

IMPACT OF METEOROLOGICAL PARAMETERS ON THE DAILY VARIABILITY OF THE GROUND-LEVEL PM_{2.5} CONCENTRATIONS ACCORDING TO MEASUREMENTS IN THE MIDDLE URALS

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ABSTRACT. The results of a comparison of the PM_{2.5} aerosol concentration daily variability for the summer and winter seasons at the urban and background monitoring sites in the Middle Urals for 2016–2019 are presented. The cluster analysis method revealed a statistically significant difference between the two groups corresponding to higher and lower concentrations of fine aerosol during the day. Studies of the daily variation of the PM_{2.5} particle concentration in the Middle Urals indicate the leading role of meteorological characteristics (in particular, air temperature, pressure and wind speed) in changing the level of aerosol suspension in the air surface layer. Distinctive typical average daily concentrations of PM_{2.5} for the Middle Urals region, corresponding to the cluster of lower values, are observed in the summer and are on average ~ 5.2 µg/m³ for the urban area and ~ 3.4 µg/m³ for the background site. In winter, these parameters are 12.8 µg/m³ for urban conditions and 10.5 µg/m³ for background site. The higher content of PM_{2.5} particles, corresponding to the cluster of higher values, are identified in winter and are on average ~32.2 µg/m³ in urban conditions and ~ 30.3 µg/m³ in the background area. In summer, these parameters are 13.6 µg/m³ for urban site and 9.6 µg/m³ for background area. Simultaneous analysis of the fine aerosol concentrations and the meteorological parameters in the surface atmospheric layer allowed to define of weather conditions, at which the occurrence of higher PM_{2.5} values is possible.

KEYWORDS: mass concentration of PM_{2.5} aerosol particles, meteorology, cluster analysis, air quality, Middle Urals

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INTRODUCTION

In recent decades, the interest in the problem of atmospheric air pollution with fine suspended particles has been growing due to the significance of their impact on human health, the state of ecosystems, and global climate change. Aerosol particles with aerodynamic diameters less than 2.5 microns (PM_{2.5}) are a complex, heterogeneous mixture of many components suspended in the air. It is well known that PM_{2.5} particles are able to penetrate into the internal environment of the body and accumulate in the upper and lower parts of the bronchi, inducing diseases of the human respiratory and cardiovascular systems (e.g., Pope et al. 2020; Vohra et al. 2021; Zhang et al. 2018; Seinfeld and Pandis 2006; Kim et al. 2015).

PM_{2.5} particles can affect shortwave radiation coming from the Sun to the Earth and longwave radiation emitted by the Earth's surface into space, participating in the processes of

absorption and scattering of radiation in the atmosphere, on the one hand, and in cloud formation, on the other hand (IPCC, 2021; Ginzburg et al. 2009)

The National Hydrometeorological Services monitor the concentration of suspended particles. As a criterion for the pollution level by fine aerosol, Russia has put into effect a hygienic standard that regulates the maximum permissible concentrations of suspended particles in the atmospheric air. According the hygienic standard, the average daily level of PM_{2.5} particles concentrations in the air should not exceed 35 µg/m³, and the average annual level should not exceed 25 µg/m³ (SanPiN 1.2.3685-21, 2021).

One of the effective methods of protecting the health of the population is the forecast of unfavorable meteorological conditions contributing to an increase in the concentration of atmospheric impurities. According to the estimates of various authors (e.g., Hooyberghs et al. 2005; Stern et al. 2008; Tai et al.

2010), a significant part of the average daily variability of aerosol concentration is determined by the entire set of meteorological parameters.

The air pollution forecast schemes are developed based on the results of theoretical and experimental studies, in which the statistical relationships between atmospheric pollution and the corresponding meteorological factors are studied. For example, Gubanov et al. (2018) have investigated the relationships between $PM_{2.5}$ and meteorological factors in the Moscow. According to the correlation analysis results, $PM_{2.5}$ concentrations was negatively correlated with wind speed (correlation coefficient $R = -0.56$), positively correlated with air temperatures (0.55).

Many studies have already proven that the correlations between $PM_{2.5}$ concentration and meteorological factors vary with the seasons. For example, Chen et al. (2016) have determined that the correlation between $PM_{2.5}$ and air temperature was negative in summer (-0.03) and autumn (-0.26) and then turned to positive in spring (0.22) and winter (0.35).

However, besides seasonal variations, it has also been found that the relationships between $PM_{2.5}$ concentration and meteorological factors vary between regions (Yang et al. 2017; Novikova et al. 2017; Li et al. 2017; Kermani et al. 2020; Zhou et al. 2023; Gao et al. 2022).

In our recent work (Luzhetskaya et al. 2022) was created a prognostic model for estimating the surface $PM_{2.5}$ concentrations in the Middle Urals. The aerosol optical depth ($\tau_{0.5}$), meteorological and geographical parameters were considered as predictors. As a result, was obtained the ranked lists of the possible predictors usable in statistical models for estimating the logarithm of $PM_{2.5}$ values (the pairwise correlation coefficients between a corresponding quantity and $\ln PM_{2.5}$ are given in parentheses). The significant predictors for urban area were boundary layer height (-0.51), $\ln \tau_{0.5}$ (0.31), pressure (0.31), relative air humidity (0.29), and Normalized Difference Vegetation Index (-0.27). The possible predictors for background monitoring site were boundary layer height (-0.48), $\ln \tau_{0.5}$ (0.44), Normalized Difference Vegetation Index (-0.29), relative air humidity (0.26), and pressure (0.25).

This research is aimed at studying the impact of meteorological parameters not on the values of single concentrations, but on the daily variability of the concentration of fine $PM_{2.5}$ aerosols in the air surface layer by means of the cluster analysis method. Based measurement data set accumulated at the urban and background monitoring sites in the Middle Urals during 2016–2019, an attempt was made to reveal the specific type of daily variation and the typical values

of particle concentrations depending on a set of parameters – air pressure and air temperature, wind speed, and boundary layer height.

The results obtained can be used in numerical modeling of air quality in Yekaterinburg and other cities of the Middle Urals.

MATERIALS AND METHODS

Study area and data

The Middle Urals is located inside the Eurasian continent at the junction of two parts of the world – Europe and Asia, within the Ural ridge – the Northern and Southern Urals, as well as the East European and West Siberian plains. All seasons of the year are dominated by westerly winds, northerly winds are not uncommon, and easterly winds are a rarer occurrence. The remoteness from the Atlantic Ocean and the proximity of Siberia make the climate of the Middle Urals continental, which induces sharp changes in air temperature. The average monthly air temperature in January is $-16.2\text{ }^{\circ}\text{C}$ and in July – $+16.7\text{ }^{\circ}\text{C}$. (Morokova and Shver, 1981; Shalaumova et al. 2010; Scientific and application oriented handbook... 1990).

Yekaterinburg is the fourth most populous city in Russia, located in the central part of the Middle Urals. The main sources of industrial air pollution in Yekaterinburg are ferrous and non-ferrous metallurgy, energy, mechanical engineering, construction and chemical industries, as well as road and rail transport (mprso.midural.ru, 2019).

The results of long-term measurements of the mass concentration of atmospheric aerosols of the $PM_{2.5}$ fraction performed at the background and urban monitoring sites in the Middle Urals during 2016–2019 are used in this research. The urban monitoring site is located in Yekaterinburg on the territory of the Institute of Industrial Ecology of the Ural Branch of the Russian Academy of Sciences (56.850° N , 60.655° E). The background monitoring site is located in a forest ~ 65 km northwest of Yekaterinburg at the site of the Kourvka Astronomical Observatory (KAO) of the Ural Federal University (57.036° N , 59.546° E).

Measurements of the concentration of fine particles in the surface air layer are performed using two sets of Panasonic $PM_{2.5}$ optical sensors, which allowed estimating the concentration of aerosol particles in the size range between 0.3 and 2.5 μm (Nakayama et al. 2018). Observations of $PM_{2.5}$ particle concentrations at the urban and background monitoring sites are performed at the same height (~ 9 m above the ground).

Fig. 1 shows the schematic location of two monitoring sites of the $PM_{2.5}$ fraction of aerosol particles in the Middle Urals.

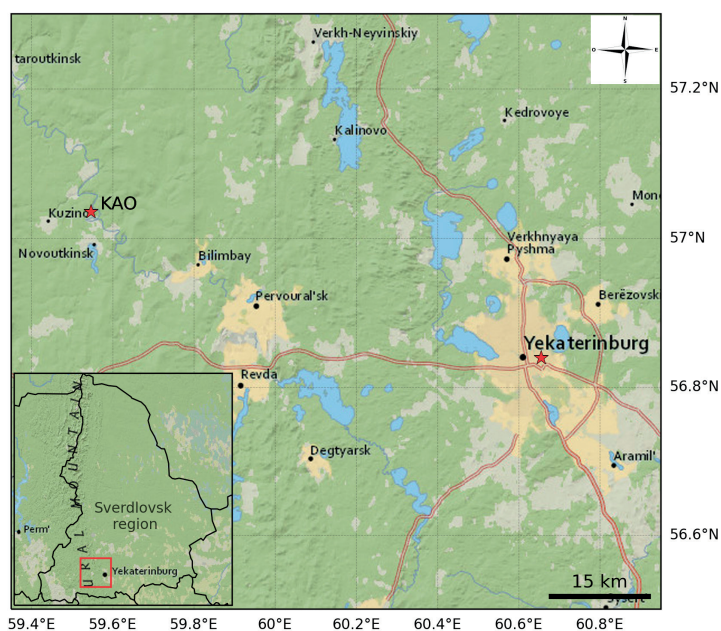


Fig. 1. Schematic location of urban (Yekaterinburg) and background (KAO) monitoring sites in the Middle Urals

The meteorological information used in the research was extracted from the reanalysis databases of the European Center for Medium-Range Weather Forecasts (ECMWF) (www.ecmwf.int). Weather data from the ECMWF Reanalysis v5 (ERA 5) database were available on a regular coordinate grid with a spatial resolution of $0.25^\circ \times 0.25^\circ$ and a temporal resolution of 1 hour. The following parameters were selected from the whole variety of reanalysis data: pressure (P , hPa); air temperature at 2 m (T , $^\circ\text{C}$); dew point temperature ($d2m$, K); horizontal wind speed components at a height of 10 m (V_x , V_y , m/s); boundary layer height (blh , km). The dew point temperature is used to calculate the relative air humidity (Hu , %). The horizontal wind speed w_s (m/s) and direction w_d (deg) are calculated from the horizontal wind components.

Cluster analysis method

Based on the selected data for each monitoring site, samples of $\text{PM}_{2.5}$ aerosol concentrations and meteorological parameters are formed with averaging over a time interval of 1 hour, corresponding to the calendar summer and winter periods. In spring and autumn, a transition of the daily variation features of the $\text{PM}_{2.5}$ aerosol concentration from winter to summer ones and vice versa occurs (Luzhetskaya et al. 2022), and such transient processes are not considered within the framework of this research.

The cluster analysis method is used to study the daily variability of $\text{PM}_{2.5}$ aerosol concentration. Recently, cluster analysis methods have become widespread for the analysis of aerosol pollution. For example, Rozwadowska et al. (2010), Hafner et al. (2007) have used air mass backward trajectory cluster analysis to investigate the transport pathways and potential sources of atmospheric aerosols at Spitsbergen island and in the Western U.S. Omar et al. (2005), Aladodo (2022) have identified main clusters of aerosol types and determined microphysical properties of aerosol groups using cluster analysis of Aerosol Robotic Network (<https://aeronet.gsfc.nasa.gov>) measurements.

In this research, the clustering procedure is performed not on the entire set of average hourly values, but on samples characterizing the daily variation of aerosol pollution of the atmosphere. Therefore, the initial time series of values of ground-level concentrations of aerosol particles is divided into samples by day. As a result, an array is formed consisting of a set of time series, each of which contained 24 average hourly values. Time series with gaps are removed. Then the time series clustering method is applied, as a result of which each such time series belonged to one or another cluster. Thus, different types of daily variation of $\text{PM}_{2.5}$ concentrations are revealed. The K-means method is used for clustering time series in this research (Aghabozorgi et al. 2015; MacQueen 1967). K-Means is the most popular unsupervised algorithm of clustering for several reasons. It is easy to use, algorithm is computationally efficient and results are easy to interpret. The method certainly has disadvantages, among which is sensitivity to outliers. For this reason, high aerosol concentrations ($\text{PM}_{2.5} > 80$) are excluded from consideration. Clustering is performed using the *TimeSeriesKMeans* method of the Python *tslearn*. clustering module (<https://tslearn.readthedocs.io/en/stable/>). The metric applied to determine the centers of clusters is the Euclidean distance.

In order to assess the quality of clustering, the average silhouette coefficient is used, which is calculated using the average distance between points within the cluster and the average distance to the points of another nearest cluster (Rousseeuw, 1987). The value of the average silhouette coefficient is in the range between -1 and +1. If the average silhouette coefficient is positive, the cluster points are on average closer to their group than to the neighboring one. The higher the value of the silhouette

coefficient is, the higher is the quality of clustering.

The number of clusters is set equal to two, since with an increase in the number of clusters, the values of the silhouette coefficients noticeably decreased, which means a decrease in the quality of clustering.

The values of the average silhouette coefficients for the measurement data samples in Yekaterinburg are 0.47 and 0.50 for the summer and winter periods, respectively. In KAO the average silhouette coefficients for the summer and winter periods are 0.42 and 0.48, respectively.

RESULTS AND DISCUSSION

The clustering results are shown in Fig. 2.

Since the initial time series are not scaled in any way, the most significant feature characterizing the two groups of samples obtained during clustering is the average value in the daily variation of concentrations. As a result of the procedure described above, clusters with typical low (cluster 1) and high values (cluster 2) of $\text{PM}_{2.5}$ aerosol concentrations are identified. It should be noted that in all the cases considered, clusters with high concentrations of $\text{PM}_{2.5}$ particles are smaller in number.

Fig. 2 demonstrates the daily variations of ground-level $\text{PM}_{2.5}$ particle concentrations, which, as a result of the procedure, are assigned to a specific cluster (gray lines), and the centers of the corresponding clusters (red lines). The figure also reveals information on how many time series fell into a particular cluster.

Fig. 3 demonstrates the daily variability of hourly mean values of ground-level $\text{PM}_{2.5}$ particle concentrations and some meteorological parameters for each of the two selected clusters. The upper and lower bounds of the boxes mark the values of the first and third quartiles of the data samples. The horizontal bar in the box corresponds to the median, and the slanted serifs at the median were a rough estimate of the 95% confidence interval for median differences. The overlap of slanted serifs allows revealing the statistical indistinguishability of the medians of the compared measurement data samples corresponding to a certain hour.

According to Fig. 3, the most pronounced changes in the daily variations are characteristic of high aerosol concentrations (cluster 2). The curves of daily variations of $\text{PM}_{2.5}$ aerosol concentrations in summer are characterized by the presence of two periods of increased values. Both in Yekaterinburg and KAO the higher values of $\text{PM}_{2.5}$ aerosol concentrations are observed in the morning and evening hours, which are separated by a segment with a lower content of particles in the afternoon hours. In summer, the maximum of daily average variations of fine aerosol concentration exceeds the minimum 1.6 times in Yekaterinburg and 2.4 times in KAO.

If the winter period is considered, then the segments of lower values in the curves of the daily variation at both monitoring sites was less pronounced. It should be noted that during the cold period, the daily variations in the $\text{PM}_{2.5}$ particle concentrations in the background region for cluster 2 are more pronounced. The maximum of daily average variations of fine aerosol concentration exceeds the minimum 1.4 times. For Yekaterinburg the difference of these values is less pronounced and their ratio is 1.2.

It should be noted that smaller changes in the daily variations in the concentrations of fine particles both in winter and in the summer period in the city could be associated with the formation of an urban heat island, which reduced daily fluctuations in the boundary level height. The research used meteorological parameters, including the height of the boundary layer, taken from the ECMWF reanalysis data with a spatial resolution of $0.25^\circ \times 0.25^\circ$. Therefore, the graphs shown in Fig. 3 do not illustrate a fundamental difference in the daily variation

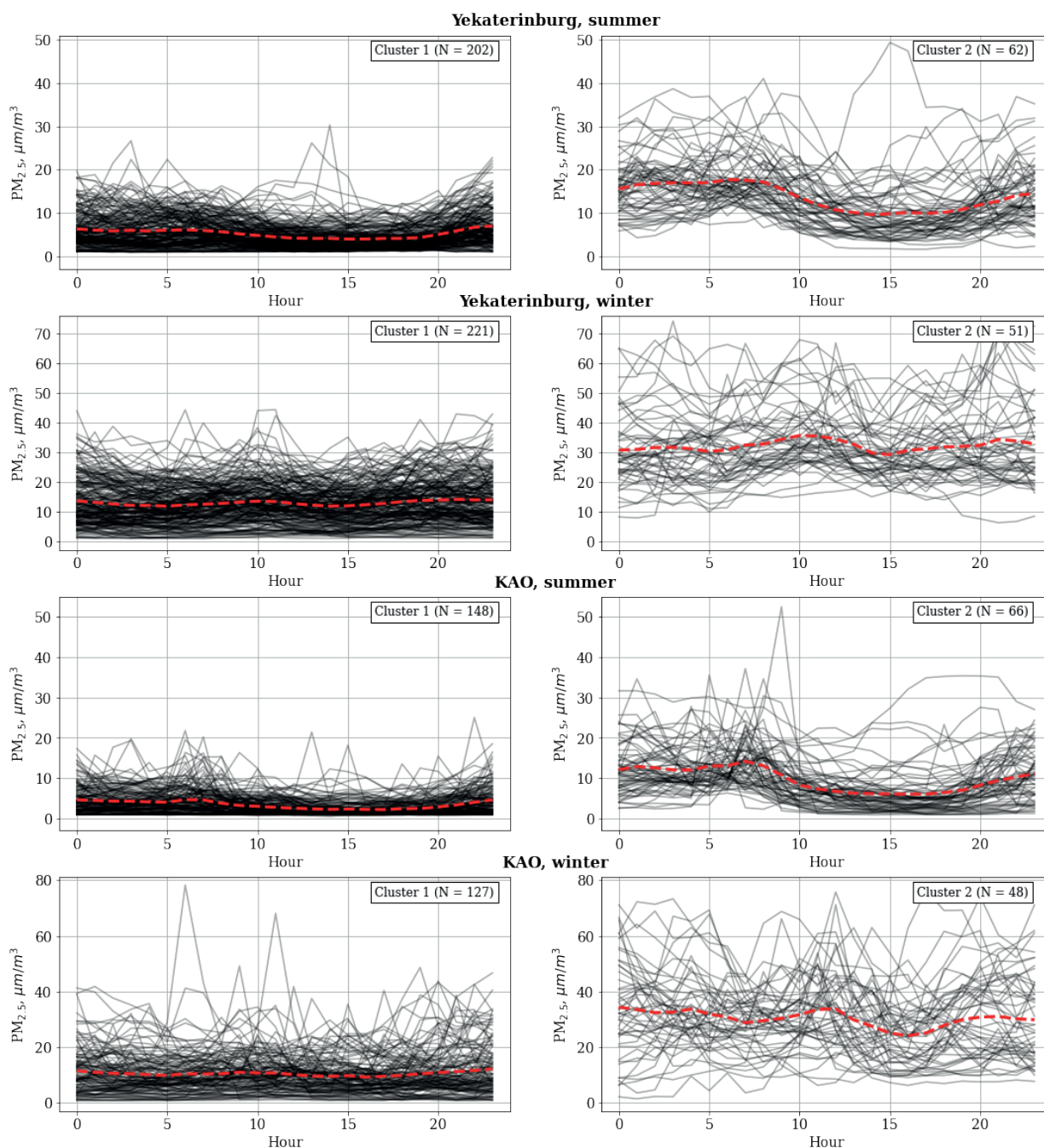


Fig. 2. Clusters identified by the K-mean method based on daily variability in the concentration of PM_{2.5} particles

of boundary layer heights for urban and background monitoring sites.

A comparison of the daily variability of PM_{2.5} particle concentrations with meteorological characteristics confirm the fact that meteorological parameters significantly influenced the level of pollution of the lower atmospheric layer with fine aerosol.

Fig. 3 shows that in all cases, the differences of median values of wind speed, air temperature, and pressure corresponding to clusters of low (cluster 1, blue boxes) and high (cluster 2, orange boxes) ground-level aerosol concentrations are statistically significant. Also, the differences between median values of the boundary layer height are statistically significant in the winter period for the entire daily variation curve. At the same time, in the summer period no statistically significant difference is revealed both in the city and in the background territory during the daytime. Therefore, in the summer period, the boundary layer height during the daytime have the same impact on the aerosol concentration values in both groups – an increase in the boundary layer height is accompanied by a decrease in the PM_{2.5} particles concentrations and vice versa.

For the daily variation of relative air humidity (Hu , %) and wind direction (wd , deg.), no statistically significant difference was found between the medians of the samples corresponding to different clusters. For this reason, Fig. 3 does not show graphs for Hu and wd .

The graphs in Fig. 3 demonstrate that in summer, both in Yekaterinburg and in KAO, the cluster with higher content of PM_{2.5} particles corresponded to clusters with higher values of air temperature (T , °C) and pressure (P , hPa), as well as to clusters with lower values of wind speed (w_s , m/s) and boundary layer height (blh , km).

It should be noted that in winter, when compared with the summer period, both in Yekaterinburg and in KAO, a cluster with higher content of PM_{2.5} particles correspond to a cluster of lower air temperature values. This is probably due to temperature inversions, which led to a weakening of the active atmospheric circulation, a decrease in the boundary layer height, and a weak manifestation of its daily variation. In winter, an increase in air temperature lead to an increase in vertical convection (boundary layer height) and, as a result, to a decrease in ground-level aerosol concentrations. In summer, higher air temperatures, on

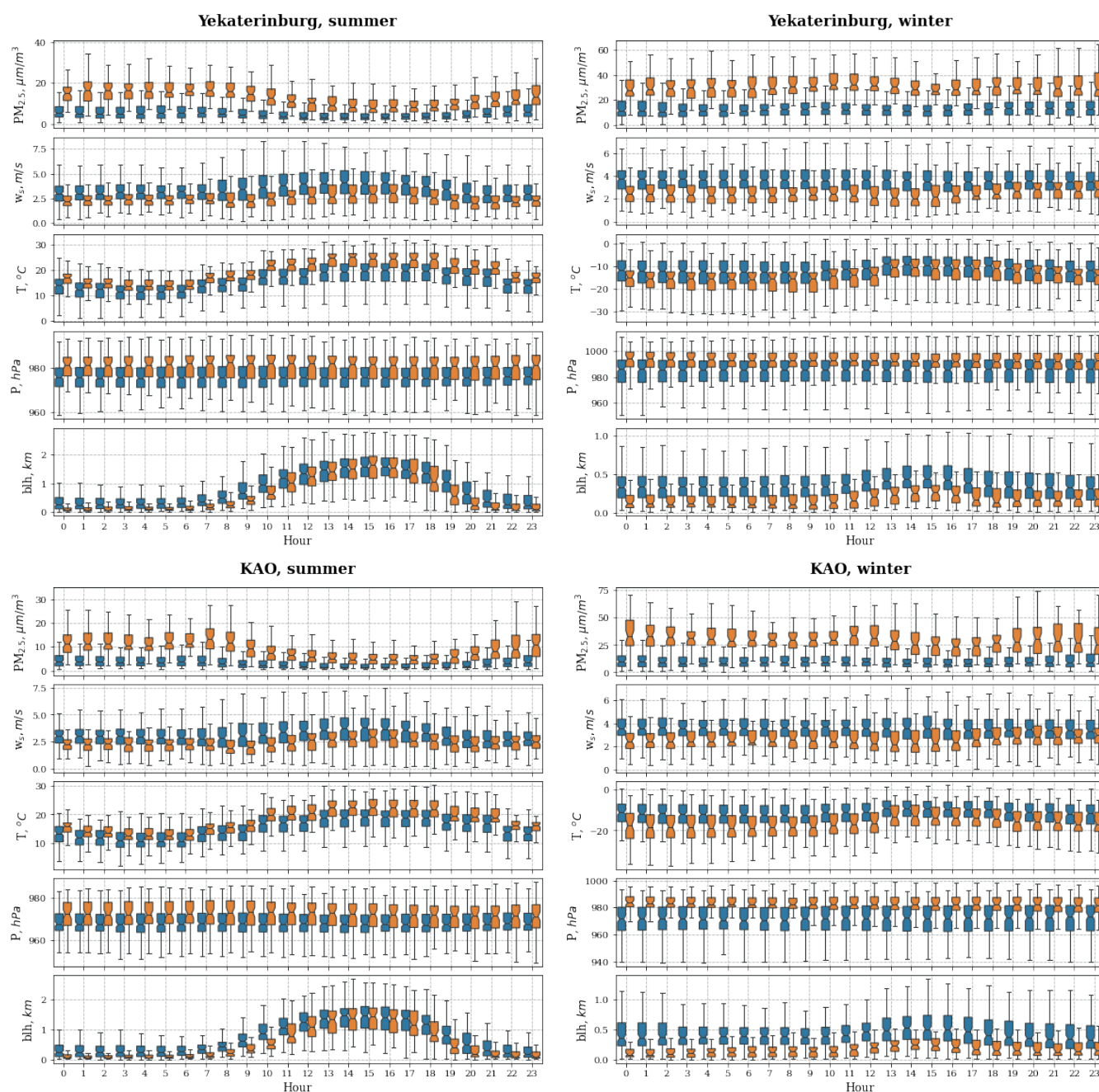


Fig. 3. Daily variability of statistical characteristics of ground-level $PM_{2.5}$ aerosol concentrations and some meteorological parameters for clusters of low (cluster 1, blue boxes) and high (cluster 2, orange boxes) values

the one hand, also caused an increase in convection, but at the same time, on the other hand, contributed to the intensification of natural fires. Wildfires lead to an increase in the aerosol content in the total atmospheric column, including in the lower atmospheric layer.

In the winter season, the range of pressure changes is wider than in the summer period, and for the atmospheric boundary layer, it is vice versa. For summer conditions, changes in the boundary layer height are significant for both the city and the background monitoring sites. At the same time, it is during the winter period that the values of atmospheric pressure and boundary layer height for clusters 1 and 2 have significant differences.

Table 1 shows the average daily values of $PM_{2.5}$ aerosol concentrations and meteorological parameters for two clusters with typical and high content of fine particles for the Middle Urals region.

Higher levels of ground-level aerosol concentrations in winter (cluster 2) are associated with the so-called unfavorable meteorological conditions – high pressure, weak winds, low air temperatures, and low atmospheric boundary

layer heights. In these situations, aerosol particles cannot rise to the upper atmosphere and accumulate in the surface air.

Moreover, a group of meteorological conditions for winter and summer, which contribute to the emergence of higher concentrations of surface aerosol for the Middle Urals region can be selected. The scatter diagrams of the average daily values of meteorological parameters of the concerned clusters were analyzed for this purpose (Fig.4).

Table 2 shows the ranges of meteorological parameters corresponding to the cluster of higher surface concentrations, which are determined on the basis of Figure 4. The higher $PM_{2.5}$ aerosol concentrations (on average $\sim 32 \mu\text{g}/\text{m}^3$ for the urban area, $\sim 30 \mu\text{g}/\text{m}^3$ for the background area) are observed in winter and are associated with pressure $> 962 \text{ hPa}$, weak winds $< 5 \text{ m/s}$, air temperatures $< -5.0 \text{ }^\circ\text{C}$, and low boundary layer heights $< 0.5 \text{ km}$. In summer, higher $PM_{2.5}$ aerosol concentrations reach values $\sim 13.6 \mu\text{g}/\text{m}^3$ in the urban area, $\sim 9.6 \mu\text{g}/\text{m}^3$ in the background area. Higher of aerosol concentrations are concerned with pressure $> 954 \text{ hPa}$, weak winds $< 5 \text{ m/s}$, air temperatures $> 12.0 \text{ }^\circ\text{C}$, and boundary layer heights $< 1 \text{ km}$.

Table 1. Average daily (\pm standard deviation) values of $PM_{2.5}$ aerosol concentrations and meteorological parameters for two clusters with typical and high content of fine particles for the Middle Urals region

Typical values of $PM_{2.5}$ (cluster 1)				
parameters	Yekaterinburg, summer	KAO, summer	Yekaterinburg, winter	KAO, winter
$PM_{2.5}$, $\mu\text{g}/\text{m}^3$	5.2 ± 2.7	3.4 ± 0.7	12.8 ± 5.7	10.5 ± 5.6
blh , km	0.8 ± 0.5	0.7 ± 0.5	0.4 ± 0.2	0.4 ± 0.2
w_s , m/s	3.5 ± 1.1	3.2 ± 1.0	3.6 ± 1.0	3.6 ± 0.9
T , $^{\circ}\text{C}$	15.4 ± 4.1	15.0 ± 3.9	-12.0 ± 5.4	-11.6 ± 4.9
P , hPa	976.0 ± 5.5	967.8 ± 5.5	984.5 ± 9.7	971.4 ± 9.8
High values of $PM_{2.5}$ (cluster 2)				
	Yekaterinburg, summer	KAO, summer	Yekaterinburg, winter	KAO, winter
$PM_{2.5}$, $\mu\text{g}/\text{m}^3$	13.6 ± 4.3	9.6 ± 4.9	32.2 ± 9.1	30.3 ± 11.0
blh , km	0.6 ± 0.5	0.5 ± 0.5	0.2 ± 0.1	0.2 ± 0.1
w_s , m/s	2.5 ± 1.1	2.4 ± 0.8	2.5 ± 0.9	2.6 ± 0.9
T , $^{\circ}\text{C}$	19.2 ± 4.3	17.6 ± 4.0	-14.6 ± 5.1	-16.7 ± 5.8
P , hPa	981.0 ± 5.9	971.9 ± 6.3	991.7 ± 7.6	982.3 ± 5.7

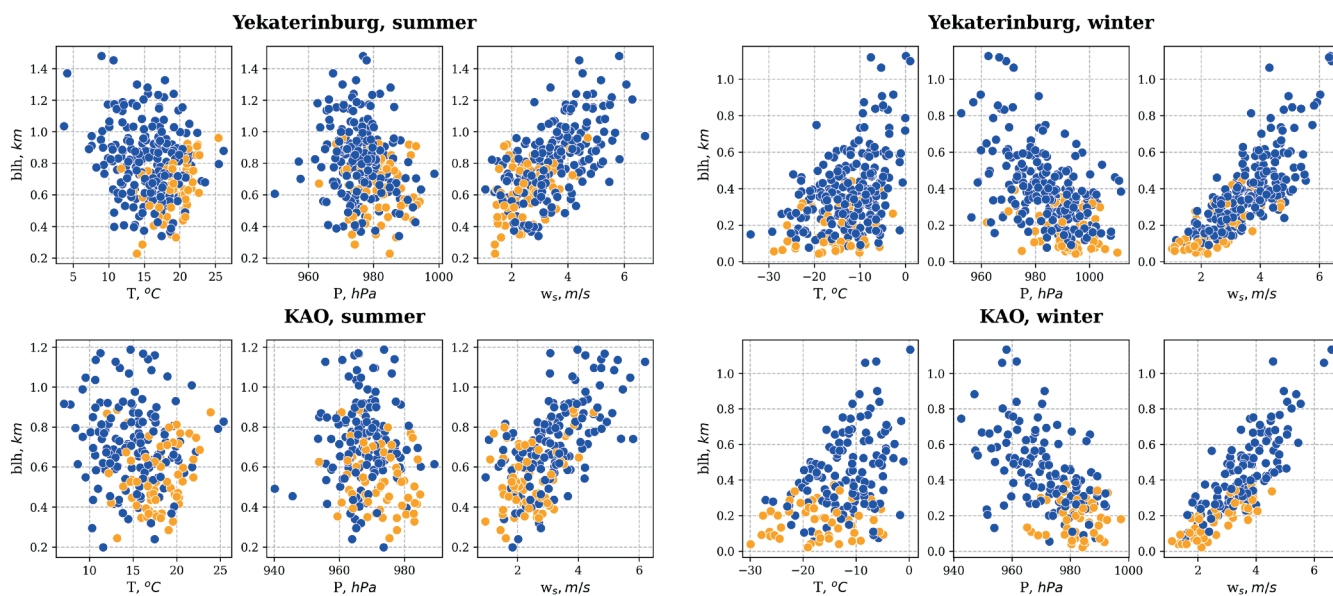


Fig. 4. Scatter diagram of average daily values of meteorological parameters for clusters of low (cluster 1, blue dots) and high (cluster 2, orange dots) values

Table 2. Meteorological conditions contributing to the appearance of higher $PM_{2.5}$ aerosol surface concentrations for the Middle Urals region for the Middle Urals region

parameters	summer	winter
blh , km	<1	<0.5
w_s , m/s	<5	<5
T , $^{\circ}\text{C}$	>12	<-5
P , hPa	>954	>962

The physical sense of this group of meteorological conditions is as follows. Under such meteorological conditions, increased surface concentrations are likely in the presence of sources of aerosol release into the atmosphere. From the point of view of mathematical logic, this is a necessary condition for the appearance of increased surface aerosol concentrations in the daily variation, but

not a sufficient one. On the contrary, when implementing meteorological parameters, the values of which do not satisfy the conditions, even in the presence of atmospheric aerosol sources, $PM_{2.5}$ surface concentration increase cannot be realized. Thus, we can speak of a necessary and sufficient condition for the appearance of typical aerosol surface concentrations in the daily variation.

CONCLUSION

This work presents a clustering approach using the K-means method to studying the daily variability of PM_{2.5} aerosol concentration of measurements at the urban and background monitoring sites in the Middle Urals region.

Cluster analysis identifies a statistically significant difference between the two groups corresponding to higher and lower concentrations of fine aerosol during the day.

The study reveals a significant dependence of the daily variability of PM_{2.5} particles concentrations on meteorological characteristics (in particular, air temperature, pressure, wind speed and boundary layer height).

Results show that distinctive typical average daily concentrations of PM_{2.5} in the air atmospheric layer for the Middle Urals region, corresponding to the cluster of lower values, are observed in the summer and were on average ~ 5.2 µg/m³ for the urban area and ~ 3.4 µg/m³ for the background area. In winter, these parameters are 12.8 µg/m³ for Yekaterinburg and 10.5 µg/m³ for KAO. Higher concentrations of PM_{2.5} aerosols, corresponding to the cluster of higher values, were observed in winter and were

on averaged ~ 32.2 µg/m³ for the urban area, ~ 30.3 µg/m³ for the background area. In summer, these parameters are 13.6 µg/m³ for Yekaterinburg and 9.6 µg/m³ for KAO.

The obtained results allow us to formulate threshold values of meteorological parameters, at which the occurrence of higher fine aerosol concentrations is possible. In summer, higher values are associated with pressure > 954 hPa, wind < 5 m/s, air temperature > 12 °C and boundary layer height < 1 km. In winter, higher values are possible with pressure > 962 hPa, wind < 5 m/s, air temperature < -5 °C and boundary layer height < 0.5 km.

The statistical regularities of the influence of meteorological parameters on the daily variability of the PM_{2.5} particles concentrations revealed during the research can be used as the basis for developing methods for assessing atmospheric pollution by fine aerosol in the Middle Urals based on weather forecasts, as well as for improving the air basin monitoring system.

The proposed approach can be used to determine the basic "background" type of weather conditions under which the levels of pollution of the lower atmospheric layer with fine PM_{2.5} aerosols can be considered typical for the analyzed region. ■

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