Composition Characteristics and Potential Regions of PM$_{2.5}$ during Winter Haze Pollution in Typical Industrial Areas, NW-China

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ABSTRACT

To investigate the causes and potential sources of fine particulate matter (PM$_{2.5}$) pollution during winter haze pollution in typical industrial areas in northwest China, PM$_{2.5}$ samples were collected during a winter extreme pollution event (from January 15 to January 29, 2016). The daily average PM$_{2.5}$ concentrations were ~210 µg m$^{-3}$ and peak daily concentrations were ~496 µg m$^{-3}$ in the Kuitun-Dushanzi-Wusu (K-D-W region) of Xinjiang Uygur Autonomous Region, China. Eighty-eight samples (including 44 quartz and 44 Teflon samples for PM$_{2.5}$) were assessed for water-soluble ions (WSIIs), organic/elemental carbon (OC/EC) and inorganic elements. The results showed that the percentage of carbonaceous compounds decreased with more severe pollution levels, and the OC and SOC decreased more rapidly than EC. The sum of 39 inorganic element concentrations (8.28% $\pm$ 3.59%) was lower than that of water-soluble ions (63.26% $\pm$ 8.78%) and carbonaceous compounds (10.95% $\pm$ 3.22%). SO$_4^{2-}$ is the component with the highest percentage, and the percentage of SO$_4^{2-}$ increases continuously in severe pollution, indicating that secondary transformation of SO$_4^{2-}$ was more significant during polluted periods. The increased pollution, combined with high relative humidity (RH) increased the liquid water content (LWC), which in turn promoted heterogeneous reactions. The Positive Matrix Factorization (PMF) analysis shows that secondary particulate matter (47%), coal combustion (19%), fugitive dust (14%), industrial sources (10%) and vehicular emissions (10%) are identified as the major emission sources during winter in the K-D-W region. Potential areas in the K-D-W region are distributed in the southeast direction of the 8th Division.

Keywords: PM$_{2.5}$, Composition characteristics, Source appointment, Potential sources

1 INTRODUCTION

PM$_{2.5}$ is a widely studied atmospheric pollutant that is mainly emitted from human activities. It has potential effects on climate change (Cheng et al., 2015), air quality (Shi et al., 2014), and public health (Li et al., 2017). PM$_{2.5}$ can be generated through various natural and human processes and can be emitted directly into the air or formed through gas-to-particulate conversions (Zhang et al., 2021).

Emission sources and adverse meteorological conditions, such as low wind speed and high relative humidity, are key factors in the formation, development, and dissipation of winter air pollution (Kong et al., 2020) In developed countries, including several European cities, secondary
and industrial sources are the main contributors to PM$_{2.5}$ pollution. Secondary particles have the highest contribution to PM$_{2.5}$ during winter (Choi et al., 2012; Vallius et al., 2005). Recent studies in China have extensively investigated the main chemical components of PM$_{2.5}$, including inorganic elements (IEs), water-soluble inorganic ions (WSIs), and carbonaceous compounds (OC/EC) (Tian et al., 2020). Regional characteristics of PM$_{2.5}$ have been studied in east-central and southern China, particularly in the Beijing-Tianjin-Hebei region (Zhang et al., 2017; Song et al., 2019), Yangtze River Delta (Pathak et al., 2009; Shi et al., 2014; Shu et al., 2017; Cheng et al., 2015), and Pearl River Delta (Cui et al., 2015; Tao et al., 2017).

Recently, some polluting enterprises in the eastern regions have been moved to the western regions, where environmental regulations are more lenient (Han et al., 2017), changing the regional industrial structure, increasing corporate pollution emissions, and boosting regional economic growth and employment. Xinjiang has experienced rapid growth in urban population density and the size of urban agglomerations (Shrestha and Luo, 2017). In addition, frequent sand and dust storm activities and long winter heating periods significantly exacerbated air pollution in Xinjiang. A previous study (Wang et al., 2020) analyzed the spatial and temporal variation of PM$_{2.5}$ based on satellite data. The results showed a significant increase in PM$_{2.5}$ concentrations on the northern slopes of Tianshan Mountain from 2001 to 2016.

The K-D-W region, including Kuitun (KT), Dushanzi (DSZ), and Wusu (WS), an area of 20,000 square kilometers, is located at the north slope of Tianshan Mountain and the southwest edge of the Junggar basin. It is one of the most central economic zones (the North Tianshan Mountain Economic Zone) and the largest petrochemical base of Xinjiang Uygur Autonomous Region, China. The K-D-W region is high in the south and low in the north and is divided into five terrain zones, which includes high mountains, medium and low mountains, hills, plains and deserts. Co-existence of coal chemical, petrochemical, iron and steel, power and concrete supply industries leading to more air pollutants (Zhang et al., 2020). Air pollution problems have become a severe concern in the K-D-W region, particularly in winter. PM$_{2.5}$ and its major components were assessed over the four annual seasons in Dushanzi. It was discovered that winter is the season with the most pollution, and coal combustion and secondary particulates were the primary sources of PM$_{2.5}$ during winter (Turap et al., 2019). A high-resolution field emission scanning electron microscope with energy dispersive X-ray spectroscopy (FESEM-EDX) was used to study the microscopic morphology of PM$_{2.5}$ in the Kuitun-Dushanzi petrochemical zone. The results showed that plant, power generation, vehicle exhaust emissions and road dust were the primary sources of PM$_{2.5}$ in the Kuitun-Dushanzi petrochemical zone (Talifu et al., 2015). Nevertheless, related studies on the K-D-W region were limited in data observations during specific periods, such as the heavy air pollution episode. This study aims to (1) investigate the impacts of meteorological factors (such as temperature, relative humidity and wind speed/direction) and related gas pollutants (NO$_2$, SO$_2$, CO, and O$_3$) to analyze the causes of pollution, (2) characterize PM$_{2.5}$ components under different pollution levels in the K-D-W region during winter, (3) apply Positive Matrix Factorization (PMF) to differentiate the sources of PM$_{2.5}$, and (4) use the MeteoInfo model to analyze the potential sources area. The key findings will provide reference data for establishing environmental policy and a regional development strategy.

2 METHODOLOGY

2.1 Sampling

Field sampling for ambient PM$_{2.5}$ was conducted in the KT, DSZ and WS environment monitoring stations, respectively (Fig. 1). The sampling location was on the building roof of the sampling sites, approximately 20 m above the ground. KT is located on the traffic fortress and encompasses the highest vehicle population. The DSZ region includes the most industries in these three cities. WS has the highest human population in the K-D-W region, with approximately 23 thousand people living in WS. All three sampling sites belong to the integrated functional area. Stores, schools, residential areas and office buildings surround the KT sampling site (44.42°N, 84.88°E). Office buildings and residential areas surround the DSZ sampling site (44.34°N, 84.90°E). The sampling sites in WS (44.45°N, 84.69°E) are surrounded by stores, residential areas and office buildings.
The offline PM$_{2.5}$ sampling campaign was undertaken from January 15 to January 29, 2016, using a low-volume gravimetric automatic sequential sampler (LVS, Comde-Derenda) with an airflow rate of 16.7 L min$^{-1}$. The samples were collected simultaneously on quartz fibers and Teflon filters from 11:00 am to 10:00 am the following day. All samples were preserved in a refrigerator immediately after sampling. The filters were weighed before and after sampling by placing them on a one-millionth automatic balance system (AWS-1, Camtek, Germany) at constant temperature [(20±1)$^\circ$C] and relative humidity [(50±5)%] for 24 h. The quality control method was developed in a previous study (Yu et al., 2020).

Meteorological data (wind speed, wind direction, temperature, and humidity) and online pollutant levels (PM$_{10}$, PM$_{2.5}$, NO$_2$, SO$_2$, CO, and O$_3$) were obtained from the automatic station.

2.2 Chemical Analysis

Quartz filter membranes were used to determine water-soluble ions (i.e., SO$_4^{2-}$, NO$_3^-$, Cl$^-$, NH$_4^+$, Na$^+$, Mg$^{2+}$, Ca$^{2+}$, K$^+$) with an ion chromatograph (ICS-1100, Dionex). Organic/elemental carbons (OC/EC) were assessed using a thermal/optical carbon analyzer (DRI Model 2001A, Desert Research Institute of US). Teflon PM$_{2.5}$ filter membranes were used to analyze inorganic elements (such as Na, Mg, and Al) with ICP-MS and ICP-OES (Agilent 7500a, Agilent company). Specific analytical methods of all components mentioned above were described in Yu’s study (Yu et al., 2020).

2.3 Statistical Analysis

2.3.1 Mass-reconstruction

PM$_{2.5}$ mass reconstruction (MR) is a method for aerosol analysis and is often used as a quality assurance tool for gravimetrically measured mass (Shahid et al., 2016). Typically, the chemical compositions of PM$_{2.5}$ can be divided into eight major types, including SO$_4^{2-}$, NO$_3^-$, NH$_4^+$, OM (organic matter), EC (elemental carbon), MD (mineral dust), TE (trace elements), and UM (unidentified matter). The calculation formula of OM and MD is as Eq. (2) and Eq. (3). TE is the sum of the elements except for the MD elements. Unidentified matter (UM) is an unidentified mass.

\[
[\text{MR}] = [\text{SO}_4^{2-}] + [\text{NO}_3^-] + [\text{NH}_4^+] + [\text{OM}] + [\text{EC}] + [\text{MD}] + [\text{TE}]
\]

(1)

\[
[\text{OM}] = 1.8 \times [\text{OC}]
\]

(2)

\[
[\text{MD}] = 1.89 \times [\text{Al}] + 2.14 \times [\text{Si}] + 1.4 \times [\text{Ca}] + 1.43 \times [\text{Fe}] + 1.67 \times [\text{Ti}] + 1.21 \times [\text{K}] + 1.66 \times [\text{Mg}]
\]

(3)
2.3.2 Ion balance

Comprehending the acidity of particulate matter (PM) holds great significance because it serves as a critical factor influencing heterogeneous reactions, hygroscopic expansion, and the toxicity of atmospheric PM. Additionally, it plays a pivotal role in the neutralization of acid rain (Shi et al., 2017). Calculations for ion balance proved valuable in analyzing the acid-base equilibrium of aerosols. Additionally, the AE (anion equivalent) to CE (cation equivalent) ratios served as indicators of atmospheric aerosol acidity. Calculation of anion and cation equivalents for particulate matter is described as follow:

\[ \text{AE} = \frac{[F^-]}{19} + \frac{[NO_2^-]}{46} + \frac{[Cl^-]}{35.5} + \frac{[NO_3^-]}{62} + \frac{[SO_4^{2-}]}{48} \]  
(4)

\[ \text{CE} = \frac{[NH_4^+]}{18} + \frac{[Ca^{2+}]}{20} + \frac{[K^+]}{39} + \frac{[Mg^{2+}]}{12} + \frac{[Na^+]}{23} \]  
(5)

The mass concentrations of [F\(^-\)], [NO\(_2\)\(^-\)], [Cl\(^-\)], [NO\(_3\)\(^-\)], [SO\(_4\)\(^{2-}\)], [NH\(_4\)\(^+\)], [Ca\(^{2+}\)], [K\(^+\)], [Mg\(^{2+}\)], and [Na\(^+\)] in the PM\(_{2.5}\) samples are denoted by the symbols. Earlier research utilized an AE/CE ratio exceeding 1 to signify acidic particle conditions, while a ratio lower than 1 indicated alkaline conditions.

2.3.3 ISORROPIA II model

The Liquid water content (LWC) of PM\(_{2.5}\) was calculated using ISORROPIA II (http://isorropia.eas.gatech.edu), which is based on the thermodynamic equilibrium formula of SO\(_4^{2-}\)-NO\(_3^-\)-Cl\(^-\)-Na\(^-\)-NH\(_4^+\)-K\(^+\)-Ca\(^{2+}\)-Mg\(^{2+}\)-H\(_2\)O (Seinfeld and Pandis, 2006). The chemical equilibrium components in the system are calculated under the given T and RH conditions. The ISORROPIA II thermodynamic model mainly includes two modes: forward (closed mode) and reverse (open mode), and two particle states: stable (steady state) and metastable (metastable state). This study chose the forward mode and metastable state, input water-soluble inorganic ion components (Na\(^+\), SO\(_4^{2-}\), NH\(_4^+\), NO\(_3^-\), Cl\(^-\), Ca\(^{2+}\), K\(^+\), Mg\(^{2+}\)) to calculate LWC.

2.3.4 Positive Matrix Factorization (PMF)

Positive Matrix Factorization (PMF v5.0 software of U.S. EPA), a usually applied source apportionment receptor model (Wang et al., 2013), was utilized in this study. The principles of PMF are described by Hsu et al. (2016), in detail.

2.3.5 Potential source contribution function (PSCF)

The MeteoInfo model and the TrajStat plug-in (meteothink.org) (Wang, 2014) were used to cluster the trajectories of the primary airflow in the K-D-W region with a simulated height of 500 m and a time of 24 h. GDAS meteorological data, PM\(_{2.5}\) concentrations, five main sources calculated from PMF are incorporated into the model to calculate air mass trajectories and potential sources. Using the Euclidean distance method, all the trajectories arriving at the receptor points were clustered and grouped, and the number of clusters was determined by using the total spatial variance (TSV) method. Potential sources for the Potential Source Contribution Function (PSCF) were analysed from January 15 to 29, 2016. The PSCF study area, ranging from 42–48°N and 76–90°E with a resolution of 0.2° × 0.2°.

3 RESULTS AND DISCUSSION

3.1 General Characteristics

Daily average PM\(_{2.5}\) mass concentrations in KT, DSZ, and WS from January 15 to January 29, 2016 are presented in Fig. 2. The concentration of PM\(_{2.5}\) at the three locations closely correlates with one another in the time series, indicating a regional pattern of PM\(_{2.5}\) pollution. The correlation coefficient of manual and online PM\(_{2.5}\) is 0.93 (\(p < 0.01\)), indicating reliable data quality. The average PM\(_{2.5}\) concentration in the K-D-W region during this pollution process is 210 \(\mu g m^{-3}\), 1.8 times higher than the daily concentration limit in the national ambient air quality standards (NAAQS) of China and
Fig. 2. Time series of (a) Wind Speed Rate and Wind Direction; (b) Temperature and RH; (c) NO2 and O3; (d) SO2 and CO; (e) online PM10, PM2.5; (f) PM2.5.

comparable to the winter PM2.5 concentration level in Shijiazhuang (Xie et al., 2019) (234 µg m⁻³, 2014–2016), higher than Harbin (Luo et al., 2021b) (111 µg m⁻³, 2017), Beijing (Luo et al., 2021a) (47.5 µg m⁻³, 2017), Chengdu (Liao et al., 2017) (149 µg m⁻³, 2013), Baoding (Sun et al., 2022) (156.9 µg m⁻³, 2017), Shanghai (Sun et al., 2022) (60.9 µg m⁻³, 2017), and Zhengzhou (Song et al., 2022) (191.35 µg m⁻³, 2017–2018). The high PM2.5 concentration level in the K-D-W region might correlate with enhanced emissions from coal combustion, as the result is similar to the so-called “heating-season” in other northern China cities. During the sampling period, PM2.5 concentrations are 267 ± 139 µg m⁻³ (KT), 172 ± 100 µg m⁻³ (DSZ), and 191 ± 121 µg m⁻³ (WS). The highest PM2.5 daily concentration is detected on January 27 (496 µg m⁻³ in KT), 28 (410 µg m⁻³ in DSZ), and 26 (418 µg m⁻³ in WS). Compared with the Grade II of China National Ambient Air Quality Standard (NAAQS), the PM2.5 concentrations in these three sites are approximately 3.56, 2.29, and 2.54 times higher, suggesting that PM2.5 pollution was heavy during winter in the K-D-W region. Relatively low PM2.5 concentrations in the DSZ were associated with lower precursor concentrations at this site. Additionally, the average value of PM2.5/PM10 is 0.8, ranging from 0.7–1, indicating that atmospheric particle consists chiefly of fine particles.

The PM2.5 concentration is significantly correlated with gaseous pollutants NO2 and SO2, with correlation coefficients of 0.82 and 0.44 (p < 0.01), respectively. These results infer that fossil fuel combustion and vehicles are important contributors to PM2.5 in the K-D-W region. Additionally, the influence of poor meteorological conditions (high relative humidity (RH) and low wind speed (WS)), which facilitates heterogeneous reactions (Xu et al., 2017), is another primary reason for the high PM2.5 concentrations (Zhang et al., 2019). During the sampling period, the wind speed was observed to be low, ranging from 0 to 1.6 m s⁻¹, the predominant wind direction (WD) was found to be focused between 70 and 236° (Fig. 2(a)). The relative humidity during the sampling
period averaged at 79%. Furthermore, the temperature during this time was relatively low, ranging from –19.9 to –5.5°C (Fig. 2(b)). The lower wind speed negatively affects the horizontal diffusion of PM$_{2.5}$. Under higher relative humidity, the participation of aqueous phase reactions can enhance the secondary conversion of trace gases, leading to the formation of secondary aerosols and exacerbating PM$_{2.5}$ pollution (Wu et al., 2022).

### 3.2 Characteristics of Chemical Compositions

This study analyzed PM$_{2.5}$ chemical compositions under five pollution levels in the K-D-W region, based on the China National Ambient Air Quality Standard. The levels ranged from clean days (Grade I) to severe pollution (Grade V) (Table S1).

#### 3.2.1 Water-soluble ions

Table S2 presents the water-soluble inorganic ion (WSII) content at different pollution levels in the K-D-W region during sampling. The contribution of WSIs to PM$_{2.5}$ varied from Grade I (66.04% ± 0.00%) to Grade V (62.14% ± 7.43%). The analysis reveals that WSIs are the primary component, with SNA ($SO_4^{2-} + NH_4^+ + NO_3^-$) accounting for 60.51% ± 8.48% of PM$_{2.5}$ and 95.37% ± 1.28% of total WSIs. The contribution of $SO_4^{2-}$ to PM$_{2.5}$ increases with pollution severity, ranging from 27.13% ± 0.00% in Grade I to 33.91% ± 4.41% in Grade V. Conversely, NO$_3^-$ and NH$_4^+$ percentages decrease from Grade I to Grade V levels, indicating that sulfate's secondary formation is the primary cause of PM$_{2.5}$ pollution.

The daily average ratio of NO$_3^-$/$SO_4^{2-}$ were 0.65 ± 0.00, 0.59 ± 0.07, 0.55 ± 0.14, 0.50 ± 0.17, and 0.35 ± 0.06 from Grade I to Grade V, respectively. The ratio of NO$_3^-$/$SO_4^{2-}$ < 1 reflects the dominant stationary combustion source for PM$_{2.5}$ (Wu et al., 2013). Additionally, from Grade I to Grade V, the higher conversion rate of $SO_4^{2-}$ concentration rather than NO$_3^-$ may cause the lower NO$_3^-$/$SO_4^{2-}$ value in more severe pollution levels.

Compared to $SO_4^{2-}$, NH$_4^+$, and NO$_3^-$, the content of other water-soluble ions (Na$^+$, K$^+$, etc.) were all relatively low, with minimal variation under different pollution levels.

The current investigation revealed strong correlations ($R^2 = 0.99$) between AE and CE across all samples (Fig. 3). The average AE/CE for all samples was 1.04 ± 0.2, indicating a slight acidity of the collected PM. This finding was consistent with previous studies in northern China (Turap et al., 2019). During this period of pollution, 52% of the samples surpassed the 1:1 line, signifying the acidic nature of the particles due to elevated levels of acid compounds (NO$_3^-$ and $SO_4^{2-}$).

#### 3.2.2 Carbonaceous compounds

OC and EC, derived from fuel combustion and motor vehicle exhaust emissions, are commonly associated with primary emissions and secondary conversion (Han et al., 2018). K$^+$ is a key
indicator of biomass combustion, while fossil fuel combustion emissions exhibit minimal K⁺ presence (Wang et al., 2013). Biomass combustion typically results in high K⁺/EC ratios ranging from 0.21 to 0.46, whereas fossil fuel combustion results in low ratios varying from 0.025 to 0.09 (Satsangi et al., 2012). In this study, the K⁺/EC ratios range from 0.083 to 0.121 under different pollution levels, indicating that fossil fuel combustion is the primary source of carbonaceous aerosols in the K-D-W region during sampling (Ji et al., 2014). The OC/EC ratio for coal combustion has been reported as 1 to 4.26, while for diesel and gasoline vehicles, it ranges from 0.5 to 4.2 (Watson et al., 2001; Zhang et al., 2010). The OC/EC ratios in this study range from 2.10 to 3.81, suggesting contributions from vehicle exhaust emissions and coal combustion to the carbonaceous component of PM$_{2.5}$.

OC may have primary and secondary sources (Satsangi et al., 2012). The calculation formula of SOC (secondary organic carbon) is defined in an earlier study (Zhang et al., 2019). The carbonaceous compound content of PM$_{2.5}$ at different pollution levels in the K-D-W region is shown in Fig. 4. The concentrations of OC, EC, and SOC are increasing as the pollution builds, with OC being the highest of the three. The OC average concentration increases gradually from Grade I (8.53 ± 0.00 µg m$^{-3}$) to Grade V (23.58 ± 6.54 µg m$^{-3}$). This increasing trend may be due to the poor atmospheric dispersion conditions, making it difficult for fossil fuel emissions to disperse. Concentrations of EC and SOC were far lower than OC and are 2.53–7.77 µg m$^{-3}$ and 2.52–6.27 µg m$^{-3}$ for Grade I to Grade V, respectively. Additionally, the percentages of OC, EC, and SOC decrease with worsening pollution, suggesting that carbonaceous composition may not be the primary driver of the increase in PM$_{2.5}$ concentrations during sampling.

3.2.3 Elements
As shown in Table S3, the sum of concentrations of 39 elements slightly increased from Grade I (6.50 ± 0.00 µg m$^{-3}$) to Grade IV (17.12 ± 6.95 µg m$^{-3}$), but the growth rate was lower than the PM$_{2.5}$, indicating that elements might not be the main cause of this pollution episode.

3.2.4 Pollution characteristics
As shown in Fig. 5, SNA is the dominant component of PM$_{2.5}$, with OM and MD being the subsequent components, accounting for 60.51%, 14.73%, and 12.23% of the PM$_{2.5}$ mass. Among the secondary inorganic particles, SO$_4^{2-}$ constitutes the largest proportion, accounting for 30.85% of PM$_{2.5}$, followed by NH$_4^+$ and NO$_3^-$, accounting for 14.94% and 14.53% of PM$_{2.5}$, respectively. SO$_4^{2-}$ was the dominant component, contributing 12.15%–40.92% to PM$_{2.5}$ under different pollution levels. As discussed in Section 3.2.1, the percentage of SO$_4^{2-}$ contribution increases, while the percentage of NO$_3^-$ and NH$_4^+$ decreases with worsening pollution levels. The observed trends can be attributed to the burning of coal for winter residential heating in the K-D-W region and unfavorable meteorological conditions, which enhance secondary transformation and worsen air
quality. The percentage of OM and MD decreased with the worsening pollution levels, accounting for a range of 24.14% and 16.21% (Grade I) to 11.32% and 7.95% (Grade V) of PM$_{2.5}$. EC and TE accounted for a small proportion, and the proportion gradually decreased with increasing pollution. Fig. 5 shows that the UM/PM$_{2.5}$ values increased as pollution worsened. The UM can probably be attributed to aerosol-bound water, systematic errors in chemical quantification and unanalyzed chemical components (Zhao et al., 2022).

The LWC was calculated using the ISORROPIA II model. The LWC is significantly positively correlated with relative humidity ($r = 0.42$, $P < 0.01$). Previous studies have demonstrated that hygroscopic components, like SNA, can increase aerosol LWC, resulting in elevated PM$_{2.5}$ concentrations (Peng et al., 2021). In this study, SNA concentration peaks during Grade V pollution, leading to the highest LWC concentration at constant RH (Fig. 6(b)). In conclusion, the rise in hygroscopic components like SNA and high RH increased the liquid water content (LWC), which in turn promoted heterogeneous reactions (Zhang et al., 2021).

### 3.3 Sources Apportionment

#### 3.3.1 Positive Matrix Factorization (PMF)

PM$_{2.5}$ and its components’ data were used in the PMF model, and five factors were chosen. Fig. 7 shows the modeled source profiles for each source, and their source profiles are shown in Fig. 8.

Factor 1 has a high abundance of Cl$^-$, with OC and EC having substantial content. Coal combustion usually has higher OC, EC, and Cl$^-$ concentrations (Liu et al., 2016), so this factor can be interpreted as a coal combustion source.

Factor 2 has a high content of Cr, Ni, Cu. Ni and is related to industrial sources, petrochemical plants have been associated with elevated levels of Ni (Talifu et al., 2015). Cr and Cu primarily originate from various industrial activities such as the leather industry, brick lining, chrome plating, textiles, copy machine toner, pigments for paints, inks, anti-corrosion coatings, stainless steel, textile dyes, and wood preservatives (Khan et al., 2020). Possible sources of Cu may include metal working factories, electroplating materials, Cu-containing fungicides, the iron and steel industry, wire burning, and incineration (Manoli et al., 2002). Therefore, factor 2 is considered an industrial source.
Fig. 6. Variation of aerosol liquid water concentration (LWC) at varying humidity conditions, colored according to PM$_{2.5}$ concentration.

Fig. 7. Profiles of sources identified from the PMF model. The bars and points represent the absolute concentrations and the percentages of species in the factors, respectively.

Factor 3 represents vehicular exhaust, featuring elevated levels of Ti, Fe, Zn, Ca, Cu, and Pb, with OC and EC components also present. Higher Fe and Ca usually come from dust, also found in vehicular exhaust emissions (Li et al., 2017). Previous studies used minor aerosol components (such as Zn, Pb, and Cu) as marker species (Fung and Wong, 1995; Wang et al., 2016). Pb is used...
as an important anti-detonator in gasoline (Ravindra et al., 2008) and Zn is emitted from lubricant oil, brakelinings, tires, and steel smelting (Salvador et al., 2004). Vehicle exhaust is also reported to contain significant OC and EC levels (Ji et al., 2019).

Factor 4 is characterized by high proportions of SO$_4^{2-}$, NH$_4^+$, and NO$_3^-$ in PM$_{2.5}$, which are secondary particulate matter, which could also contribute to the secondary source via the emission of their precursor gases.

In factor 5, K, Ca, and Mg$^{2+}$ have a relatively high proportion, and Al, Si, and Ca$^{2+}$ also have a certain proportion. The above components are all crustal elements, so this factor is interpreted as a fugitive dust source, related to soil blown by the wind and road dust (Begum et al., 2005).

As shown in Fig. 8(a). The secondary source, coal combustion, fugitive dust, and industrial and vehicular emissions, contribute 47%, 19%, 14%, 10%, and 10% to the PM$_{2.5}$, respectively. Comparison of source apportionment results (Table S4) with other domestic cities and South Asian countries revealed that the secondary particulate fraction in the K-D-W area during this pollution event was higher than in other study areas. The industrial source fraction was similar to that of Delhi, and higher than in other regions. The vehicular source fraction was similar to Lahore, lower than in Beijing, Dhaka, and Delhi, and higher than in Chengdu. The coal combustion source fraction was lower than in Chengdu but higher than in Beijing. The fugitive dust source fraction was similar to Chengdu, Baoshan, and Delhi, lower than in Beijing and Dhaka. In summary, during this pollution event, the fraction of secondary particulate matter and industrial sources were relatively high, the vehicular and coal combustion sources were at a moderate level, and the fugitive dust source fraction was relatively low.

As shown in Figs. 8(b), 8(c), and 8(d), with a contribution of 42% to 51%, secondary particulate matter is the most significant source of emissions. The secondary contribution of particulate matter in KT is the highest (51%), resulting in the highest PM$_{2.5}$ concentration. A previous study has shown that coal combustion was the dominant source of fine particles around China (Yao et al., 2010), resulting from coal still being a significant energy source in China. The contribution of coal combustion sources, fugitive dust and industrial source to PM$_{2.5}$ at the three sites range from 16% to 21%, 11% to 19%, and 7% to 12%. The contribution of motor vehicles to PM$_{2.5}$ (12%) is slightly higher in KT, owing to being an important transportation hub and communication power hub connecting the economic zone of the northern slope of the Tianshan Mountains, KT has seen a significant increase in traffic-related emissions due to its excellent geographical location for transportation (Wang, 2020).

Fig. 8. Relative contributions from five identified PM$_{2.5}$ sources.
3.3.2 Potential sources

Previous studies (Wang, 2020) have shown that the dominant winter wind direction in the K-D-W region is westerly, and the wind speed is higher, resulting in longer transmission distances. In contrast, wind speeds are lower for southerly and other wind directions, leading to shorter transmission distances. As shown in Fig. 9(a), Cluster 1 and Cluster 5 (blue line and black line) came from the southwestern direction, the transmission distance is relatively long. Cluster 1 came from central Xinyuan County, accounting for 32.41% of the air mass. Cluster 5 comes from Northeast Karakor, Kyrgyzstan, accounting for 1.94% of the air mass. Cluster 1 has a secondary particulate matter percentage of 35% (PM$_{2.5}$ 139 µg m$^{-3}$), while Cluster 5 has a percentage of 23% (PM$_{2.5}$ 114 µg m$^{-3}$). The air masses in Cluster 1 and Cluster 5 carry relatively low levels of PM$_{2.5}$ and SO$_{4}^{2-}$. The percentage of coal combustion, fugitive dust, vehicular exhaust, industrial source in Cluster 1 and Cluster 5 is 29% and 29%, 15% and 21%, 9% and 11%, 11% and 16%, respectively.

Clusters 2–4 have relatively short transmission distances. Cluster 2 (green line) air masses had shorter air quality transport pathways, accounting for 19.26% of the air mass. Cluster 3 (yellow line)

Fig. 9. (a) Mean 24 h backward trajectories of each trajectory cluster and the percentage of allocation to each cluster; (b) Analysis of potential source regions of PM$_{2.5}$ in the K-D-W region.
came from the southeasterly direction, accounting for 22.96% of the air mass. Cluster 4 (red line) came from the northeast, with a percentage of 23.43%. Cluster 2 (181 \(\mu g \, m^{-3}\)), Cluster 3 (178 \(\mu g \, m^{-3}\)), and Cluster 4 (155 \(\mu g \, m^{-3}\)) exhibit relatively high levels of PM\(_{2.5}\). These three air masses have the highest percentages of secondary particulate matter, ranging from 40% to 55%. Cluster 2, Cluster 3, and Cluster 4 show percentages of 11% to 17%, 14% to 20%, 10% to 13%, and 7% to 14% for coal combustion, fugitive dust, vehicular exhaust, and industrial sources, respectively. These findings highlight the significance of secondary particulate matter and polluting air masses originating from the eastern regions.

The PSCF analysis requires the definition of pollution trajectories. In this study, pollution trajectories were defined based on a PM\(_{2.5}\) concentration of 75 \(\mu g \, m^{-3}\), which corresponds to Grade II of China's National Ambient Air Quality Standard (NAAQS). The contribution factor of the potential source region of PM\(_{2.5}\) was calculated. A higher WPSCF value indicates a greater contribution of the area to the atmospheric particulate matter concentration in the K-D-W region. Fig. 9(b) reveals that the potential source regions of WPSCF in the K-D-W region are predominantly situated in the southeast direction of the 8th Division. The K-D-W region has a relatively low elevation, making it vulnerable to the influence of high mountains, which hinders the diffusion of pollutants to other areas. As a result, polluted air mass tend to accumulate and stagnate in the K-D-W region (Wang, 2020). These findings underscore the significance of implementing collaborative regional measures to mitigate air pollution.

4 CONCLUSIONS

The PM\(_{2.5}\) pollution was severe in the K-D-W region from January 15 to January 29, 2016, with average daily concentrations of 210 ± 109 \(\mu g \, m^{-3}\). PM\(_{2.5}\) pollution may have been influenced by increased emissions, while unfavorable meteorological conditions exacerbated the secondary generation, which is another significant factor contributing to pollution formation. SNA (SO\(_4^{2-}\) + NH\(_4^+\) + NO\(_3^-\)) are the dominant contributors to PM\(_{2.5}\), comprising 60.51% of the PM\(_{2.5}\) mass. The percentage of SO\(_4^{2-}\) contribution increases, while the percentage of NO\(_3^-\) and NH\(_4^+\) decreases with worsening pollution levels. Moreover, the increase in pollution combined with high RH increased LWC, further promoting heterogeneous reactions.

Using the PMF model, the secondary source, coal combustion, fugitive dust, industrial source, and vehicular emissions were identified as the major emission sources during winter in the K-D-W region, contributing 47%, 19%, 14%, 10%, and 10% to PM\(_{2.5}\), respectively. Secondary particulate matter and polluting air masses transmitted from the eastern regions cannot be ignored. The potential sources in the K-D-W region are distributed in the southeast direction of the 8th Division. These findings indicate the importance of regional joint prevention and control measures to control air pollution.

ACKNOWLEDGMENTS

This work was funded by Xinjiang Special Project for Air Pollution Prevention and Control: The Establishment of Heavy Pollution Weather Emergency Controls in Xinjiang Uygur Autonomous Region. The authors wish to thank the editor and reviewers for their valuable comments.

ADDITIONAL INFORMATION AND DECLARATIONS

Disclaimer

The authors declare that they have no conflicts of interest.

Supplementary Material

Supplementary material for this article can be found in the online version at https://doi.org/10.4209/aaqr.230290
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