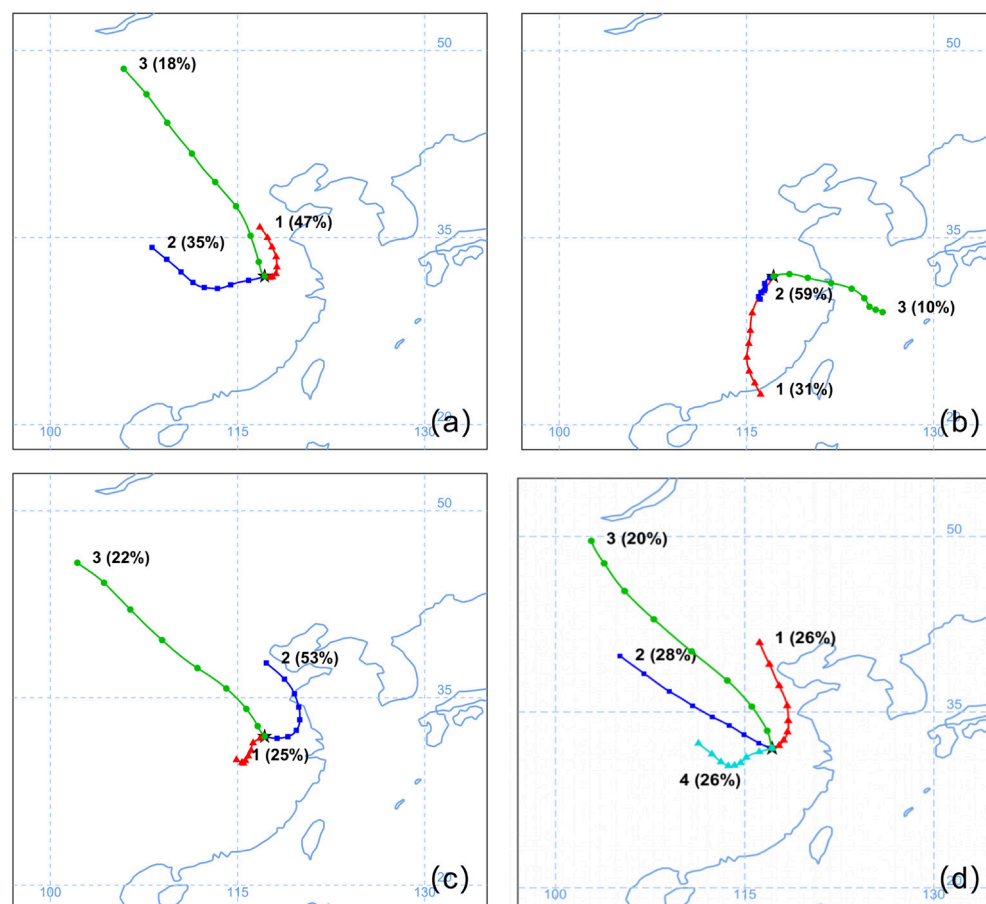


Figure 9. Backward trajectories of air masses during SF₆ observations in different seasons: (a) spring; (b) summer; (c) autumn; (d) winter.

Figure 10 presents the backward trajectories of long-distance air masses during high-SF₆ events. For the high-SF₆ events analysis, the trajectory arrival time was set according to the corresponding high-SF₆ events observation time at an hourly resolution. To examine the spatial relationship between atmospheric transport pathways and potential anthropogenic source regions, the EDGAR 2024 SF₆ emission inventory was incorporated into the analysis. EDGAR (Emissions Database for Global Atmospheric Research) is a global anthropogenic emission inventory developed by the Joint Research Centre of the European Commission,

providing greenhouse gas emissions as both national totals and gridded spatial distributions. In this study, gridded SF₆ emission data with a spatial resolution of $0.1^\circ \times 0.1^\circ$ were used as an independent dataset to provide additional spatial context for interpreting the backward trajectory results during high-SF₆ events [30].

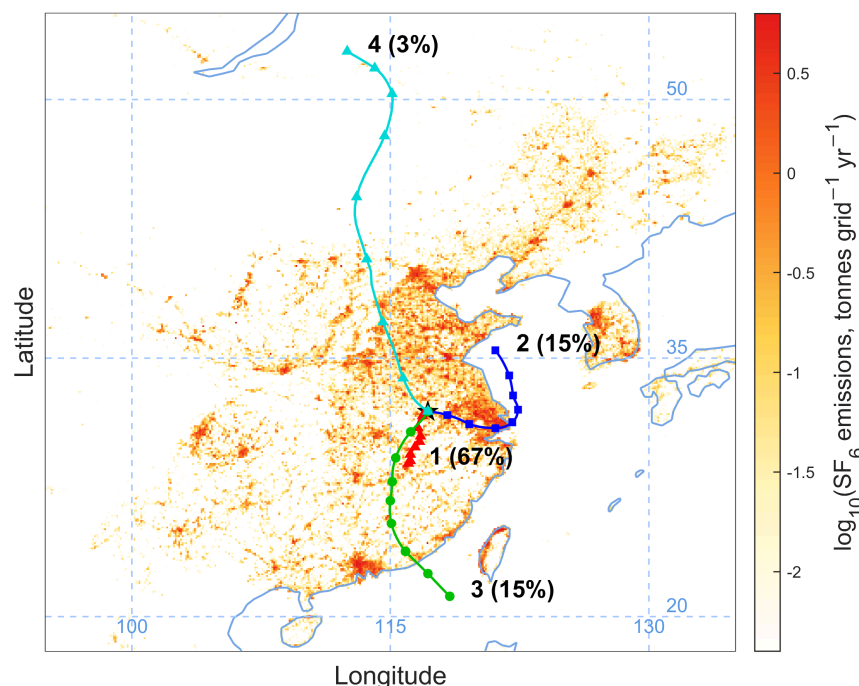


Figure 10. Backward trajectories of air masses during high SF₆ with the EDGAR SF₆ emissions.

The results indicate that the majority of high-concentration SF₆ air masses originate from nearby southern regions of the site (about 67%), passing through southern Anhui Province. About 15% of the air masses come from the east, including the eastern coastal regions of China, passing through southern Jiangsu and eastern Anhui. Another 15% originate from the South China Sea, traveling across southern China and southern Anhui. A small fraction about 3%, is attributed to long-distance transport from northern regions.

The SF₆ emission inventory developed by Fang et al. showed that SF₆ emissions in China mainly originate from the electrical equipment, magnesium production, semiconductor manufacturing, and SF₆ production sectors. Among these sectors, the electrical equipment sector is the dominant source, accounting for approximately 70% of total SF₆ emissions in China, whereas the magnesium production, semiconductor manufacturing, and SF₆ production sectors each contribute approximately 10% [31]. The EDGAR emission inventory indicates that relatively high SF₆ emissions are concentrated in eastern China, particularly in the Yangtze River Delta and its surrounding regions. In addition, Chen et al. estimated SF₆ emissions over southeastern China (covering Anhui, Jiangsu, Zhejiang, Shanghai, Jiangxi, Fujian, Guangdong, and Hainan) for 2021–2023 using high-frequency in situ SF₆ observations at the Xichong regional background station combined with the FLEX-PART transport model and a Bayesian inversion framework. The estimated SF₆ emissions in southeastern China were approximately 2.38 Gg yr^{-1} in 2023, indicating substantial anthropogenic emissions in this region [26]. The wind statistics indicate that high-SF₆ events mainly occurred under easterly wind conditions, whereas the HYSPLIT backward trajectory analysis showed that the corresponding air masses mainly originated from nearby regions to the south of Hefei. In particular, the dominant trajectory cluster accounted for 67% of the high-SF₆ events and showed relatively short transport pathways, suggesting that near-regional air mass transport and limited dispersion may also have contributed to

the accumulation of SF₆ around the observation site. These results suggest that regional anthropogenic emissions, near-regional accumulation and atmospheric transport may have jointly contributed to elevated SF₆ column concentrations over Hefei.

Considering that the FTIR SF₆ retrieval mainly provides column concentration information, backward trajectories initialized at different starting heights were further calculated using HYSPLIT. The trajectories initialized at 5 km and below generally showed similar transport characteristics, mainly indicating transport from the eastern to southern sectors of the site; however, the trajectories initialized at 10 km and above showed relatively large differences. Since SF₆ mainly originates from anthropogenic surface emissions, lower and middle tropospheric trajectories are more directly related to the influence of regional surface emissions, whereas upper-level trajectories may more likely reflect the effects of upper-level atmospheric circulation, vertical mixing, and stratosphere–troposphere exchange on the column concentration. However, due to the lack of SF₆ vertical profile observations and related meteorological diagnostic data, it is difficult to determine the specific contributions of transport processes at different altitude layers to the column concentration variations. Therefore, the HYSPLIT results in this study are mainly used to help identify the low-level transport directions and potential influence regions that may be affected by surface emissions during high-SF₆ events.

5. Conclusions

In this study, atmospheric SF₆ column concentrations during 2023–2025 were retrieved using mid-infrared solar absorption spectra measured by ground-based high-resolution FTIR spectroscopy at the Hefei site. The seasonal variation characteristics and recent trends of SF₆ were analyzed, and the influence regions and transport characteristics of high-SF₆ events were further investigated through wind statistics and HYSPLIT backward trajectory cluster analysis.

For SF₆ spectral retrieval, the spectral window of 946.5–949.0 cm^{−1} was selected. To improve the stability of the retrieval results and suppress the influence of noise on the retrieved profiles, the Tikhonov L1 regularization method was introduced to reduce profile oscillations. The uncertainty analysis showed that the total retrieval uncertainty of the SF₆ column concentrations was approximately 5.70%, with smoothing error, measurement error, and temperature error representing the major contributions. Based on the observational time series, the variations in SF₆ column concentrations over Hefei during 2023–2025 were analyzed. The results showed that higher concentrations mainly occurred in summer, while lower concentrations appeared in winter. In addition, the SF₆ column concentrations exhibited an overall increasing trend in three years, with an average total column concentration of 2.80×10^{14} molec·cm^{−2} and an average annual growth rate of $6.33 \pm 0.28\%$ yr^{−1}. The dry-air column-averaged mole fraction X_{SF_6} was further calculated from the retrieved total column concentrations, yielding an average annual growth rate of 0.88 ppt yr^{−1} during 2023–2025. Comparison with observations at other sites showed that the X_{SF_6} values at the Hefei site were close to the annual mean surface concentrations measured at the Waliguan and Shangdianzi background stations in 2024, whereas the annual growth rate at Hefei was higher than observed at the two background stations. Comparisons with SF₆ simulations from the WACCM further indicated that both the simulated dry-air mole fraction and annual growth rate were lower than the background observations at the Hefei, Waliguan, and Shangdianzi stations, suggesting that the WACCM generally underestimates the background concentration and growth trend of atmospheric SF₆.

High-SF₆ events at the Hefei site were identified using a threshold of the mean value plus two standard deviations. The results showed that high-value SF₆ events mainly occurred in summer, followed by autumn and spring, while no high-value events were

observed in winter. Wind statistics indicated that high SF₆ concentrations were mainly associated with winds from the northeast to southeast directions, suggesting that easterly to southeasterly flow may have favored the occurrence of high-SF₆ events. Further HYSPLIT backward trajectory cluster analysis revealed that the majority of high-concentration air masses originated from nearby southern transport pathways, accounting for approximately 67%, indicating that short-range transport and near-regional accumulation may have contributed to the observed enhancements. In addition, long-distance transport pathways from eastern China, the eastern coastal regions, and southern China were also identified. Seasonal transport analyses further demonstrated that air mass origins differed among seasons. In particular, summer, when relatively high SF₆ concentrations were observed, exhibited more pronounced transport influences from nearby southern air masses and regional transport from southern to eastern sectors, whereas other seasons showed greater contributions from long-range transport originating from northern and northwestern regions. Wind statistics mainly reflect local wind field conditions near the observation site during high-value events, while backward trajectories describe the regional transport pathways of air masses before arriving at the site. Together, these analyses reveal the transport characteristics associated with high-SF₆ events. Overall, regional anthropogenic emissions over eastern and southeastern China, together with short-range transport, near-regional accumulation, and atmospheric transport processes, may have jointly contributed to elevated SF₆ column concentrations over Hefei. These findings provide observational evidence for understanding the variation characteristics of atmospheric SF₆ column concentrations, the potential influencing regions of high-value events, and the influence of regional transport processes over Hefei.

This study still has some limitations. Since the vertical degrees of freedom of FTIR SF₆ retrieval are limited, the retrieval results mainly reflect column concentration variations, while wind statistics and HYSPLIT backward trajectories are mainly used to characterize lower tropospheric transport processes. Therefore, the interpretation of vertical transport processes and their relationship with column concentration variations remains limited. Future studies combining in situ SF₆ observations and higher resolution emission data would help improve the reliability of regional SF₆ source identification and transport interpretation.

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