Exploring coupling effect between urban heat island effect and PM$_{2.5}$ concentrations from the perspective of spatial environment

Yunhao Fang$^{1}$, Kangkang Gu$^{1,2}$

$^1$School of Architecture and Planning, Anhui Jianzhu University, Hefei 230022, China
$^2$Anhui Collaborative Innovation Center for Urbanization and Construction, Hefei 230022, China

Abstract

The coupling effect between urban PM$_{2.5}$ concentrations and urban heat island effect has been paid more and more attention to. Previous studies mostly focused on the analysis of data correlations, lacking the interpretation of the formation texture. Taking Hefei as the subject, this study combined the spatial statistical model with the coupling coordination degree model to explore the influence of spatial environment-related indicators on the coupling effect of cities. In addition, at the micro level, the paper used grid unit to verify the relevance and made a comprehensive analysis on the formation texture of coupling effect. The results indicated that: (1) there is a significant coupling effect between the urban heat island intensity and PM$_{2.5}$ concentrations in the main urban area of Hefei with significant spatial heterogeneity. (2) to some extent, the indicators of urban spatial environment, including vegetated areas, buildings, residential land, commercial land, industrial land, building density, floor area ratio, building form ratio, the densities of road junctions and sub-arterial roads, have different effects on the coupling effect. In general, the higher the degree of human activity, the higher the degree of coupling effect. (3) the coupling effect may be influenced by a variety of spatial environment factors.

Keywords: Coupling coordination degree model, PM$_{2.5}$, Spatial statistical model, Urban heat island effect, Urban planning strategy, Urban spatial environment

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† Corresponding Author
E-mail: kangkanggu@163.com
Tel:+86-0551-15855118329
ORCID: 0000-0001-7606-9651
1. Introduction

Climatic problems in cities are becoming increasingly serious, most which are urban heat island effect and air pollution [1, 2]. Multiple studies have confirmed that excessive heat and air pollution particles in the city such as PM_{2.5} (particulate matter in the air that is less than 2.5 mm in aerodynamic diameter) will continue to affect the lives of the residents, and, in turn, lead to greater health risks [3–6]. Research on urban heat island and urban air quality has become a heated topic in relevant research.

Researchers in different fields are trying to find a solution to the urban heat island intensity (UHII) and air pollutant concentrations [7–10]. Part of the results indicate that there is a close coupling effect between the UHII and urban air pollutant concentrations, which has been confirmed by relevant research [11–13]. For instance, Estournel et al. [14] found out that the temperature of urban and rural areas in Toulouse varies with the aerosol based on the results of solar radiation. Similar results are reported by Jauregui and Luyando for Mexico City [15], Robaa for the Greater Cairo region and Wang et al. for Beijing [16, 17]. Total Suspended Particles (TSP) plays an important role in the UHII as well [18, 19]. Furthermore, this process depends on the urban form, e.g. on the multiple bounces that may occur inside canyons. In turn, temperature determines the concentration of aerosols. For example, Sarrat et al. [20] studied the results of Paris, proving urban heat islands change the spatial distribution of regional pollutants (ozone and nitrogen oxides) by changing the atmospheric boundary layer. Besides, ozone is produced by the photooxidation of VOCs in the presence of nitrogen oxides (NOx) [21]. Based on related research, the cluster effect is governed by the amount of population, which is typically larger over dense urban areas [22]. Some researchers also used regression analysis to explore the
correlation between changes in SO\textsubscript{2} and NO\textsubscript{2} concentrations and temperature from the perspective of data analysis [23]. However, the method only considers the influence of numerical value, ignoring the connections among various factors in the region [24–26]. Therefore, some scholars used the method of spatial statistics to combine the spatial distribution of air pollution and thermal pollution and performed correlation analysis because such method incorporates spatial factors in the analysis and can consider the impact of air pollution or thermal pollution on its neighborhood [27, 28].

With the understanding of climate issues deepens, the research focus on the relationship between the UHII and air pollutant concentrations has gradually shifted to forming texture. Theoretically, on the one hand, the temperature difference between urban areas and suburbs has led to atmospheric circulation and the pollutants removal, which has affected the distribution of pollutants [29, 30]. On the other hand, the spatial distribution of air pollutant concentrations indirectly affects the UHII by influencing the radiation within the city [31, 32]. And when the air quality is poor, the high concentration of pollutants reduces the radiation from the sun to the ground during the day and the long-wave radiation from the ground at night, thus reducing the heat emission, leading to the temperature rise in the city. In addition, some studies have shown that pollutants in the air will result in cooling [33]. The reason is that the "dust dome" formed by excessive particulate matter will affect the solar radiation, which will lead the temperature to drop [34, 35].

However, UHII and air pollution are not only the opposite side of the synergistic effect, the process of which is also affected by the underlying surface spatial environment [36]. Although a large number of studies in the past have shown that UHII or air pollution is related to
the spatial environment, they all indicate the relationship between the two. For example, Yuan et al. [28] used the spatial measurement model to explore the impact of PM$_{2.5}$ and built environment, while Yin et al. [27] explored the impact of urban form and urban heat island effect. In a word, they focused on the spatial environment but neglected its impact on the interaction between UHII and air pollution.

The purpose of this study is to analyze the interaction between urban heat island and air pollution according to spatial environment in order to improve urban climate and human settlements. Accordingly, we choose the main urban area of Hefei as the subject research object and try to explore the influence of urban spatial environment on the coupling effect of UHII and PM$_{2.5}$ by combining the coupling coordination degree model and spatial statistical model. In addition, we also used the combined perspective of macro and micro to give further guidance on the optimization of urban spatial environment.

2. Research Area and Methods

2.1. Research Area

Hefei (116°41′E-117°58′E, 30°57′N-32°37′N) lies in the eastern China, the middle latitude zone (Fig. 1). The terrain mostly consists of plains, hills and mountains. It has humid subtropical climate, with distinctive four seasons and an annual temperature average of 15.7°C. Its average annual precipitation is about 1,000 mm, and relative humidity 77%. An annual mainstream prevails north and northwest throughout the year. In the end of 2018, the number of the permanent residents in Hefei reached 8.087 million, and the building area 460 km$^2$. In recent years, with the expansion of cities and the increase in construction intensity, haze weather
condition in urban areas has increased. According to the 2016 World Health Organization (WHO)'s air pollution statistics on Chinese cities, Hefei has serious air pollution, ranking 14th worst. In addition, the phenomenon of urban heat islands has intensified year by year, especially the long-lasting high temperature in summer. The data from China National Meteorological Observation Station showed that the average annual temperature increased in urban areas by 0.89°C/10 years, compared to the 0.44°C/10 years after 2,000 in the suburban areas, and the gap showed a trend of increasing. In general, the urban air pollution problem and the urban heat island effect have become the two major climatic problems in Hefei, and their interaction and impact pose a threat to the living environment of the urban residents.

2.2. Research Methods and Data
This study focused on the urban spatial environment and its influence on the interaction degree between thermal environment and air pollution. As Fig. 2 showed, we took the main urban area of Hefei as a sample and divided it into a grid of 500 m*500 m. Urban remote sensing data and related urban air quality data were used to calculate UHII and PM$_{2.5}$ concentrations. It was worth noting that UHII referred to UHII at the surface rather than UHII in the atmosphere. Specifically, we analyzed the relationship between UHII and PM$_{2.5}$ concentrations through the coupling coordination degree model, and analyzed the size of the UHII -PM$_{2.5}$ coupling result CCD. Furthermore, spatial statistical model was used to explore the link between CCD and four spatial environmental indicators (including land cover indicators, land use indicators, building form indicators and road traffic indicators). Finally, we supplemented the effects of the mixed effects
of spatial environmental indicators and other indicators uncovered in the analysis on the micro
scale.

2.2.1. Urban heat indicators and air pollution indicators
Considering PM$_{2.5}$ and UHII in Hefei spring are obvious and easy to interact with others, we
selected the data of April 2018 as samples for spatial processing. The sources and selection
methods of each data are as follows:

Based on the remote sensing image data, we selected the Landsat8 Thermal Infrared
Sensor (TIRS) data (https://atmcorr.Gsfc.nasa.gov/) at 2:42 am on April 11, 2018, which was a
date with less cloud cover and no rainfall. At the same time, the atmospheric visibility was high,
and it had the conditions for good surface temperature inversion [37, 38]. For the calculation of
surface UHII, we used atmospheric correction. Landsat8 TIRS data were processed using
Envi5.3 software to invert the surface temperature. This removed the effects of atmospheric
radiation on the surface based on real-time atmospheric sounding data to obtain a true ground
heat radiation intensity [39, 40]. The algorithm also considers that the thermal infrared radiation
brightness value ($L_d$) comprises of the atmospheric upward radiance ($L_u$), the atmospheric
downward radiance ($L_d$) and the true radiation received by satellite sensor from the ground.

\[ L_d = [\varepsilon L_T + (1 - \varepsilon)L_d] \tau + L_u \]  

where $\varepsilon$ is the surface specific emissivity; $L_T$ is the radiant brightness of a black body with
temperature ($T (K)$) in the thermal infrared band; $\tau$ is the atmospheric transmittance, which can
be obtained using online values of $L_u$ and $L_d$. Based on the $L_T$ obtained from the formula (1), the
surface temperature \((T_s)\) was obtained using formula (2). The relevant parameters for each satellite are given in Table 1.

\[
T_s = K_2/\ln[1 + K_1/L_T]
\]  

The heat island intensity was then calculated using the UHI intensity index (UHII) algorithm, and the UHI scale index formula is shown in formula (3).

\[
UHII_i = T_i - \frac{1}{n} \sum_{1}^{n} T_{\text{crop}}
\]

where \(UHII_i\) is the heat island intensity corresponding to the \(i\)th pixel on the image; \(T_i\) is the surface temperature; \(n\) is the number of effective pixels in the suburban farmland; and \(T_{\text{crop}}\) is the surface temperature in the suburban farmland, which is meant to the average surface temperature of all surrounding agricultural and forest land.

PM\(_{2.5}\), as the most commonly used air pollution detection indicator, can reflect the degree of urban air pollution [41]. The higher the PM\(_{2.5}\) concentration, the higher the air pollution indicator, and the greater the harm to the human health [5]. At present, the 10 state-controlled ambient air automatic monitoring stations in Hefei cannot evaluate the spatial distribution of PM\(_{2.5}\), and large-scale monitoring is not in line with the reality. However, related studies have shown that remote sensing images are of importance to the study of the spatial distribution of PM\(_{2.5}\) in cities, especially in built-up areas [28, 42]. Specifically, the method combined aerosol optical depth (AOD) data with the scattering characteristics of the aerosol vertical profile through a CEOS-Chem transport simulation with good precision \((r^2 = 0.81; \text{slope} = 0.68)\) [43]. Therefore, we used this method to obtain 2018 PM\(_{2.5}\) data from Atmospheric Composition Analysis Group (http://fizz.phys.dal.ca/~atmos/martin/?page_id=140) in Hefei. The study obtained processed China-wide PM\(_{2.5}\) raster data from the above website, calibrated and adjusted
by ArcGIS Software. In addition, we also clipped high-precision PM$_{2.5}$ spatial distribution data within the main urban area of Hefei.

2.2.2. Urban spatial environment-related indicators

In the study, the selection of spatial environmental indicators included two aspects that affect urban air environment and urban thermal environment. Specifically, we summarized four types of indicators: land cover, land use, building form, and road traffic to reflect the urban spatial environment through Geographic Information System (GIS) (Table 2). In addition, 500 m*$^2$ grids in Hefei were selected as samples.

Land cover indicators influence urban climate through transpiration of vegetation and radiation of hardened land surface [44, 45]. This information on land cover was obtained from high resolution remote sensing data. In this study, vegetated areas, waters, buildings and soils were counted in the study area, respectively.

The proportions of different land use indicators were used to reflect urban functions in each grid [46, 47]. We used Hefei urban planning dataset in 2016 to represent land use indicators because of the accuracy of their classification. Based on this, we counted four types of indicators, including administration land (AL), business land (BL), residential land (RL), and industrial land (ML).

Building form indicators, including building height (BH), building density (BD), floor area ratio (FAR), and building form ratio (BFR), can not only change the ventilation performance of the block, but also affect the pollutant concentration and surface temperature around the buildings [48, 49]. They were also obtained from the Hefei urban planning dataset in
2016. It was worth noting that what we calculated was the average value within the grid, where BH and BD reflected the average height and density within the unit grid, FAR reflected the ratio of the total building area within the unit grid to the land area, and BFR reflected the ratio of the building surface area within the unit grid to the total volume.

Road traffic indicators reflected the influence of automobile exhaust emissions on street air and surface temperature [50]. We obtained the relevant vector from OpenStreetMap (http://download.geofabrik.de/), as the arterial road data and the sub-arterial road data. Based on this, we conducted intersection processing with road data through 500m*500m grids in ArcGIS software to calculate the length of all arterial roads and sub-arterial roads in each grid. The ratio of the length to the area of all arterial roads in the grid will be regarded as the arterial road density (AD), and the ratio of the length to the area of all sub-arterial roads in the grid will be the sub-arterial road density (SAD). In addition, the study also counted the number of road intersections in the cell grid and set it as the road junction density (RJD).

2.2.3. Coupling coordination degree (CCD) model

The coupling coordination degree (CCD) of UHII-PM$_{2.5}$ represented the degree of interaction between urban thermal environment and urban air environment through different spatial elements. Besides, CCD ignores the pros and cons of the elements, which indicates the benign coupling in the interaction process, that is, the CCD performs numerical normalized analysis on the elements in the model [51]. The larger the value, the greater the degree of interaction between them [52]. In this study, CCD calculation was derived from remote sensing data and air quality data in April 2018. The consistency of the timing sequence avoids the construction
indicators conflict, thus ensuring the accuracy of coupling results. By establishing a CCD model, we can not only explain the state of UHII and PM$_{2.5}$, but also analyze the texture and mechanism of interaction in the spatial environment. The CCD was calculated using the following expression:

\[ C = 2 \times \left[ \frac{U_1 \times U_2}{(U_1 + U_2)^2} \right]^{0.5} \]  

(4)

\[ T = aU_1 + bU_2 \]  

(5)

\[ CCD = (C \times T)^{0.5} \]  

(6)

Where the CCD is between 0 and 1, a larger value indicates a stronger interaction between the UHII and PM$_{2.5}$ concentration; $C$ is the general coupling degree, which can only reflect the strength of the interaction, but cannot filter out benign coupling. For example, when both PM$_{2.5}$ concentration and UHII are at a low level, there is also a high degree of coupling. Overall, it is difficult to reflect an accurate interaction compared to the CCD; $T$ is the comprehensive evaluation value of PM$_{2.5}$ concentration and UHII; $a$ and $b$ are parameters to be determined. In this study, $a = b$ is set, which indicates that PM$_{2.5}$ concentration is as important as the UHII in the CCD model; $U_1$ represents the normalized value of UHII and $U_2$ the normalized value of PM$_{2.5}$ concentration. Because of the inconsistency of dimensions, the above factors should be normalized with the following formula:

\[ U_i = \frac{U - U_{\text{min}}}{U_{\text{max}} - U_{\text{min}}} \]  

(7)

where $U_i$ is a normalized value for the ith pixel (500m spatial resolution), $U$ represented the value of the PM$_{2.5}$ concentration or UHII, and $U_{\text{min}}$ and $U_{\text{max}}$ are the minimum and maximum values of these factors, respectively.
2.2.4. Spatial statistical model

The spatial statistical model was used because it incorporated spatial factors in statistical analysis, which made the results more accurate [25, 53]. Compared with traditional statistical methods (such as the Spearman correlation), the spatial statistical model can take into account the heat transfer and air flow on the land surface [54].

First, this study calculated a global autocorrelation index (Moran's I) using values for all the grids in the study area to evaluate whether patterns of spatial data distribution are clustered, dispersed, or random. We further used local Moran's I (LISA) to show the relationship of spatial data between each grid and its surrounding grids across the study area. The LISA is a space based on statistical technique which can give an indication of the extent to a significant spatial clustering of homogeneous values, existing around a particular observation [55]. Depending on the application, the high-high (HH) locations have been used to detect clusters of high CCD values, while high-low (HL) locations have been incorporated to locate local high outliers in the study area. The HH and HL locations are considered as hot spots whereas the low-low (LL) and low-high (LH) locations are indicative of the local cold spots and are not considered in detail in this study. Furthermore, The LISA can also serve as a prerequisite for the use of spatial statistical model.

Then, the study established a Queen contiguity weights matrix and used the test of Lagrange Multiplier (LM) index and the Robust Lagrange Multiplier (robust LM) index to select spatial statistical models, including spatial error model (SEM, Eq. (9)) and spatial lag model (SLM, Eq. (8)) [56, 57]. In detail, the test contains four statistical variables, including LM lag, LM error, Robust LM lag and Robust LM error. It also leads to an important parameter P, and
the smaller the value is, the stronger the significance. In the process of modeling, SEM model is selected when LM-error statistics are significant, while SLM model is selected when LM-lag statistics are significant. If both of the two statistics are significant, we need to judge the remaining two statistics. SEM model is selected if the Robust LM-error statistics are significant, while SLM model is selected if the Robust LM-lag statistics are significant.

Finally, based on the appropriate spatial statistical model, we analyzed the statistical results. It should also be noted that all modelling was performed using GeoDa software and all variables were standardized before statistical analysis. Specific formulas included:

\[ Y = \rho W_y + \sum a_i X_i + \epsilon \]  
\[ Y = \sum a_i X_i + u(u = \lambda W_u + \epsilon) \]

Where \( Y \) is dependent variable, representing the CCD of the grid; \( \rho \) is a spatial autocorrelation parameter; \( X_i \) is independent variable, representing the spatial environment-related indicator in the grid; \( a_i \) is the parameter of the corresponding independent variable; \( \epsilon \) is the error term; \( u \) is the regression residual vector; \( \lambda \) is the spatial autocorrelation parameter reflecting the residual; \( W_y \) and \( W_u \) are the spatial matrices for \( Y \) and \( u \), respectively.

### 3. Results and Analysis

#### 3.1. Spatial Distribution Pattern of UHII and PM\(_{2.5}\) Concentrations

It is indicated that UHII of different areas were diversified, showing the pattern of "double peaks and double bottoms" with significant difference in temperature (Fig. 3). Most main urban areas exhibited generally high temperature at about 31.78°C in general. Specifically, the heat peak areas took the form of patches in the figure, clustered in the Luyang area in the north and the
Jingkai area in the southwest of the city. Meanwhile, Dongpu Reservoir and Dafangying Reservoir were two bottoms in the figure, located in the northwest of the main urban area with the lowest temperature, namely 12.62°C. In general, the UHII in the main urban area of Hefei demonstrated a spatial pattern of "cold outside but hot inside", and temperature gradually decreased from the inside out.

In the study area, PM$_{2.5}$ concentrations ranged from 55.23 to 115.07μg/m$^3$ with a mean value of 78.95μg/m$^3$. It showed the pattern of "double bottoms and multiple peaks" in general, and the average value of some grids was higher than the national standard of 75.00μg/m$^3$. As Fig. 3 showed, the PM$_{2.5}$ concentrations were high in some areas, such as the center of Xinzhan area in the northeast and old city in the middle, with the highest concentration reaching 115.07μg/m$^3$. Jingkai area in the southwest ranked the second, and the PM$_{2.5}$ concentrations were in the range of 70.65~90.00μg/m$^3$.

This study prioritized the determination of Moran's I indicator before exploring the spatial correlation analysis between the UHII and PM$_{2.5}$ concentrations. According to the displayed results, some areas such as the Luyang area in the north, the Jingkai area in the southwest and the Gaoxin area in the west were considered the high-high clusters of the UHII, while other areas, such as the Old city in the central and the Xinzhan area in the northeast, demonstrated the spatial pattern of PM$_{2.5}$ concentration as high-high clusters. In addition, the Moran’s I of the UHII and the Moran's I of PM$_{2.5}$ concentrations were 0.77 (P < 0.001) and 0.31 (P < 0.001) in the study area, respectively, which indicated that spatial autocorrelation for the UHII and PM$_{2.5}$ concentrations across all grids were significant. More importantly, the spatial distribution of the UHII and PM$_{2.5}$ concentrations in each grid was not random, and may also be
affected by neighboring areas, which is consistent with the theory of the spatial statistical model [54].

3.2. Spatial Correlation Pattern of UHII and PM$_{2.5}$ Concentrations

The results of the spatial statistical analysis between UHII and PM$_{2.5}$ concentrations were shown in Table 3. Unexpectedly, either UHII or PM$_{2.5}$ concentration was taken as the independent variable, and both demonstrated a significant positive correlation. At the same time, the correlation parameters R$^2$ were 0.57 and 0.83, indicating that the UHII and PM$_{2.5}$ concentrations in cities were not spatially independent, and they often influenced each other [12]. Besides, the intensity of their interaction was significant, which was probably caused by the same reasons [7]. According to the results of spatial statistics, the analysis of the CCD of UHII-PM$_{2.5}$ was performed in this study, as shown in Fig. 4. The distribution of the CCD in the main urban area of Hefei had obvious spatial differences, and showed a spatial pattern of "double peaks and double bottoms". Furthermore, CCD ranged from 0 to 0.97 with the average value of 0.71, which means that UHII and PM$_{2.5}$ concentrations have a significant correlation in the study area. It also validated the analysis results obtained by the spatial statistical model.

It can also be seen from spatial distribution (Fig. 4) that Old city in the central and the Jingkai area in the southwest had the highest CCD value, mainly in the range of 0.81~0.97, belonging to "double peaks". The northern part of Xinzhan area ranked the second, and its range was maintained at 0.75~0.81, which was generally higher than the average. The "double bottoms" in the city, that was, grids with low CCD values, were mostly distributed in the Shushan area and the Binhu area, while a few were distributed in the Dongpu Reservoir and
Dafangying Reservoir. Overall, the spatial distribution of CCD in the main urban area of Hefei formed a three-pole peak zone of "Xinzhan area-Old city-Jinkai area", which gradually decreased to the northwest and southeast sides.

LISA cluster distribution is found to be approximate and asymptotic while deriving the exact distribution for the global statistics [55]. According to LISA results, the Moran's I of CCD is 0.95 (P < 0.001), which means that a significant local cluster of CCD values locations is detected. Specifically, HH areas, such as Xinzhan area in the northeast, old city in the middle and Jingkai area in the southwest, on LISA map reflected the high-value clustering distribution of CCD while LL areas, such as Shushan area, on LISA map demonstrated the low-value clustering distribution of CCD. In addition, there were only three grids with a high level of CCD values surrounded by low levels of CCD (three high-low outliers) and one grid with a low level of CCD values surrounded by high levels of CCD (a low-high outlier).

3.3. Association between Urban Spatial Environment and UHII-PM$_{2.5}$ Coupling Coordination

3.3.1. Urban land cover indicators

The spatial statistical results of land cover indicators were shown in Table 4 and Figure S1. Vegetated areas and CCD showed a significant negative correlation, with the corresponding coefficient R$^2$ of 0.75, which indicated that green vegetation can alleviate the degree of interaction between urban heat island effect and PM$_{2.5}$ [58]. Unexpectedly, the proportion of waters within grids was not correlated to CCD. On the one hand, the cooling effect of water can inhibit the UHII enhancement process caused by PM$_{2.5}$ [59]. Meanwhile, the space above water
also reduced collisions among PM$_{2.5}$ particles caused by UHII. Both processes mean that they weaken the effects between UHII and PM$_{2.5}$. On the other hand, higher humidity around the water can provide an environment that intensified the interaction between UHII and PM$_{2.5}$ [60]. The results presented by buildings showed that building agglomeration had a positive effect on surface temperature and PM$_{2.5}$, with a correlation coefficient of 0.75. This also reflected that urban climate problems caused by the interaction between urban heat island effect and air pollution were closely related to human activities in built-up areas. In terms of soils, there was no significant correlation with spatial coupling coordination of UHII-PM$_{2.5}$.

3.3.2. Urban land use indicators
The spatial statistical results of land use indicators are shown in Table S1 and Figure S2. There is no obvious correlation between administration land (AL) and CCD, which may be related to the geographical division of administration land itself. Both BL and RL have a significant positive correlation, with a correlation coefficient of 0.65 and 0.76, respectively. This may be because residential land and commercial land are more densely populated, intensifying the interaction between heat island effect and PM$_{2.5}$ in cities. At the same time, this result also indirectly indicates that a large number of crowded places are exposed to thermal pollution and air pollution [46]. While the proportion of industrial land (ML) in the grid has a positive correlation with the CCD, this is related to the industrial land itself having the function of emitting a large amount of pollutant haze and heat.

3.3.3. Urban building form indicators
The spatial statistical results of building form indicators are shown in Table S2 and Figure S3. There is a low correlation between BH and CCD, reflecting the differentiation effect of building height. Specifically, when the building height is too low, polluted gas and heat cannot interact with each other; while when the city buildings exceed a certain height, the closed interval formed impedes the contact with other areas [61]. Meanwhile, BD and FAR affect the interaction between UHII and PM$_{2.5}$, with the correlation coefficients for 0.73 and 0.83. The reason for this is that when the index was too high, more building surfaces can store a lot of heat and block the movement of aerosol molecules, leading to the heat island effect in the region and the deterioration of air quality [62, 63]. Besides, the correlation coefficient R$^2$ of BFR is 0.78, reflecting the connection between surface area and volume. For example, it is more difficult for panel buildings to ventilate than point buildings. As a result, high thermal inertia and impermeability provide an interaction site for local heat islands and PM$_{2.5}$ [29].

3.3.4. Urban road traffic indicators

The spatial statistical results of road traffic indicators were shown in Table S3 and Fig. S4. The significance of AD was not high, with a P value of 0.05. Despite the roads developed rapidly in Hefei in recent years, traffic flows were still concentrated in Old city when the main roads were being built outward which can indirectly explain the current unbalanced development [64]. In addition, the densities of road junctions (RJD) and sub-arterial roads (SAD) showed significant positive correlation with CCD, and the corresponding correlation coefficients were 0.61 and 0.58, respectively. The above data indicated that cars in cities produced a large amount of heat energy
while emitting exhaust gas, intensifying the interaction between temperature and PM$_{2.5}$ in cities [50].

4. Discussion

The interaction between urban heat island effect and PM$_{2.5}$ concentrations has become one of the most important phenomena in urban climate environment. Studies have shown that these interactions worsen urban climate. Exploring the influence of urban spatial distribution on this interaction provides a new research perspective for mitigating urban climate problems. The CCD between UHII and PM$_{2.5}$ concentrations indicated that there was a significant coupling effect between thermal environment and air environment. In this study, four types of urban spatial environment control group were selected, including land cover, land use, building form and road traffic. Specifically, vegetated areas, buildings, residential land, commercial land, industrial land, building density, floor area ratio, building form ratio, the densities of road junctions and sub-arterial roads all had an impact on the coupling effect to some extent. But the actual situation was often more complicated. In different regions, the CCD between UHII and PM$_{2.5}$ concentrations was affected by a variety of spatial environment indicators [36].

Taking the above situations into consideration, in order to further study the impact of urban spatial environment, the paper verified the impact of spatial environment on the CCD in a micro-scale grid. In terms of geographical location selection, according to the spatial distribution of CCD, we chose the area with a higher degree of interaction between UHII and PM$_{2.5}$, which was more representative. In terms of the selection of specific indicators, the paper selected the indicators of building form and road traffic. On the one hand, in the spatial layout strategy, these
two indicators were more feasible and had more obvious benefits to urban development, while the cost of optimizing land cover and land use indicators was too high. On the other hand, there was no significant difference between the land cover indicators and the land use indicators of adjacent plots on the micro scale.

As shown in Fig. S5, the paper selected a set of adjacent grids in Old city to compare their building forms. After data statistical analysis, the CCD value of grid A and B is 0.87 and 0.76, respectively, and the value of A is greater than B. Meanwhile, we excluded the influence of floor area ratio, building density, the densities of road junctions and sub-arterial roads because the difference between FAR and BD values in the comparison was both relatively small, and both units were close to the main road except a few roads in the residential areas. By combining data and visualization results, the building form ratio (BFR) in grid A was 0.56 lower than the value of grid B (0.73), so the CCD between UHII and PM$_{2.5}$ had a significant negative effect, verified the previous spatial statistical analysis of the study area. Therefore, in the urban spatial planning and optimization strategy, we should reduce rough architecture, effectively improve the building form ratio, so as to optimize the climate environment.

The coupling effect of road traffic on UHII and PM$_{2.5}$ concentrations depends on the number of different types of roads and intersections. Under the same regional conditions, the more road intersections in the city, the more likely it is to generate vehicle exhaust and heat [64]. Based on this, we also selected the adjacent grids of Old city to compare with their road traffic. Meanwhile, we ensured that their urban building forms and other indicators were all similar (Fig. S6). The results showed that grid D has two more intersections than grid C, but its CCD is not very different. There are many reasons for this. On the one hand, the increase of road
intersections means the increase of urban main roads, which can lead to the increase of open
spaces, affecting the synergy between UHII and PM$_{2.5}$ concentrations. On the other hand, the
pattern of streets and lanes under grid D may also change the microclimate, such as wind
direction and wind speed. These local climate variations may weaken the interaction between
PM$_{2.5}$ concentrations and UHII [65].

5. Conclusions

There is a coupling effect between the urban heat island intensity (UHII) and PM$_{2.5}$
concentrations, which will aggravate the deterioration of climate environment and endanger the
health of residents. In the study, we selected the main urban area of Hefei as the research object.
From the perspective of spatial environment, including land cover, land use, building form and
road traffic, spatial statistical model and coupling coordination degree model were combined to
explore the relationship between spatial environment and UHII-PM$_{2.5}$ coupling effect. This study
provides a new perspective for the spatial layout strategies of urban planning and draws the
following conclusions:

(1) There is a significant coupling effect between the urban heat island intensity and
PM$_{2.5}$ concentrations in the main urban area of Hefei with significant spatial heterogeneity.

(2) Urban spatial environment can greatly influence the coupling effect between urban
heat island intensity and PM$_{2.5}$ concentrations. The region with strong coupling effect has
relatively strong spatial environment index significance, which means that the more intense the
underlying surface activity is, the higher the synergistic effect is. To deal with this coupling
effect, it is necessary for urban planners to develop a polycentric urban structure to balance high
population density and reduce traffic emissions in downtown areas. Road and bus networks should be optimized simultaneously to reduce traffic jams, and more public transits (such as subways) should be built to link urban sub-centers to the downtown. In general, the exploration of spatial environmental indicators should be the focus of research to mitigate this coupling effect.

(3) The coupling effect between urban heat island intensity and PM$_{2.5}$ concentrations is complex, which may be influenced by a variety of spatial environmental indicators. Our study proved that relevant indicators have a certain impact and put forward some strategies, but there are still some limitations. Firstly, due to the time limitation of remote sensing image data, the timeliness of the research is affected to some extent. In addition, studies from the macro perspective may not be comprehensive enough, and the microclimate effects such as wind speed and direction are ignored. The combination of macro and micro methods can provide deeper comprehension of the mechanism of UHII-PM$_{2.5}$ coupling effect.

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Author Contributions
Y.F. (PG. student) conducted all the data analysis and wrote the manuscript. K.G. (Professor) wrote and revised the manuscript.
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Fig. 1. Location and study area.

Fig. 2. Flowchart of the study.
Table 1. Parameters Used in the Radiative Transfer Equation-Based Method

| Landsat type | $K_1 / (W/(m^2 \cdot sr \cdot \mu m))$ | $K_2/K$ |
|--------------|---------------------------------|---------|
| Landsat 5    | 607.76                          | 1.260.56|
| Landsat 7    | 666.09                          | 1.282.71|
| Landsat 8    | 774.89                          | 1.321.08|

Fig. 3. Spatial distribution of UHII and PM$_{2.5}$ concentrations.

Fig. 4. CCD and spatial autocorrelation analysis.
Table 2. Statistics of All the Variables

| Category       | Metrics          | Min  | Max   | Mean  | Std.D | Note                                      |
|----------------|------------------|------|-------|-------|-------|-------------------------------------------|
| UHII           |                  | 19.14| 47.96 | 33.36 | 3.95  |                                           |
| PM$_{2.5}$     |                  | 55.23| 115.07| 78.95 | 4.15  |                                           |
| Land cover     | Vegetated areas  | 0    | 1.00  | 0.19  | 0.08  | Sum of forest and grassland               |
|                | Waters           | 0    | 1.00  | 0.09  | 0.06  | Sum of rivers, reservoirs and lakes       |
|                | Buildings        | 0    | 0.32  | 0.05  | 0.09  |                                           |
|                | Soils            | 0    | 0.54  | 0.27  | 0.29  |                                           |
| Land use       | AL               | 0    | 1.00  | 0.04  | 0.12  | Administration land                        |
|                | BL               | 0    | 0.92  | 0.02  | 0.08  | Business land                              |
|                | RL               | 0    | 0.97  | 0.10  | 0.19  | Residential land                           |
|                | ML               | 0    | 1.00  | 0.09  | 0.21  | Industrial land                            |
| Building form  | BH               | 0    | 90.00 | 7.39  | 12.86 | Building height (m)                        |
|                | BD               | 0    | 0.52  | 0.05  | 0.09  | Building density (%)                       |
|                | FAR              | 0    | 4.71  | 0.29  | 0.54  | Floor area ratio                          |
|                | BFR              | 0    | 0.97  | 0.15  | 0.21  | Building form ratio                        |
| Road traffic   | AD               | 0    | 2.00  | 0.35  | 0.08  | Arterial road density (km/km$^2$)          |
|                | SAD              | 0    | 2.00  | 0.75  | 0.14  | Sub-arterial road density (km/km$^2$)      |
|                | RJD              | 0    | 5.70  | 1.03  | 0.26  | Road junction density                     |

Table 3. Spatial Correlation between UHII and PM$_{2.5}$ Concentrations

| Type  | Variable | Model | LM lag | Robust LM lag | LM error | Robust LM error | $R^2$ | P   |
|-------|----------|-------|--------|---------------|----------|-----------------|-------|-----|
| UHII  | PM$_{2.5}$ | SLM   | 0      | 0             | 0.12     | 0               | 0.57  | 0   |
| PM$_{2.5}$ | UHII    | SLM   | 0      | 0             | 0.18     | 0               | 0.83  | 0   |

Note: The results indicate metrics statistically significant at P < 0.01 level.

Table 4. Statistical Results of Land Cover Indicators
| Type                          | Variable       | Model | LM lag | Robust LM lag | LM error | Robust LM error | R²  | P    |
|-------------------------------|----------------|-------|--------|---------------|----------|-----------------|-----|------|
| Coupling coordination degree (CCD) | Vegetated areas | SLM   | 0      | 0             | 0        | 0               | 0.75| 0    |
|                               | Waters         | SLM   | 0      | 0             | 0        | 0.13            | 0.31| 0.25 |
|                               | Buildings      | SEM   | 0      | 0.45          | 0        | 0.01            | 0.75| 0.02 |
|                               | Soils          | SLM   | 0      | 0.48          | 0        | 0.69            | 0.01| 0.81 |

Note: The results indicate metrics statistically significant at P < 0.01 level.