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Spatial distribution characteristics of PM$_{2.5}$ and PM$_{10}$ in Xi’an City predicted by land use regression models

Li Han$^a$, Jingyuan Zhao$^{a*}$, Yuejing Gao$^a$, Zhaolin Gu$^{b,*}$, Kai Xin$^a$, Jianxin Zhang$^a$

$^a$ Chang An Univ., Coll Architecture, 161 Chang An Rd., Xian, 710061, Shaanxi, People’s Republic of China
$^b$ Xi An Jiao Tong Univ., Sch Human Settlement & Civil Engn, Xian, 710049, Shaanxi, People’s Republic of China

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ABSTRACT

PM$_{2.5}$ and PM$_{10}$ could increase the risk for cardiovascular and respiratory diseases in the general public and severely limit the sustainable development in urban areas. Land use regression models are effective in predicting the spatial distribution of atmospheric pollutants, and have been widely used in many cities in Europe, North America and China. To reveal the spatial distribution characteristics of PM$_{2.5}$ and PM$_{10}$ in Xi’an during the heating seasons, the authors established two regression prediction models using PM$_{2.5}$ and PM$_{10}$ concentrations from 181 monitoring stations and 87 independent variables. The model results are as follows: for PM$_{2.5}$, $R^2 = 0.713$ and RMSE = 8.355 μg/m$^3$; for PM$_{10}$, $R^2 = 0.681$ and RMSE = 14.842 μg/m$^3$. In addition to the traditional independent variables such as area of greenspace and road length, the models also include the numbers of pollutant discharging enterprises, restaurants, and bus stations. The prediction results reveal the spatial distribution characteristics of PM$_{2.5}$ and PM$_{10}$ in the heating seasons of Xi’an. These results also indicate that the spatial distribution of pollutants is closely related to the layout of industrial land and the location of enterprises that generate air pollution emissions. Green space can mitigate pollution, and the contribution of traffic emission is less than that of industrial emission. To our knowledge, this study is the first to apply land use regression models to the Fenwei Plain, a heavily polluted area in China. It provides a scientific foundation for urban planning, land use regulation, air pollution control, and public health policy making. It also establishes a basic model for population exposure assessment, and promotes the sustainability of urban environments.

1. Introduction

The rapid economic development and accelerated urbanization process in China have been accompanied by high energy consumption and excessive pollutant emission, this has caused serious air pollution issues and hindered the sustainable development of urban areas (Liu, Sun, & Feng, 2020; Ortolani & Vitale, 2016). As main air pollutants, PM$_{2.5}$ and PM$_{10}$ are the most harmful to human health and thus, of the most concern to the general public. They are the focus of smog control in China at the current stage. The concentrations of PM$_{2.5}$ and PM$_{10}$ are impacted by urban space morphology, land use layout, and adverse meteorological factors and are thereby likely to accumulate in cities (Jin et al., 2019). Long-term exposure to contaminated atmosphere increases the risk of cardiovascular and respiratory diseases (Barzeghar, Sarbakshah, Hassanvand, Faridi, & Gholampour, 2020; Berman, Burkhardt, Bayham, Carter, & Wilson, 2019; Feng, Gao, Liao, Zhou, & Wang, 2016). Properly planned commuting routes can reduce human exposure to pollution (Ahmed, Adnan, Janssens, & Wets, 2020; Pilla & Broderick, 2015; Qiu et al., 2017). The variations in spatial distribution of urban air pollutants have become a widespread concern in several fields such as urban and rural planning, environmental science, and medicine (Son et al., 2018; Yang et al., 2020; Yuan, Song, Huang, Shen, & Li, 2019; Zou, Wilson, Zhan, & Zeng, 2009).

Land use regression (LUR) models have proven to be an effective method for predicting the spatial distribution of pollutants (Jerrett et al., 2005). LUR models work using pollutant concentration data collected at a limited number of monitoring stations in conjunction with characteristic variables such as land use information to evaluate pollutant concentrations in areas that lack monitoring stations. A main feature of LUR models is the correlation of land use characteristics to the concentrations of target pollutants, which can be used to determine the relationship between air pollutant concentrations and other geographic variables to simulate the spatial distribution of air pollutants in urban areas and identify the causes of pollutants to a certain extent.
The interpretation of the relationship can guide urban land use adjustment. By adjusting the layout of industrial land, intensive land use is achieved to reduce pollutant emission, and ultimately accomplish sustainable urban land use.

One of the earliest LUR models was developed by Briggs et al. (1997) to predict NO\textsubscript{2} concentrations in three European cities and plot pollution maps. Owing to the simplicity of model construction and ease of data acquisition as well as improvement in the modeling technology and content and higher diversity in the allowed variable types, LUR models have also been applied to the prediction of air pollutants such as NO\textsubscript{2}, PM\textsubscript{10}, and PM\textsubscript{2.5} in Europe and North America (Allen, Amram, Wheeler, & Brauer, 2011; Briggs et al., 2000; Eeftens et al., 2012; Moore, Jerrett, Mack, & Kunzli, 2007; Song, Jia, Li, Tang, & Wang, 2019). Two early studies in 2010 (Chen, Bai et al., 2010, 2010b) predicted the concentrations of PM\textsubscript{10}, NO\textsubscript{2}, and SO\textsubscript{2} in two Chinese cities (Tianjin and Jinan) and plotted pollutant distribution maps. Since 2013, China has begun to gradually establish and improve its air quality monitoring network, an action accompanied by a growing body of LUR-model-based studies investigating the spatial distribution of air pollutants in Chinese cities such as Chengdu, Changsha, Beijing, and Shanghai, with a particularly large number of studies in the latter two cities (Ji, Wang, & Zhuang, 2019; Liu et al., 2015; Meng et al., 2015, 2016; Wu et al., 2015; Xiao, Wang, Wu, Fu, & Zhu, 2018). Compared with the research results of other cities, this study is the first to apply land use regression models to the Fenwei Plain, a region in China with severe air pollution. The number of monitoring stations used in this study is the greatest so far. The dependent variables are selected specifically during the heating seasons. It explains the reasoning behind the selection of buffer zones. It applies comprehensively all aspects of regression model diagnosis, cross-validation and verification of LUR applicability in different heating seasons. Hence, to a certain extent, it has enriched the application of land use regression models in the prediction of the spatial distribution of atmospheric pollutants.

Xi’an is an important western Chinese city located on the west of the rift basin of the Fenwei Plain, encompassing 11 cities; a plain subjected to smog in large areas and considered one of the most atmospherically polluted areas in China. The national air quality report released by the Ministry of Ecology and Environment of China revealed that between January and December 2018, Xi’an ranked 158 out of 169 cities in terms of air quality and was under severe air pollution. Xi’an has special natural conditions (i.e., unique topography and unfavorable meteorological conditions) with a special land use status, economic development level, and industrial layout. Thus, the air pollution is further exacerbated (Huang, Zhang, Tang, & Liu, 2015; Song et al., 2015). Therefore, a deep insight into the spatial distribution characteristics of the concentrations of PM\textsubscript{2.5} and PM\textsubscript{10} during the heating seasons of Xi’an is the key to supporting air pollution control.

The purpose of this study is to establish a regression prediction model for PM\textsubscript{2.5} and PM\textsubscript{10} in the heating seasons of Xi’an to test the applicability of the land use regression models, and to reveal the spatial distribution characteristics of these pollutants. Further, it aims to
analyze the relationship between the spatial distributions of PM$_{2.5}$ and PM$_{10}$ and land use characteristics and therefore provides a scientific foundation for urban planning, land use regulation, air pollution control, and public health policy-making. It also establishes a basic model for population exposure assessment. The application of the land use regression models to areas requiring heating in winter and heavily polluted areas plays a positive role in achieving sustainable urban environment and promoting sustainable development in urban environments.

2. Materials and methods

The air quality data used in this study were the daily mean concentrations of PM$_{2.5}$ and PM$_{10}$ at 181 air quality monitoring stations under the Xi’an Ecology and Environment Bureau. The concentration measurements were conducted during the winter heating season from November 15, 2018 to March 15, 2019, and the period-averaged concentrations of PM$_{2.5}$ and PM$_{10}$ obtained from each monitoring station were used as the dependent variables, as depicted in Fig. 1. A total of 86 factors in the five categories of land use, road traffic facilities, socioeconomic development, emission source, and geospatial information were considered as independent variable candidates. For a particular monitoring station, independent variable candidates were extracted in two ways: (1) with the monitoring station as the center, circular buffer zones at various distances were delineated using GIS, and the independent variable candidates were the length, number, or area within the buffer zones, Fig. 2 shows the length of the roads in the 3000 m buffer zone around the New Software City station; (2) the independent variable candidates were the distances from the monitoring stations to notable objects or the characteristic values of monitoring stations, Fig. 3 displays the distance from the New Software City station to the nearest highways. After the extraction of variables, correlation analysis was performed between the independent and dependent variables using SPSS software. Variable screening was performed based on the magnitude of the Pearson correlation coefficients, and the selected independent variables were included in multiple stepwise regression analyses using R software. The established models were subjected to cross-validation to test their generalizability using R software. The procedure followed in this study is depicted in Fig. 4.

2.1. Study area and its characteristics

Xi’an, the capital of Shaanxi Province and an important central city in western China, is located in the Guanzhong Basin in the middle of Yellow River watershed and has the largest variations in elevation within its administrative areas among all Chinese cities. Xi’an is composed of 11 districts with two counties and has been entrusted the administration of the Xi Xian New District, having a total area of 10,752 km$^2$, approximately 204 km long in the east-west direction and approximately 116 km wide in the south-north direction. By the end of 2018, the resident population had reached 10,003,700, and the city’s GDP in 2018 was 834.986 billion Chinese RMB. The prevailing winds in Xi’an are the northeasterly winds with low speed in Fig. 5. Thus, the meteorological conditions are not favorable for the diffusion of pollutants. A stagnation zone of anticyclonic airflow is prone to form owing to obstruction by mountains and the sinking of the leeward airflow. When pollution occurs, the pollutants accumulate mostly near the surface, where diffusion is difficult. The Fenwei Plain is located in a valley region, and any city in the plain is under the direct impact of pollutant emissions from other cities. In terms of the energy consumption structure, coal consumption accounts for a relatively high proportion of total energy consumption in the Fenwei Plain. Shaanxi and Shanxi Provinces are large coal producers as well as consumers. In particular, coal consumption is more centralized in the Fenwei Plain, accounting for nearly 90% of its total energy consumption, far greater than the national average of 60%.

2.2. Dependent variables

The daily mean concentrations of PM$_{2.5}$ and PM$_{10}$ obtained from 181 air quality monitoring stations of Xi’an Ecology and Environment Bureau were used in this study, which were measured during the winter heating season from November 15, 2018 to March 15, 2019, with period-averaged concentrations at each station used as the dependent variables. As illustrated in Figs. 6 and 7, the concentrations of PM$_{2.5}$ and PM$_{10}$ from the 181 stations display a normal distribution. The mean is the average value of the concentrations, and Std. Dev. is the standard deviation of the concentrations. Xi’an has cold weather in winter, and the local government implements central a heating system, which requires combustion of a substantial amount of coal and natural gas. This aggravates the PM$_{2.5}$ and PM$_{10}$ pollution in the city. In addition, due to frequent calm days in winter plus the adverse terrain in Xi’an for pollution dispersion, the occurrence of heavy pollution is concentrated during this period, causing great harm to human health. Considering these factors, the authors select the PM$_{2.5}$ and PM$_{10}$ concentration data of the heating season from November 15, 2018 to March 15, 2019.
2.3. Independent variables

2.3.1. Land use information

The land use data used in this study were derived from the remote sensing monitoring data of China’s land use, built by the Chinese Academy of Sciences. The Landsat TM/ETM/OLI remote sensing images are the main data source. After going through processes such as image fusion, geometric correction, image enhancement and stitching etc., the land use types were classified into 6 first-level categories, 25 second-level categories and certain third-level categories according to the land use/cover classification system in China, via human-computer interactive visual interpretation. In this study, five types of land-use data were extracted, namely, those from farmland (paddy fields + dry land), green land (forest land + grassland), waterbodies (waterways + lakes + reservoirs + ponds), industrial and mining land (factories and mines + industrial areas + airports), and construction land (urban land + rural residential areas). The shape and size selection of a buffer zone was based on the diffusion range of the pollutants in the atmosphere and the impact of geographical elements on the pollutants. However, because of the complexity and uncertainty of atmospheric pollution diffusion, previous research results were usually referenced when determining a new buffer zone. In this study, the correlation
coefficients of most independent variables increased with respect to pollutant concentrations as the buffer zones increased in size until the distance of 5000 m, a limiting distance beyond which the correlation coefficients would not increase. Thus, the maximum distance of buffer zones was set to 5000 m. GIS software was employed to establish station-centered circular buffer zones for each of the 181 monitoring stations at successive distances of 100, 300, 500, 1000, 2000, 3000, 4000, and 5000 m and then to extract the length or area data associated with each type of land use in each buffer zone.

2.3.2. Road traffic facility information

Road traffic facility information referred to road networks, parking lots, and bus stops. In this study, five types of road network data were extracted from OpenStreetMap, namely, motorways, primary roads, secondary roads, tertiary roads, and trunk lines. The road network data in a buffer zone were extracted using two metrics: extraction of the length of motorways in the buffer zone or extraction of the total length of the five types of roads in the buffer zone. The parking lot data and bus stop data were obtained from Gaode map, i.e., the number of parking lots and bus stops in each buffer zone were calculated.

2.3.3. Socioeconomic information

The socioeconomic information consisted of GDP and population data. The GDP data came from the kilogram grid dataset of the spatial distribution of China’s GDP (GDP Grid China) constructed by the Chinese Academy of Sciences. It has a raster data form, with each raster representing the total GDP output value within the grid range (1 square kilometer) in the unit of ten thousand yuan/km². The GDP value of each grid with a monitoring site was extracted from GIS data. The population data were derived from the sixth national census and used to calculate the population of each abovementioned sub-district or town.

2.3.4. Emission source information

The emission sources consisted of air-polluting enterprises, restaurants, and motorways. Air-polluting enterprise information was obtained from the Monitoring Information Release Platform of Key Pollutant-discharging Enterprises in Shaanxi Province and the List of Key Pollutant-discharging Units released by Xi’an Ecology and Environment Bureau. There were 37 pollutant-discharging enterprises. The distance between each monitoring station and the nearest pollutant-discharging enterprise from it was calculated. Also the number of pollutant-discharging enterprises in each buffer zone was counted. Restaurant data were obtained from Gaode map by calculating the number of restaurants in each buffer zone. Motorway data were obtained by calculating the distance from each monitoring station to its nearest motorway.

2.3.5. Geospatial information

Geospatial information consisted of the elevation of each monitoring station and its distance to a water surface. Elevation data were obtained by extracting Digital Elevation Model (DEM) topographic data with a precision of 30 m. Considering the effect of water–land breeze on atmospheric pollution transport, the distance from each monitoring station to the nearest water bodies was calculated.

2.4. Model construction

A total of 87 independent variables were extracted. Bivariate correlation analysis was performed among the 87 independent variables and the dependent variables PM$_{2.5}$ and PM$_{10}$ using SPSS 17.0 to obtain the Pearson correlation coefficients of each independent variable with respect to PM$_{2.5}$ and PM$_{10}$. Independent variables that are significantly correlated to the dependent variables ($P < 0.05$) were selected. In each category of independent variables, the variables with the largest Pearson correlation coefficient were selected, which led to the selection of 13 independent variables for PM$_{2.5}$ (Table 1) and 14 for PM$_{10}$ (Table 2). Multiple stepwise regression of PM$_{2.5}$ and PM$_{10}$ was separately performed on these independent variables using R software to remove independent variables with a $p$-value > 0.01 while performing
collinearity diagnostics to remove independent variables with Variance Inflation Factor (VIF) > 4.

2.5. Model diagnostics

The models were subjected to regression diagnostics using R software. For regression diagnostics, the results of model fitting were presented in four plots: (1) a Residual-versus-Fitted plot to test the assumption that the independent variable in question was linearly correlated to the dependent variable in question; (2) a Normal Q-Q plot to test the normality of residuals; (3) a Scale-Location plot, intended to test the homoscedasticity assumption; and (4) a Residual-versus-Leverage plot to identify outliers, high-impact points, and high-leverage points.

2.6. Model cross-validation

The models were subjected to cross-validation using R software. Model validation was performed using the 10-fold cross-validation method aimed at testing the generalizability of the models. Thus, the samples in question were divided into 10 equal-sized subsamples, of which one subsample was retained as the validation group, whereas the remaining nine subsamples were used as the training group; repeating this process in turn for each subsample as the validation group finally led to a total of 10 prediction equations, whose \( R^2 \) values and RMSEs were averaged. The equations for RMSE and \( R^2 \) calculations are listed as follows:

\[
RMSE = \sqrt{\frac{1}{m} \sum_{i=1}^{m} (y_{i}^{(i)} - \hat{y}_{i}^{(i)})^2}
\]

\[
R^2 = 1 - \frac{\sum_{i=1}^{m} (y_{i}^{(i)} - \bar{y})^2}{\sum_{i=1}^{m} (y_{i}^{(i)} - \bar{y})^2}/m
\]

In the RMSE equation, \( y_{i}^{(i)} \) represents the monitoring concentration of the i-th monitoring station in the test set, \( \hat{y}_{i}^{(i)} \) refers to the predicted concentration of the i-th monitoring station in the test set, and \( m \) is the number of monitoring stations in the test set. In the \( R^2 \) equation, \( \hat{y}_{i}^{(i)} \) and \( y_{i}^{(i)} \) represent the predicted and monitoring concentrations of the i-th monitoring station respectively in the training set, \( \bar{y} \) represents the average concentration of the training set, and \( m \) indicates the number of monitoring stations in the training set.

2.7. Industrial land

The results section analyzed the relationship between the industrial land layout of the study area and the Regulatory Management Zone (RMZ) and the spatial distributions of PM\(_{2.5}\) and PM\(_{10}\) in the heating seasons in Xi’an. The definition of industrial land in urban and rural planning is applied here, which refers to land for production shops, warehouses and auxiliary facilities of industrial and mining enterprises, including land for special railways, docks and auxiliary roads, and parking lots. The information of industrial land layout was from the central urban area land use plan map from Xi’an’s Urban Master Plan (2008–2020) and the remote sensing monitoring data of China’s land use.

### Table 1

| Category | Sub-category | Buffer zone | Unit | Code   | Mean   | Standard deviation | Min  | Max   |
|---------|--------------|-------------|------|--------|--------|--------------------|------|-------|
| Land use information | Green space | 4000 m | m\(^2\) | GS-4000 | 5991739 | 9151113 | 0 | 45787914 |
|         | Industrial and mining land | 5000 m | m\(^2\) | IM-5000 | 1796676 | 2565877 | 0 | 12036045 |
|         | Built-up area | 1000 m | m\(^2\) | BA-1000 | 1639066 | 1146245 | 0 | 3141593 |
| Road traffic information | Major road | 5000 m | m | MR-5000 | 186615 | 121895 | 6738 | 417015 |
|         | Parking lot | 5000 m | Number | PA-5000 | 1013 | 1548 | 0 | 5080 |
|         | Bus stop | 4000 m | Number | BS-4000 | 98 | 108 | 0 | 354 |
| Socioeconomic information | Population | No | Number | PO | 58588 | 46813 | 2264 | 223840 |
| Emission source information | Distance to the nearest air-polluting enterprise | No | m | DIS-MO | 4528 | 5094 | 21 | 43354 |
|         | Distance to the nearest motorway | 5000 m | Number | RE-5000 | 3122 | 4489 | 0 | 14736 |
|         | Restaurant | 5000 m | Number | PE-5000 | 0.91 | 1.14 | 0 | 5 |
| Geospatial information | Elevation | No | m | EL | 467 | 154 | 345 | 1124 |
|         | Distance to nearest water bodies | No | m | DIS-WA | 2716 | 2209 | 17 | 8796 |

### Table 2

| Category | Sub-category | Buffer zone | Unit | Code   | Mean   | Standard deviation | Min  | Max   |
|---------|--------------|-------------|------|--------|--------|--------------------|------|-------|
| Land use | Green space | 5000 m | m\(^2\) | GS-5000 | 9814783 | 14460656 | 0 | 71238521 |
|         | Industrial and mining land | 5000 m | m\(^2\) | IM-5000 | 1796676 | 2565877 | 0 | 12036045 |
|         | Built-up area | 1000 m | m\(^2\) | BA-1000 | 1639066 | 1146245 | 0 | 3141593 |
| Road traffic information | Motorway | 5000 m | m | MO-5000 | 19906 | 21388 | 0 | 88843 |
|         | Major road | 5000 m | m | MR-5000 | 186615 | 121895 | 6738 | 417015 |
|         | Bus stop | 5000 m | Number | BS-5000 | 145 | 162 | 0 | 550 |
| Socioeconomic information | Population | No | Number | PO | 58588 | 46813 | 2264 | 223840 |
| Emission source information | Distance to the nearest air-polluting enterprise | No | m | DIS-MO | 4528 | 5094 | 21 | 43354 |
|         | Restaurant | 5000 m | Number | RE-5000 | 3122 | 4489 | 0 | 14736 |
| Geospatial information | Elevation | No | m | EL | 467 | 154 | 345 | 1124 |
|         | Distance to nearest water bodies | No | m | DIS-WA | 2716 | 2209 | 17 | 8796 |
3. Results

3.1. Significant independent variables

Bivariate correlation analysis indicated that 44 of the 87 independent variables were significantly correlated to PM2.5 and 42 to PM10. Among these 44 and 42 independent variables, those with the largest correlation coefficients in the respective categories were selected, ultimately leading to 13 and 14 independent variables selected for PM2.5 and PM10, respectively, which included 10 in common, as presented in Tables 1 and 2.

The independent variables demonstrated positive correlation to the concentration of PM2.5, except for four independent variables, which demonstrated negative correlation, namely, GS-4000, reflective of the area of greenspaces in buffer zones at a distance of 4000 m; DIS-PE, reflective of the distances from the stations to their respective nearest air-polluting enterprises; DIS-MO, reflective of the distances from the stations to their respective nearest motorways; and EL, reflective of the elevation of the stations, as depicted in Fig. 8. Similarly, GS-5000, DIS-PE, DIS-MO, and EL demonstrated negative correlation to the concentration of PM10, as depicted in Fig. 9. The negative correlation coefficient \( r \) of GS-4000 with respect to PM2.5 was the largest among the four negative correlation coefficients with respect to PM2.5. The negative correlation coefficient \( r \) of GS-5000 with respect to PM10 was smaller than that of only EL, indicating that larger the greenspaces in buffer zones, smaller were the concentrations of PM2.5 and PM10 at the stations. The negative correlation coefficient \( r \) of EL with respect to PM2.5 and PM10 was the second largest (after that of GS-4000) and the largest, respectively, which was attributed to the special terrain of Xi’an, i.e., stations with higher EL had larger green spaces. The correlation coefficient \( r \) of DIS-PE and DIS-MO with respect to the pollutants was large and significantly negative, indicating that closer the air-polluting enterprises and motorways, higher were the concentrations of PM2.5 and PM10.

3.2. LUR models

3.2.1. Multiple stepwise regression

Bivariate correlation analysis confirmed that three independent variables, GS-4000, RE-5000, and PE-5000, should be included in the PM2.5 LUR model. The regression coefficient was significant at the \( p < 0.05 \) level, and the adjusted \( R^2 \) value (Adj-\( R^2 \)) was 0.713, indicating that 71.3 % of the variance of the concentration of PM2.5 was accounted for by the model. The model RMSE was 8.355 \( \mu \text{g/m}^3 \) and the VIF of each variable was less than 4, indicating that there was no multicollinearity among the three independent variables (Table 3). The observed and predicted concentrations of PM2.5 were compared (Fig. 10).

For the PM10 LUR model, bivariate correlation analysis confirmed that four independent variables, GS-5000, MO-5000, BS-5000, and PE-5000, should be included in the model. The regression coefficient was significant at the \( p < 0.05 \) level, and the Adj-\( R^2 \) was 0.681, indicating that 68.1 % of the variance of the concentration of PM10 was accounted for by the model. The model RMSE was 14.842 \( \mu \text{g/m}^3 \), and the VIF of each variable was less than 4, indicating that there was no multicollinearity among the four independent variables (Table 4). The observed and predicted concentrations of PM10 were compared (Fig. 11).

3.2.2. Model evaluation

The model evaluation measures included regression diagnostics, cross-validation, and the spatial autocorrelation test. Regression diagnostics were performed by checking four plots, namely, a residual-versus-fitted plot, normal Q-Q plot, scale-location plot, and residual-versus-leverage plot. Figs. 12a and 13a depict that there was no correlation between the residuals and fitted values, and the dependent and independent variables were linearly correlated. In Figs. 12b and 13b all the data points of the plots fall on a straight line at an angle of 45°, indicating the fulfillment of the normality assumption. Figs. 12c and 13c present a random distribution of data points around the horizontal line, indicating the fulfillment of the homoscedasticity assumption. Fig. 12d depicts that the PM2.5 regression model was free of outliers, highly influential points, and high-leverage points. Fig. 13d indicates that for the PM10 model there was an outlier data point—sample 164, but it was not advisable to delete this outlier. In the multivariate LUR models for PM2.5 and PM10, the coefficient of multiple determination (Mul-\( R^2 \), Adj-\( R^2 \), and RMSE were all less than the respective averages in the 10-fold cross-validation, which indicated that there was no overfitting and underfitting and the LUR models had good generalizability. For the spatial autocorrelation test of PM2.5 residuals, the \( p \)-value was greater than 0.05 (95 % confidence level) and the z-score was above the threshold of -1.65, indicating that the PM2.5 residuals were randomly distributed in space without spatial clustering. For the PM10 residuals, the \( p \)-value of the spatial autocorrelation test was greater.
than 0.05 (95% confidence level) and the z-score did not exceed the threshold of 1.65, indicating that the PM$_{10}$ residuals were also randomly distributed in space without spatial clustering (Table 5).

### 3.2.3 Model verification for different heating seasons

To verify the applicability of the land use regression models in different heating seasons in Xi’an, the authors used the pollutant data from the recent heating season from November 15, 2019 to January 24, 2020 for verification. To exclude the impact of the novel coronavirus pandemic, only part of the data for the entire heating season of November 15, 2019-March 15, 2020 was selected. Affected by the pandemic, since Jan 24, 2020, most factories have been shut down, road traffic has declined sharply, and restaurants have been closed. The reduction in emission sources has a great impact on the distribution of pollutants. Compared with the model for the previous heating season, the independent variables of the PM$_{2.5}$ regression model of the recent heating season are the same as those of the previous heating season. Adjustable $R^2 = 0.639$, lower than 0.681, the value of the previous heating season; RMSE = 12.704 μg/m$^3$, also lower than the value from the previous heating season at 14.842 μg/m$^3$. The PM$_{2.5}$ and PM$_{10}$ land use regression models for the recent heating season exhibit reduced accuracy in fitting and smaller errors, but they still have good prediction capabilities, proving the applicability of the land use regression models in different heating seasons.

### 3.3 Spatial distribution of PM$_{2.5}$ and PM$_{10}$

Xi’an was divided into a grid of 10,525 cells using ArcGIS, each of 1 km × 1 km area, and regression mapping was performed using the PM$_{2.5}$ and PM$_{10}$ regression models. During regression mapping, the independent variables associated with a cell were extracted at the centroid of the cell and then substituted in the PM$_{2.5}$ and PM$_{10}$ regression models to predict the concentrations of PM$_{2.5}$ and PM$_{10}$ for the

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**Table 3**

Results of multiple stepwise regression for PM$_{2.5}$.

|                  | Estimate | Std error | t value | Pr (>|t|) | VIF | Result          |
|------------------|----------|-----------|---------|----------|-----|-----------------|
| Intercept        | 1.051e+02| 1.074e+00 | 97.857  | < 2e-16***|     | Multiple R-squared: |
| GS-4000          | -1.494e-06| 7.444e-08| -20.073 | < 2e-16***| 1.17| 0.718           |
| RE-5000          | -6.894e-04| 1.590e-04| -4.336  | 2.44e-05***| 1.28| Adjusted R-squared: 0.713 |
| PE-5000          | 1.964e+00| 5.975e-01| 3.288   | 0.00122**  | 1.17| RMSE: 8.355 μg/m$^3$ |

*Note: ***,** and * indicate significant levels of significance at 0, 0.001, and 0.01 respectively.*

**Table 4**

Results of multiple stepwise regression for PM$_{10}$.

|                  | Estimate | Std error | t value | Pr (>|t|) | VIF | Result          |
|------------------|----------|-----------|---------|----------|-----|-----------------|
| Intercept        | 1.606e+02| 2.282e+00 | 70.364  | < 2e-16***|     | Multiple R-squared: |
| MO-5000          | 1.832e-04| 5.352e-05| 3.423   | 0.00077***| 1.04| 0.688           |
| GS-5000          | -1.520e-06| 8.540e-08| -17.803 | < 2e-16***| 1.21| Adjusted R-squared: 0.681 |
| BS-5000          | -3.309e-02| 8.159e-03| -4.056  | 7.49e-05***| 1.39| RMSE:14.842 μg/m$^3$ |
| PE-5000          | 3.635e+00| 1.106e+00| 3.286   | 0.00123**  | 1.26|                |

*Note: ***,** and * indicate significant levels of significance at 0, 0.001, and 0.01 respectively.*

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**Fig. 10.** Scatter plots showing observed and predicted PM$_{2.5}$ using LUR model.

**Fig. 11.** Scatter plots showing observed and predicted PM$_{10}$ using LUR model.
Fig. 12. Regression diagnostic plots of PM$_{2.5}$ LUR model.

Fig. 13. Regression diagnostic plots of PM$_{10}$ LUR model.

Table 5
Cross-validation of models and spatial autocorrelation test of residuals.

|       | PM$_{2.5}$ |       | PM$_{10}$ |
|-------|------------|-------|-----------|
|       | LUR | Cross- | Spatial | LUR | Cross- | Spatial |
| Mul $R^2$ | 0.718 | 0.719 | Moran I: -0.129 | Mul $R^2$ | 0.688 | 0.691 | Moran I: 0.589 |
| Adj $R^2$ | 0.713 | 0.713 | z score: -0.216 | Adj $R^2$ | 0.681 | 0.682 | z Score: 1.043 |
| RMSE   | 8.355 | 8.660 | p-value: 0.828 | RMSE   | 14.842 | 15.609 | p-value: 0.297 |

Table 6
Results of multiple stepwise regression for PM$_{2.5}$ in the new heating season.

| Estimate | Std.Error | t value | Pr(>|t|) | Vif | Result          |
|----------|-----------|---------|---------|-----|----------------|
| Intercept | 7.566e + 01 | 9.906e-01 | 76.381 | < 2e-16 *** | Multiple R-squared: |
| GS-5000  | -7.405e-07 | 4.302e-08 | -17.212 | < 2e-16 *** | 0.642 |
| RE-5000  | -6.666e-04 | 1.450e-04 | -4.596 | 8.15e-06 *** | Adjusted R-squared: |
| PE-5000  | 1.083e+00 | 5.433e-01 | 1.994 | 0.0477 * | 0.636 |

Note: ***, ** and * indicate significant levels of significance at 0.001, 0.01 and 0.05 respectively.
The spatial distribution maps (Figs. 14 and 15) of the concentrations of PM$_{2.5}$ and PM$_{10}$ in Xi’an were generated using the visualization function of ArcGIS, which presented significant differences between the spatial distributions of the concentrations of PM$_{2.5}$ and PM$_{10}$ in Xi’an.

4. Discussion

4.1. Comparison with other studies

The correlation coefficients of the green-space area with respect to the concentrations of PM$_{2.5}$ and PM$_{10}$ were largest in each buffer zone, and the coefficients increased with the increase in the area of the buffer zone, which indicated that with increase in green space, the negative correlation between the pollutant concentrations and the green spaces was more significant. The independent variable shared by the PM$_{2.5}$ and PM$_{10}$ land use regression prediction models of Xi’an is the number of polluting enterprises with a buffer area of 5000 m. Moreover, the results indicated that while green-space area was the most critical independent variable in both the models, it exerted its largest impact at various buffer-distance zones. In addition to the green-space area, the PM$_{2.5}$ LUR model also included the number of restaurants in the 5000-m-distance buffer zone as an independent variable.

### Table 7

| Estimate         | Std.Error | t value | Pr(>|t|) | Vif | Result       |
|------------------|-----------|---------|----------|-----|--------------|
| Intercept        | 1.195e+02 | 2.129e+00 | 56.368   | < 2e-16 *** | Multiple R-squared: |
| MO-5000          | 1.504e-04 | 5.483e-05 | 2.743    | 0.0067 **   | 0.647         |
| GS-5000          | -1.220e-06 | 5.384e-08 | -22.659  | < 2e-16 *** | 1.21          |
| BS-5000          | -2.935e-02 | 5.769e-03 | -5.088   | 9.22e-07 *** | 0.639         |
| PE-5000          | 1.810e+00 | 7.489e-01 | 2.4167   | 0.0167 *    | 1.26          |

Note: ***, ** and * indicate significant levels of significance at 0, 0.001, and 0.01 respectively.

Fig. 14. Spatial distribution map of PM$_{2.5}$ in urban areas of Xi’an and regulatory management zone.
whereas the PM$_{10}$ LUR model included the number of bus stops and the length of motorways in the 5000-m-distance buffer zone as two independent variables. The reason green-space area was the most critical independent variable in both models was that Xi'an has a unique terrain and urban morphology. That is to say, the forest coverage of Xi'an is as high as 48%, with a large area of green spaces and vegetation in the Qinling and Li Mountains. There is a strong negative correlation between the concentration of pollutants and the green-space area of the buffer zone and a significant positive correlation between the green-space area of the buffer zone and its elevation with a correlation coefficient of 0.86. The green-space area in a buffer zone around a station with a high elevation tends to be big. It indirectly reflects the strong negative correlation between the elevation of the monitoring station and the concentration of pollutants. Comparison with the studies of other cities in Table 8 indicates that there are similarities among Beijing, Czech-Poland and Xi'an in that a great number of mountains and green-space areas exist in the territories of these study areas. These researches also contain the independent variable of green-space area, which shows that the pollutant distributions are all impacted by the mountains and green space (Bitta, Pavlíková, Svozilík, & Jančík, 2018; Ji et al., 2019; Wu et al., 2015). Those studies, except for that in Beijing by Wu et al. (2015) did not include industry-related independent variables. Other studies included the independent variable of pollution emission or industrial land area. In this study, two industry-related independent variables were selected, namely the area of industrial land and the distance from air-polluting enterprise, and the distance from air-polluting enterprises was finally included in the model. Moreover, studies in Beijing and the other Chinese cities of Shanghai and Tianjin also included road length as an independent variable (Chen, Bai et al., 2010; Liu, Henderson, Wang, Yang, & Peng, 2016; Meng et al., 2016; Wu et al., 2015), consistent with the present study. The Adj-$R^2$ values of the PM$_{2.5}$ and PM$_{10}$ LUR models of Xi'an were 0.713 and 0.681, respectively, lower than the Adj-$R^2$ values of 0.877 and 0.81, respectively, obtained in LUR models of Shanghai (Liu et al., 2016) and Beijing (Ji et al., 2019) but higher than 0.43–0.65 and 0.54, respectively, for Beijing in another study (Wu et al., 2015) and Hong Kong (Lee et al., 2017). Therefore, the Adj-$R^2$ value obtained in this study was considered to represent a moderate level compared with other reports. This study used data observed at 181 monitoring stations—the largest number and density of monitoring stations among studies of this type. However, the higher density of monitoring stations in this study did not lead to improvement in fitting accuracy compared with other studies, suggesting that fitting accuracy may not be simply dependent on the number and density of monitoring stations.
| Author               | City     | Research object | Variables entered into the model                                                                 | Independent variables                                                                 | Result            | Monitoring period          | Buffer zone                                      | Number of stations | Area of study zone |
|----------------------|----------|-----------------|---------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------|-------------------|---------------------------|-------------------------------------------------|-------------------|-------------------|
| This study 2019      | Xi'an    | PM$_{2.5}$      | Green space, 4000 m Restaurant, 5000 m Distance to the nearest air-polluting enterprise Green space, 5000 m Motorway, 5000 m Bus stop, 5000 m Distance to the nearest air-polluting enterprise | Land use, road, traffic facilities, emission sources, geospatial information, socioeconomic information | Adjusted $R^2$: 0.713 RMSE: 8.355 | 2018.11.15-2019.03.15 | 100 m, 300 m, 500 m, 1000 m, 2000 m, 3000 m, 4000 m, 5000 m | 181               | 10,752 km$^2$     |
|                       |          | PM$_{10}$       |                                                                                                  |                                                                                        | Adjusted $R^2$: 0.681 RMSE: 14.842 |                       |                                                 |                                                |                   |                   |
| Liu et al. (2016)    | Shanghai | PM$_{2.5}$      | Long Distance to the coast High way intensity, 300 m Water body area, 500 m Industrial land area, 300 m | Land use, population density, road networks, distance from monitors to the ocean, major air pollution sources, longitude, latitude | Adjusted $R^2$: 0.877 RMSE: 194.59 | One year                   | 100 m, 300 m, 500 m, 1000 m, 3000 m | 35                | 5512 km$^2$       |
| Meng et al. (2016)   | Shanghai | PM$_{10}$       | Distance to the coast Emission, 7000 m Green space, 1000 m | Land use, aerosol optical depth, meteorological data                                      | Adjusted $R^2$: 0.80 RMSE: 4.2 | 2008                         | 100 m, 300 m, 500 m, 1000 m, 2000 m, 3000 m, 5000 m | 28                | 6300 km$^2$       |
| Wu et al. (2015)     | Beijing  | PM$_{2.5}$      | Major road length Water area, 500 m Natural vegetation area, 300 m Crop area, 3000 m | Street network, land cover, population density, catering services distribution, bus stop density, intersection density | Adjusted $R^2$: 0.43-0.65 RMSE: 6.5–19.1 | 2013.03-2014.03 | 100 m, 200 m, 300 m, 500 m, 750 m, 1000 m, 2000 m, 3000 m, 5000 m | 35                | 16,411 km$^2$     |
| Ji et al. (2019)     | Beijing  | PM$_{2.5}$      | Industrial-mining-warehouse land, 200 m Average temperature Forest-grassland, 500 m Wetland, 3000 m | Land use, road, terrain, Population, meteorological factors | Adjusted $R^2$: 0.81 RMSE: 15.7 | Heating season | 100 m, 200 m, 300 m, 1000 m, 2000 m, 3000 m, 4000 m, 5000 m | 35                | 16,411 km$^2$     |
| Lee et al. (2017)    | Hong Kong| PM$_{2.5}$      | Expressway, 25 m Distance to Shenzhen Car park density, 1000 m Car park density, 25 m Government, 100 m Industrial, 25 m | Annual average traffic density, road length, traffic loading, urban build-up, land use, point value variables, point feature, value extracted at point, distance | Adjusted $R^2$: 0.54 RMSE: 4.0 | 2014.04.24-2014.05.15 | 50 m, 100 m, 200 m, 300 m, 500 m, 1000 m, 2000 m, 3000 m, 4000 m, 5000 m | 80                | None              |
| Chen, Bai et al. (2010)| Tian Jin| PM$_{10}$       | Major roads, 2000 m Residence, 2000 m Population density Distance to sea Wind speed | Major road, land use, population, meteorological factors, distance to sea | Adjusted $R^2$: 0.72 | 2006 Heating season | 500 m, 1000 m, 1500 m, 2000 m, 2500 m | 30                | 11,920 km$^2$     |
| Bitta et al. (2018)  | Czech-Polish border | PM$_{10}$      | Emissions from industrial sources, 2000 m Emissions from domestic heating, 2000 m | Pollution source, land use | Adjusted $R^2$: 0.65 RMSE: 8.34 | None | 100 m, 200 m, 500 m, 1000 m, 2000 m | 27 | 8832 km$^2$ |
| Sabzevar             | PM$_{2.5}$ | Industrial, 500 m Distance to religion/ | Traffic surrogates, land use, urban morphology, distance variables, | | Adjusted $R^2$: 0.68 | 2017.04.20-2018.03.06 | 100 m, 200 m, 300 m, 400 m, 500 m, 750 m, 1000 m, 1250 m, 1500 m | 26 | None |

(continued on next page)
4.2. Spatial distribution characteristics of pollutants in Xi'an

The concentrations of PM$_{2.5}$ and PM$_{10}$ had a strong correlation, with the Pearson correlation coefficient as high as 0.864. Accordingly, the concentrations of PM$_{2.5}$ and PM$_{10}$ in Xi'an presented basically the same trend in spatial distribution except for in some local regions and each pollutant demonstrated an overall decreasing trend of concentration from the north to the south. The concentrations of PM$_{2.5}$ and PM$_{10}$ in the Qinling Mountains south of Xi'an and Li Mountains east of Xi'an were significantly lower than those in other areas, which was attributed to the fact that the reduction of pollutant emission sources and increase in vegetation have a mitigating effect on the concentrations of PM$_{2.5}$ and PM$_{10}$. You et al. (2016) performed the MODIS aerosol inversion to derive the spatial distribution of the concentration of PM$_{10}$ in Xi'an during 2011–2013, finding a high concentration of PM$_{10}$ accumulated in the west and northeast of the main urban district of Xi'an, consistent with the results of this study. However, You et al. (2016) did not observe the accumulation of high-concentration PM$_{10}$ in the High-tech Industry Development Zone (HIDZ) southwest of the main urban district of Xi'an but observed it in the area east of the main urban district, which is significantly different from the observations in this study. This inconsistency may be attributed to the various data acquisition times and data types used by You et al. (2016), i.e., MODIS AOD data, compared with those used this study.

Outside the Qinling and Li Mountains, the concentrations of PM$_{2.5}$ and PM$_{10}$ were closely related to the layout of industrial land use and the locations of air-polluting enterprises. Fig. 16 presents the layout of industrial land use and the locations of air-polluting enterprises in Xi'an. In particular, a large amount of industrial land existed in the HIDZ southwest of the main urban district and the Huyi District (HYD) and Caotang Science & Technology Zone (CSTZ) southwest of the regulatory management zone (RMZ), and a large number of industrial enterprises were present in the Fengdong New City (FDNC) west of the RMZ, leading to significantly higher concentrations of PM$_{2.5}$ and PM$_{10}$ in these areas compared with other areas. The Lintong District (LTD), Gaoling District (GLD), and Yanliang District (YLD) in the northeast of the RMZ were home to the Lintong District of Modern Industry (LTDMI), Gaoling District of Equipment Industry (GLDEI), and Yanliang District of Aviation Industry (YLDAI), respectively, with significantly higher concentrations of PM$_{2.5}$ and PM$_{10}$ compared with other areas. Huang et al. (2015) confirmed that the accumulation of PM$_{2.5}$ in Xi'an was closely related to industrial production. Wang et al. (2014) reported that as high as 58% of the concentrations of PM$_{2.5}$ in Xi'an in the heavy pollution months were caused by industrial activities. Song et al. (2015) revealed that transportation and industrial emissions were the main sources of PM$_{2.5}$ in Xi'an. However, the correlation coefficients between the areas of industrial and mining land use and the concentrations of PM$_{2.5}$ and PM$_{10}$ were quite small, and the correlation was not statistically significant, which may be attributed to the possibility that the information collected on industrial and mining land use was not truly reflective of the actual situation.

4.3. Spatial distribution characteristics of pollutants in RMZ of Xi'an

The spatial distribution characteristics of PM$_{2.5}$ and PM$_{10}$ were investigated in the RMZ, which is larger than the main urban district. Fig. 17 presents the layout of industrial land use, water systems, green spaces, and roads, all of which were factors related to the distribution of the concentrations of PM$_{2.5}$ and PM$_{10}$. The highest concentrations of PM$_{2.5}$ and PM$_{10}$ were observed in the area named WREWTR, which lies between the West Urban Ring Motorway and the West Third Ring Road, and in the HIDZ area. Both of these areas and their adjacent spaces contain a large industrial land and a large number of air-polluting enterprises, which also exist in the area north of the RMZ (NRMZ). However, there was no accumulation of high concentrations of PM$_{2.5}$ and PM$_{10}$ in NRMZ, which may be attributed to the presence of large
Fig. 16. Layout of industrial land use and positions of air-polluting enterprises in Xi’an.

Fig. 17. Layout of industrial land use, water systems, green spaces, and ring roads in RMZ of Xi’an.
water bodies and green spaces around the area due to its proximity to the Wei River. On one hand, the large water bodies can generate water–land breeze through a mechanism similar to sea–land breeze (Bouchlaghem, Mansour, & Elourragin, 2007; Zhu & Zhou, 2019), which, coupled with the open terrain and low building density of NRMZ, facilitates the diffusion of the pollutants. On the other hand, vegetation, green spaces, and wetlands can improve the removal efficiency of PM$_{2.5}$ and PM$_{10}$ (Amini Parsa, Salehi, Yavari, & van Bodegom, 2019; Feng, Zou, & Tang, 2017; Selmi et al., 2016; Zhu & Zeng, 2018). As depicted in Fig. 12, another high-concentration area of PM$_{2.5}$ and PM$_{10}$ was ERMZ, which lies on the east of RMZ, in close proximity to the Hongqing Industrial Zone (HQIZ), which is home to a large number of industrial enterprises. The concentrations of PM$_{2.5}$ and PM$_{10}$ in most areas within the Second Ring Road were generally lower than those in the surrounding areas. The southern part of the RMZ (SRMZ) and the Qiujiang New Zone (QNJZ) in the southeastern part also had significantly lower concentrations of PM$_{2.5}$ and PM$_{10}$ than those in surrounding areas. Vehicular emissions serve as a substantial source of PM$_{2.5}$, leading to rapidly increasing concentration of PM$_{2.5}$. A study by Dai et al. (2018) demonstrated that motor vehicles provided a continuously growing contribution to the concentrations of PM$_{2.5}$ during 2006–2014 in Xi’an. However, except for the WREWTR and HIDZ most areas in the RMZ did not demonstrate the accumulation of high concentrations of PM$_{2.5}$ and PM$_{10}$, indicating that industrial emissions were still the main contributor to the concentrations of PM$_{2.5}$ and PM$_{10}$ in Xi’an. Wang et al. (2019) reported that motor vehicles accounted for 11.13% of the concentrations of PM$_{2.5}$ in Xi’an in the winter of 2017, significantly lower than the contribution of 51.02% through the combustion of coal.

4.4. Limitations

Owing to the limited time available for data collection, this study focused on the heating season of Xi’an for investigating the spatial distribution of PM$_{2.5}$ and PM$_{10}$, thus being unable to address the distribution in other seasons and, thereby, making it impossible to understand inter-seasonal differences in the spatial distribution of PM$_{2.5}$ and PM$_{10}$. The land-use data employed in this study were mainly retrieved from remote sensing images as the main data source. However, these images were generated in an earlier time period than the pollution data, and, therefore, a certain degree of inter-period differences were noticed in land use, possibly introducing errors into the results of correlation analysis between the independent and dependent variables. Owing to the lack of corresponding meteorological monitoring data at the monitoring stations, this study did not consider the impact of meteorological factors such as wind direction, wind speed, air temperature, and humidity on the concentrations of PM$_{2.5}$ and PM$_{10}$. Further, the accuracy of model fitting can be improved using pollutant concentration data observed under lower wind speeds.

5. Conclusions

This study is the first to apply land use regression models to the Fenwei Plain, a heavily polluted area in China, and analyzes 87 factors from five categories of information including land use information, road traffic facility information, socioeconomic information, geospatial information, and emission source information in Xi’an. The correlation between the factors and the PM$_{2.5}$ and PM$_{10}$ concentrations of 181 monitoring stations were investigated. Based on the correlation analysis results of independent variables and dependent variables, the land use regression prediction models of PM$_{2.5}$ and PM$_{10}$ in Xi’an were established. Cross-validation confirms that the model exhibits good performance in spatial prediction and generalization, and the verification with various time periods proves the applicability of LUR models in different heating seasons. The model successfully predicted the PM$_{2.5}$ and PM$_{10}$ concentrations in 10,525 grids, revealing the variations in the spatial distribution of PM$_{2.5}$ and PM$_{10}$ concentrations in Xi’an.

Within the city limit of Xi’an, the PM$_{2.5}$ and PM$_{10}$ concentrations generally show a trend with high values in the north and low values in the south. The concentrations of PM$_{2.5}$ and PM$_{10}$ in the Qinling Mountains in the south and Li Mountains in the east are significantly lower than those in other regions. The spatial distribution of PM$_{2.5}$ and PM$_{10}$ is closely related to layout of industrial land and the location of polluting enterprises. The spatial distribution of PM$_{2.5}$ and PM$_{10}$ in the Regulatory Management Zone (RMZ) further confirms that large area of green space can effectively reduce the concentrations of PM$_{2.5}$ and PM$_{10}$. The RMZ has large traffic flow however only a small part of the zone seems to have high concentration of pollutants, indicating that industrial emissions are the main source of PM$_{2.5}$ and PM$_{10}$ in Xi’an, followed by traffic emissions. This study enriches the application of land use regression models in the prediction of the spatial distribution of atmospheric pollutants and provides a scientific foundation for urban planning, land use regulation, air pollution control, and public health policy making. It presents a basic model for population exposure assessment and promotes the application of land use regression models in areas requiring heating in winter and heavily polluted areas. It plays a positive role in achieving sustainability of urban environment and promoting sustainable development in urban areas.

Declaration of Competing Interest

All authors declare no conflict of interest.

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