



Article Spatial Distribution of Primary and Secondary PM_{2.5} Concentrations Emitted by Vehicles in the Guanzhong Plain, China

Pan Lu^{1,2,3}, Shunxi Deng^{1,4,*}, Guanghua Li¹, Jianghao Li¹, Ke Xu¹ and Zhenzhen Lu¹

- ¹ School of Water and Environment, Chang'an University, Xi'an 710064, China; 2019028015@chd.edu.cn (P.L.); 2019029020@chd.edu.cn (G.L.); jianghaoli@chd.edu.cn (J.L.); 2018229047@chd.edu.cn (K.X.); 2016029014@chd.edu.cn (Z.L.)
- ² School of Energy and Architecture, Xi'an Aeronautical Institute, Xi'an 710077, China
- ³ School of Architectural Engineering, Chang'an University, Xi'an 710064, China
- ⁴ Key Laboratory of Subsurface Hydrology and Ecological Effect in Arid Region of Ministry of Education, Chang'an University, Xi'an 710064, China
- * Correspondence: dengsx@chd.edu.cn; Tel.: +86-029-8233-4207

Abstract: With the rapid increase of the vehicle population in the Guanzhong Plain (GZP), the fine particulate matter ($PM_{2.5}$) emitted by vehicles has an impact on regional air quality and public health. The spatial distribution of primary and secondary $PM_{2.5}$ concentrations from vehicles in GZP in January and July 2017 was simulated in this study by using the Weather Research and Forecasting (WRF) model and the California Puff (CALPUFF) air quality model. The contributions of vehicle-related emission sources to total $PM_{2.5}$ concentrations were also calculated. The results show that although the emissions of primary $PM_{2.5}$, NOx, and SO₂ in July were greater than those in January, the hourly average concentrations of primary and secondary $PM_{2.5}$ in January were significantly higher than those in July. The highest concentrations of primary and total $PM_{2.5}$ were mostly located in the urban areas of Xi'an and Xianyang in the central region of GZP. The contributions of exhaust emissions, secondary nitrates, brake wear, tire wear, and secondary sulfate to the total $PM_{2.5}$ concentrations in GZP were 50.37%, 34.76%, 10.79%, 4.06%, and 0.04% in January and 71.91%, 11.14%, 11.89%, 5.03%, and 0.03% in July, respectively. These results will help us to further control $PM_{2.5}$ pollution caused by vehicles.

Keywords: PM_{2.5}; vehicle emissions; CALPUFF; concentration distribution

1. Introduction

With the rapid growth of the economy and urbanization, the high concentration of fine particulate matter ($PM_{2.5}$) has been frequently occurring in many regions of China [1–3]. Considering that high $PM_{2.5}$ concentrations not only worsen air quality and visibility [4,5], but also threaten human health and the regional climate [6–8], the Chinese government has engaged in reducing the annual average $PM_{2.5}$ concentrations to 35 µg/m³ by 2030 to meet the requirement by the World Health Organization (WHO) during the "transition period". To achieve this goal, it is particularly important to investigate the influences of anthropogenic sources on ambient $PM_{2.5}$ concentrations. Over the last decades, the vehicle population in China has rapidly increased and eventually reached a number of 372 million in 2020 [9]. Domestic and overseas studies have shown that vehicle emissions have become one of the major sources of $PM_{2.5}$ pollution [10,11]. For example, vehicle emissions accounted for 16%, 25%, and 26% of the ambient $PM_{2.5}$ concentrations in New York [12], San Joaquin Valley [13], and Beijing [14], respectively.

Air quality dispersion models are usually used to simulate the spatial and temporal distribution of air pollutants and provide effective means for formulating emission control policies. The California Puff model (CALPUFF), an advanced multi-layer, non-steady-state



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Copyright: © 2022 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). Lagrangian puff dispersion model, is recommended by the US Environmental Protection Agency (EPA) and many other international regulatory agencies to simulate the atmospheric dispersion of pollutants from various emission sources. The CALPUFF model can be run for any specified time period and for any region worldwide by considering the effects of complex three-dimensional meteorological and topographic conditions [15]. The flexibility of the CALPUFF model has made it widely applied to assess and simulate the distribution and dispersion of pollutant concentrations emitted by vehicles on one particular road or street. Shiva Nagendra et al. simulated the concentration distributions of PM2.5, sulfur dioxide (SO_2) , and nitrogen dioxide (NO_2) near a national highway passing through an industrial complex in the state of Tamil Nadu, India by applying the CALPUFF model [16]. Joo et al. adopted the Motor Vehicle Emission Simulator (MOVES) model to estimate nitrogen oxide (NOx) and PM_{2.5} emissions from vehicles on a freeway and used the CALPUFF model to simulate the dispersion of the pollutants in crash-free and crashinvolved traffic accidents on the outer ring expressway in Seoul, South Korea [17]. In addition, many studies have evaluated the dispersion of pollutants from multiple road sources based on the CALPUFF model. Fallah-Shorshani et al. integrated the CALPUFF model and a street-canyon model to calculate the NO₂ concentration distribution from 28 road segments of a dense urban neighborhood in Montreal, Canada [18]. Shekarrizfard et al. and Fallah-Shorshani et al. employed the CALPUFF model to simulate the dispersion of pollutants from all roads in the urban areas of Montreal [19,20]. Charabi et al. used the CALPUFF model to calculate the effect of monsoon and non-monsoon season on the dispersion of carbon monoxide (CO), carbon dioxide (CO₂), and NOx emitted by vehicles in the Salalah City of Oman [21]. Numerous existing studies have simulated the dispersion of pollutants under different road conditions on an urban scale or multiple urban regional scales [22–25]. However, previous simulations on the $PM_{2.5}$ dispersion from vehicles focused on the exhaust emissions, with less consideration of the contributions of nonexhaust sources (i.e., the gas-to-particle chemical conversion of tailpipe gaseous precursors, tire wear, brake wear, and road dust resuspension). Studies have shown that non-exhaust emissions have an important contribution to the total PM_{2.5} emissions of vehicles [26–29].

Guanzhong Plain (GZP) is located in northwestern China and consists of five cities: Xi'an (XA), Xianyang (XY), Weinan (WN), Baoji (BJ), and Tongchuan (TC). PM_{2.5} pollution in some cities in this region is often serious in winter [30–32]. The Three-Year Action Plan to Win the Blue Sky Defense War was issued by the State Council of China in 2018, and the GZP is one of the key areas of this plan [33]. Many researchers have carried out numerous studies on the chemical characteristics [30,34], contribution to environmental pollution [35,36], and emission reduction measures of PM_{2.5} emitted by vehicles in GZP [37,38]. Nevertheless, few studies have considered the distribution and dispersion of pollutant concentrations from vehicles in GZP.

This study employed the MOVES model to estimate primary $PM_{2.5}$, NOx, and SO_2 emissions from vehicle exhaust and non-exhaust emissions in the GZP in January and July 2017. The Weather Research and Forecasting (WRF) model and the CALPUFF air quality model were used to simulate the spatial distribution of primary $PM_{2.5}$, secondary $PM_{2.5}$, and total $PM_{2.5}$ concentrations. In addition, the contributions of vehicle-related emission sources to the total $PM_{2.5}$ concentrations were analyzed. It is hoped that the results from this study will help to formulate $PM_{2.5}$ reduction strategies in the GZP.

2. Methodology

2.1. Study Area

The Guanzhong Plain is on the eastern side of the Qinghai-Xizang Plateau and is surrounded by the Loess Plateau in the north and the Qinling Mountains in the south, with a narrow opening to the east (Figure 1). The east-west direction is approximately 380 km, the south-north direction is approximately 260 km, and its total area coverage is 55,465 km². The average elevation is 500 m. In addition, 33 state-controlled air quality monitoring stations and 5 meteorological observation stations in GZP were employed in this study.

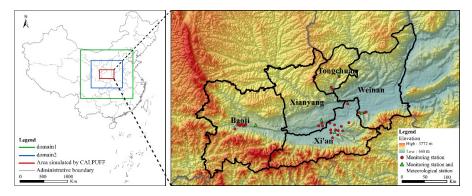


Figure 1. Location and topography of Guanzhong Plain (GZP) and the scope of simulated area.

2.2. Vehicle Emissions Model

In this study, we calculated the emissions of vehicle pollutants (primary $PM_{2.5}$, NO_X , and SO_2) using the emission factor method based on the MOVES model. The calculation formula is as follows:

$$EQ_i = \sum EF_i \times P_i \times VKT_i \times 10^{-6} \tag{1}$$

where EQ is the annual emissions of pollutants (t); EF is the vehicle emission factor (g/km); P is the vehicle population; VKT is the average annual distance in vehicle kilometers travelled (in km/vehicle); i is the pollutant type; j is the vehicle type. The calculation requires collecting relevant parameters such as the vehicle age, vehicle volume, activity level, vehicle types, and fuel types in GZP [39].

2.3. Air Dispersion Model

The WRF/CALPUFF modeling system was employed to investigate the dispersion of pollutants from vehicles in GZP. The WRF model is the latest generation mesoscale numerical weather prediction model, which has a wide range of applications in meteorological forecasting, ranging from a few kilometers to thousands of kilometers [40–42]. This model has the advantages of high precision and high operation efficiency. In this study, WRF was engaged to provide the initial guess meteorological fields for the California Meteorological Model (CALMET) in the CALPUFF model system. CALPUFF is an advanced air quality modeling system, which is suitable for modeling domains from tens of meters to hundreds of kilometers and has a good application to complex terrain, land use, and meteorological conditions. The model is open-source and has wide applicability and sufficient accuracy in the simulation of pollutant dispersion. The CALPUFF model system mainly consists of three components: CALMET (a diagnostic three-dimensional meteorological model), CALPUFF (a Gaussian smoke mass dispersion model), and CALPOST (a post-processing package). Many researchers have used this model to simulate the dispersion of pollutants from point sources [43], line sources [44,45], or area sources [46], and the model shows good reliability in the verification of simulation results.

WRF was configured with two nested domains, both of which were centered on the Bell Tower (34.26° N, 108.95° E) of XA (see Figure 1). The outer domain 1 (D1) extends from Changsha to Inner Mongolia, and the inner domain 2 (D2) covers the entire Shaanxi Province, and the area of domain D2 is 0.4 times that of D1. The domain D1 had 84×75 (1260 km \times 1125 km) grid cells with a horizontal resolution of 15 km, and D2 contained 162 \times 141 (810 km \times 705 km) grid cells with a horizontal resolution of 5 km, and the height of the two domains in the vertical direction included 32 layers. Initial conditions and boundary conditions were obtained from the Final Operational Global Analysis (FNL) of the National Center for Environmental Prediction (NCEP), and these conditions had a spatial resolution of 1° (approximately 111 km) at 6-h intervals [47,48]. Data in WRF output files were converted to a format compatible with CALMET by the interface program of CALWRF.

CALMET was utilized to generate hourly wind and temperature fields on the threedimensional gridded modeling domain. The model requires the input of high-resolution terrain elevation, land-use data, and meteorological data [49]. The terrain elevation and land-use data were obtained from United States Geological Survey (USGS) data. CALMET was configured with a domain covering the whole Guanzhong Plain (see Figure 1); the simulated domains had $250 \times 150 (500 \text{ km} \times 300 \text{ km})$ grid cells with a horizontal resolution of 2 km and 8 vertical layers, which corresponded to the physical heights of 2 m, 10 m, 40 m, 80 m, 100 m, 300 m, 1500 m, and 3000 m. CALMET's handled output data file was applied to drive the operation of CALPUFF.

In CALPUFF, the MESOPUFF chemical transformation module was used to simulate the oxidation of SO₂ and NO_X from vehicle tailpipes to form secondary SO₄²⁻ and NO₃⁻, respectively. The process involved five pollutant species: SO_2 , SO_4^{2-} , NO_X , hydrogen nitrate (HNO₃), and NO₃⁻. This chemical transformation can occur in both gas and liquid media. In the daytime, ozone (O_3) is used to replace hydroxyl radicals (OH) to oxidize SO_2 and NO_X. Therefore, the SO₂ and NO_X oxidation are hourly varying functions related to the background O₃ concentration, solar radiation, background ammonia (NH₃) concentration, relative humidity, and atmospheric stability. At nighttime, the oxidation rates of SO_2 and NO_X are very low compared with that during the day, so these parameters were set to default values of 0.2% and 2.0%, respectively, in the model [50]. In this paper, we obtained hourly background O₃ concentrations from state-controlled air quality monitoring stations in GZP. The background NH_3 concentrations were entered based on the monthly averages obtained by Wu et al. through an experimental method in GZP in 2017 [51], with the concentrations of $25 \pm 9.9 \ \mu g/m^3$ in January and $38 \pm 9.4 \ \mu g/m^3$ in July. The secondary sulfate and nitrate concentrations generated in the MESOPUFF conversion mode were multiplied by coefficients of 1.374 and 1.29, respectively, to obtain the secondary $PM_{2.5}$ concentrations [52]. The total $PM_{2.5}$ concentrations were equal to the sum of the primary PM_{2.5} concentrations and the secondary PM_{2.5} concentrations. In this simulation, we also considered the dry deposition and wet deposition of $PM_{2.5}$.

For the input of emission source intensity in the CALPUFF model, because the road network in GZP is dense and complex (Figure 2), and the line source input in the model is limited to straight-line form, and the maximum number is limited to 24, we allocated the road lines as an area source according to the spatial distribution of vehicle emissions through the ArcGIS software. Moreover, the number of area sources should be less than the maximum limit of 200 specified by the CALPUFF model. To reflect the hourly change of the pollutant emission source intensity of vehicles, as a simplified calculation, we allocated the pollutant emissions of all area sources by time, according to the change of hourly traffic flow. Then, the hourly emission rates of pollutants were input into the CALPUFF model as the source intensity.

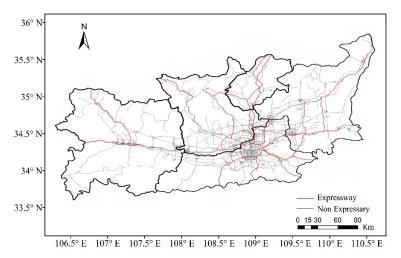


Figure 2. Distribution of the road network in GZP.

3. Results and Discussion

3.1. Analysis of Vehicle Emissions

The pollutant emissions from vehicles are an important input to the CALPUFF model. Table 1 shows the pollutant emissions of vehicles in the GZP obtained by running the MOVES model, and January and July represent winter (the most serious period of particulate pollution) and summer (the minimum period of particulate pollution) in 2017, respectively. In this research, pollutants emitted by vehicles included primary PM_{2.5}, SO₂, and NO_x. The primary PM_{2.5} chiefly came from exhaust emissions, brake wear, and tire wear. In Table 1, the emissions of primary PM_{2.5}, NO_x, and SO₂ in July increased by 10.78%, 1.96%, and 26.71%, respectively, compared with January. This was mainly because the local government implements the vehicle restriction policy in winter in Xi'an. Primary PM_{2.5} emissions in January and July were mostly from exhaust emissions, accounting for 87.70%, while brake wear and tire wear accounted for only 10.12% and 2.18%, respectively. According to the spatial distribution of pollutant emissions, we obtained 168 area sources through allocation, as shown in Figure 3. The relevant input parameters required by all area sources in CALPUFF for primary PM_{2.5} from exhaust emissions are shown in Table 2.

Table 1. Emissions of primary PM_{2.5}, NOx, and SO₂ from vehicles in Guanzhong Plain (GZP) in January and July 2017 (t).

Manth	NOv	SO_2	Primary PM _{2.5}				
Month	NO _X	50_{2}	Exhaust Emission	Brake Wear	Tire Wear		
January	6168.3	14.6	301.6	34.2	7.3		
July	6289.4	18.5	332.8	38.9	8.4		
Average	6228.9	16.6	317.2	36.6	7.9		

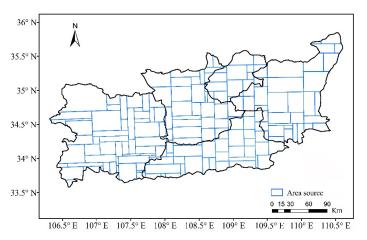


Figure 3. The result of area source allocation.

Table 2. Relevant input parameters required by all area sources for primary PM_{2.5}.

Time		Area Source Location						Source		Smoke	Effective	Dispersion	PM2.5 from Exhaust	
	x ₁ (km)	X2 (km)	х ₃ (km)	x ₄ (km)	Y ₁ (km)	Y2 (km)	Y ₃ (km)	Y ₄ (km)	Height (m)	Altitude (m)	Temperature (K)	Radius (m)	Height (m)	Emissions (g/m·s)
0:00~1:00	-2.07	-2.08	19.13	19.05	18.23	-8.72	-8.69	18.26	1	435	287.65	0	10	1.5×10^{-7}
	-19.47	-19.53	-1.36	-1.35	3.11	-17.92	-17.94	3.09	1	406	287.65	0	10	1.4×10^{-7}
	50.82	50.84	83.33	83.29	28.21	24.84	25.14	28.51	1	415	287.65	0	10	1.3×10^{-7}
													•••	
1:00~2:00	-2.07	-2.08	19.13	19.05	18.23	-8.72	-8.69	18.26	1	435	287.65	0	10	1.8×10^{-7}
	-19.47	-19.53	-1.36	-1.35	3.11	-17.92	-17.94	3.09	1	406	287.65	0	10	9.0×10^{-8}
	50.82	50.84	83.33	83.29	28.21	24.84	25.14	28.51	1	415	287.65	0	10	1.0×10^{-7}

3.2. Evaluation of Meteorological Simulation Results

The performance of the CALMET model was evaluated by comparing the simulation results with observation values from five meteorological observation stations in GZP. The locations of five meteorological observation stations (Xiaozhai, Xianyang meteorological station, Chencang District Environmental Protection Bureau, Tongchuan Party School, and Weinan Gymnasium) are shown in Figure 1. Figure 4 shows the wind rose plots at the Xiaozhai observation station in January and July 2017. Overall, the simulation results of wind speed and direction were in good agreement with the observed data. The prevailing wind directions were northeast and southwest in January, and the prevailing wind directions were southwest and southeast in July. This was caused by the topography and monsoon of GZP.

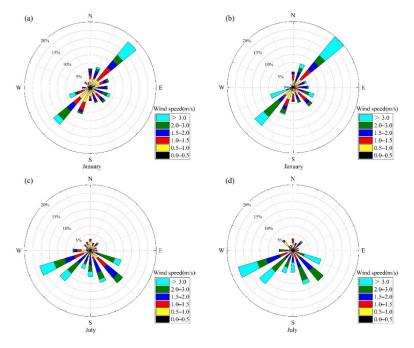


Figure 4. Windrose plots at the Xiaozhai station obtained by observation (a,c) and simulation (b,d).

Table 3 lists the validation statistics of the hourly temperature at a 2 m height and hourly wind speed at a 10 m height among all observation stations. Four statistical indexes, including the mean bias (MB), the index of agreement (IOA), the root mean square error (RMSE), and the Pearson correlation coefficient (R), were selected to verify the reliability of the model. It can be seen that temperature and wind speed were overestimated, because their MBs were 2.41 °C and 0.52 m/s in January and 2.16 °C and 0.51 m/s in July, respectively. The average IOA values were 0.93 for temperature and 0.79 for wind speed, indicating that there was a high degree of correlation and agreement between simulated and observed values. All RMSE values were close to 0, and R values were close to 1, showing that the meteorological simulation results had sufficient accuracy and reliability. Therefore, the CALMET model provided reliable meteorological condition parameters for predicting the dispersion and concentration distribution of PM_{2.5}.

Table 3. Verification statistics of the hourly temperature and wind speed in January and July 2017.

Variable	Period -	Me	ean	MB	ΙΟΑ	RMSE	R
variable		Obs.	Sim.	WID			
T (°C)	January	4.49	4.64	2.41	0.94	1.45	0.89
T (°C)	July	31.12	32.54	2.16	0.91	1.93	0.76
-1	January	0.94	1.22	0.52	0.80	0.61	0.74
$\mathrm{Ws}(\mathrm{m}\mathrm{s}^{-1})$	July	1.01	1.38	0.51	0.78	0.62	0.71

Owing to the special topographic conditions of GZP (see Figure 1), the prevailing northeast wind and low average wind speed in January easily resulted in a convergence center in the basin, which facilitated the accumulation of air pollutants, while the prevailing southwest and southeast wind and high average wind speed in July made air pollutants more easily transported from the basin to the outside [53–55]. In addition, the different temperatures in winter and summer had an important influence on the generation efficiency of secondary particulate matter [56,57].

3.3. Spatial Distribution of PM_{2.5} Concentrations

Understanding the spatial distribution of pollution concentration is conducive to the formulation of emission reduction measures. The dispersion and distribution of $PM_{2.5}$ concentrations in this research were mainly affected by emissions, meteorological conditions, and chemical transformation. To study the spatial distribution characteristics of $PM_{2.5}$ concentrations emitted by vehicles in January and July, the hourly average concentration was adopted in our paper, and the results are shown in Figure 5. In this study, the primary $PM_{2.5}$ concentrations were from exhaust emissions, tire wear, and brake wear; the secondary $PM_{2.5}$ concentrations included sulfate and nitrate concentrations generated by the gas-to-particle chemical conversion of SO_2 and NOx from vehicle tailpipes; the total $PM_{2.5}$ concentrations were obtained by summing the primary and secondary $PM_{2.5}$ concentrations.

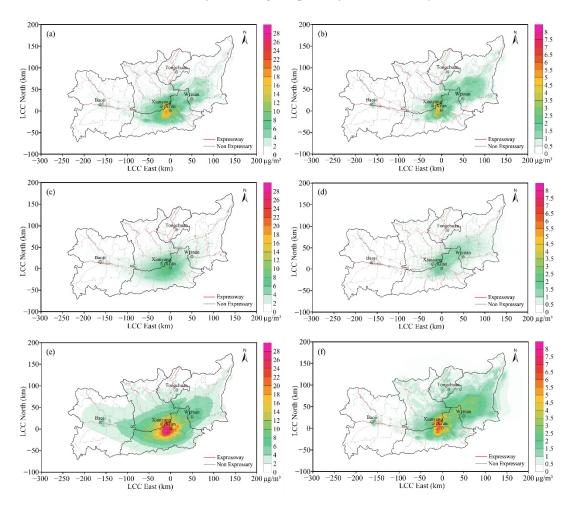


Figure 5. Spatial distribution of the primary $PM_{2.5}$ concentrations in January (**a**) and July (**b**); spatial distribution of the secondary $PM_{2.5}$ concentrations in January (**c**) and July (**d**); spatial distribution of the total $PM_{2.5}$ concentrations in January (**e**) and July (**f**).

As shown in Figure 5, the primary $PM_{2.5}$ concentrations in January were significantly higher than those in July, with the maximum values being 18.32 μ g/m³ and 4.55 μ g/m³,

respectively. However, Table 1 shows that the emissions of primary $PM_{2.5}$ in July were greater than those in January. The main reason for the difference in the primary $PM_{2.5}$ concentrations between these two months was that the prevailing northeast wind (see Figure 4) and lower wind speed (see Table 3) in January were not conducive to the dispersion of $PM_{2.5}$ compared with July. Furthermore, the unfavorable meteorological conditions in winter in GZP also include a relatively stable atmospheric stratification, low boundary layer height, and frequent temperature inversion phenomenon [53,54,58]. Due to the prevailing southwest wind and high wind speed in summer (see Figure 4), the distribution of primary $PM_{2.5}$ concentrations tended to spread to the northeast of WN in July. Except for WN in July, the primary $PM_{2.5}$ concentrations in five cities gradually decreased from urban areas with dense road networks to suburbs in January and July. The high concentrations of primary $PM_{2.5}$ mostly occurred in the west of the main urban area of XA and the southeast of the main urban area of XY.

The concentrations of secondary $PM_{2.5}$ were less than those of primary $PM_{2.5}$, and the maximum concentrations of secondary $PM_{2.5}$ were 9.06 µg/m³ and 1.37 µg/m³ in January and July, respectively. Among the gaseous precursors of secondary inorganic aerosols emitted by vehicles, NOx emissions were two orders of magnitude higher than SO₂ (see Table 1). Therefore, NO₃⁻ was the main component of secondary $PM_{2.5}$ from vehicles. Although there was little difference in NOx emissions from vehicles between January and July, the great difference in NO₃⁻ concentration was primarily due to the influence of winter and summer meteorological conditions on the gas-to-particle chemical conversion efficiency in GZP [35,59]. In particular, temperature is one of the dominant elements that impacts NO₃⁻ formation in fine particles; the lower temperature (<15 °C) in winter can favor the transformation of gaseous NOx to particulate NO₃⁻, while the higher temperature (>30 °C) in summer will enhance the volatilization of NO₃⁻ to gaseous nitric acid [56,57,60,61]. The simulated average temperature was 4.64 °C in January and 32.54 °C in July (see Table 3). In addition, during PM_{2.5} pollution in winter, the increase of water content also facilitates the formation of nitrate [62,63].

The spatial distribution trend of total $PM_{2.5}$ concentrations was similar to that of primary $PM_{2.5}$ concentrations, and its dispersion characteristics were more obvious. The maximum concentration of total $PM_{2.5}$ in January was 29.47 µg/m³, which was 4.37 times that of 6.75 µg/m³ in July. The concentration dispersion plume of total $PM_{2.5}$ was largely concentrated in the simulated GZP, and only a few exceeded the eastern boundary of WN, illustrating that the dispersion of $PM_{2.5}$ pollutions from vehicles in GZP had little impact on other regions.

3.4. Contributions of Vehicle-Related Emission Sources to Total PM_{2.5} Concentrations

To determine the contributions of vehicle-related emission sources to the hourly average total $PM_{2.5}$ concentrations, we simulated the hourly average $PM_{2.5}$ concentrations fields caused by each source separately and extracted the concentrations at the location of 33 state-controlled air quality monitoring sites in each concentration field. Then, these extracted concentrations were counted to analyze the contribution of each source to the total $PM_{2.5}$ concentrations in each city or the whole study area. Figure 6 shows the contribution values and proportions of vehicle-related emission sources in five cities and Guanzhong Plain in January and July. In this study, vehicle-related emission sources mainly included exhaust emission, brake wear, tire wear, secondary sulfate, and secondary nitrate.

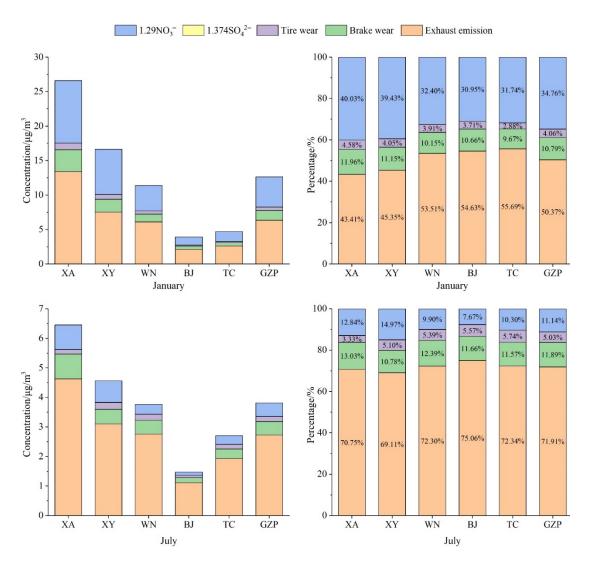


Figure 6. The value and proportion of the contributions of vehicle-related emission sources to the hourly average total PM_{2.5} concentrations.

The order of the $PM_{2.5}$ concentrations produced by each vehicle-related emission source in five cities followed XA > XY > WN > TC > BJ, and the total $PM_{2.5}$ concentrations also had the same order. This was chiefly caused by the difference in the vehicle population and road network density in the five cities. In the bar chart of the proportion of total PM_{2.5} concentrations, the contributions of exhaust emissions, secondary NO_3^- , brake wear, tire wear, and secondary SO₄²⁻ in January were 50.37%, 34.76%, 10.79%, 4.06%, and 0.04%, respectively. Their contributions in July were 71.91%, 11.14%, 11.89%, 5.03%, and 0.03%, respectively. The proportion of secondary SO_4^{2-} in these two months was very small, so the NO_3^- was the main component of secondary $PM_{2.5}$, converted from vehicle tailpipes. Generally, in the source apportionment studies of ambient $PM_{2.5}$, the ratio of NO_3^- to SO_4^{2-} is used by many researchers to indicate the relative contribution of mobile and stationary sources to PM_{2.5} pollution [64,65]. In January and July, the main changes in the contributions for total PM2.5 concentrations in five cities were exhaust emissions and secondary NO₃⁻. The contribution of secondary NO₃⁻ increased in January and decreased in July, while the contribution of exhaust emissions was the opposite. The contributions of brake wear and tire wear to total PM_{2.5} concentrations changed relatively little in these two months. Although the contribution of tire wear was small, it could not be ignored.

4. Conclusions

In this paper, the primary PM_{2.5}, NOx, and SO₂ emissions from vehicles were calculated by employing the MOVES model, and the spatial distribution characteristics of PM_{2.5} concentrations and the contributions of vehicle-related emission sources to the total PM_{2.5} concentrations were investigated by utilizing a WRF/CALPUFF modeling system. By comparing the simulation results with the observation data at five meteorological observation stations, the results showed that the meteorological simulation of the WRF/CALMET model had sufficient accuracy. In the distribution of PM_{2.5} concentrations, although the emissions of primary PM_{2.5}, NOx, and SO₂ in July were greater than those in January, the concentrations of primary and secondary $PM_{2.5}$ in January were significantly higher than those in July, indicating that the local topography, meteorological conditions, and gas-to-particle chemical conversion efficiency had important effects on the dispersion of $PM_{2.5}$ from vehicles. In January and July, the highest concentrations of primary $PM_{2.5}$ and total PM_{2.5} were mostly concentrated in the west of the main urban area of XA and the southeast of the main urban area of XY, which could be related to the direct influence of the road network density. The dispersion of total PM_{2.5} concentrations was restricted within GZP, indicating that the PM_{2.5} pollution from vehicles had little impact on other areas. From the ranking (XA > XY > WN > TC > BJ) of the total $PM_{2.5}$ concentration emitted by vehicles in the five cities, local vehicle emission intensity played a dominant role in the concentration distribution compared to pollutant transport. The analysis of the contributions of vehicle-related emission sources to the total PM2.5 concentrations showed that the contribution of exhaust emission was the largest, accounting for 50.37–71.91%, and the contribution of secondary SO_4^{2-} was the least, accounting for less than 0.1%. Besides this, the contribution of secondary NO₃⁻ was significant for the total PM_{2.5} concentrations, especially in January, accounting for 34.76%. The spatial distribution of PM_{2.5} concentrations from vehicles and the contributions of vehicle-related emission sources have an important guiding significance for the prevention and reduction of PM_{2.5} in GZP.

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