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Multivariate Analysis for Air Contamination and Meteorological Parameters in Zonguldak, Turkey

Kadir Ulutaş [1)], Abbas F. M. Alkarkhi [2)*], Sohaib K M Abujayyab [3)] and Salem S. Abu Amr [3)]

[1)] Karabuk University, Faculty of Engineering, Department of Environmental Engineering, 78050, Karabuk, Turkey.
[2)] Universiti Kuala Lumpur Business School (UniKL Bis), 50250, Kuala Lumpur, Malaysia.
* Corresponding Author. E-Mail: abbas@unikl.edu.my
[3)] International College of Engineering and Management, 111 Seeb, Muscat, Oman.

ABSTRACT

This study evaluates the concentration of PM_{10}, $PM_{2.5}$, NO_x, NO_2, CO and SO_2 parameters and the four climatological parameters (temperature, wind speed, humidity and net radiation flux) during the four seasons. Various statistical techniques were utilized to study the behavior of the selected parameters during the seasons. Descriptive statistics exhibited that the studied parameters have high concentrations in winter, except for NO_2 (which has a high concentration in autumn), while the concentrations of those parameters were the lowest in summer, except for NO_2 and NO_X (which have high concentrations in spring). Factor analysis (FA) showed that more than 80% of the total variation belongs to two factors, where 19.47% of the variation was due to wind speed and humidity, while other parameters were responsible for 62.90% of the total variation. Cluster analysis (CA) evaluated the similarity and dissimilarity between various elements through identifying four clusters representing the seasons; cluster 1: autumn, cluster 2: winter, cluster 3: spring and cluster 4: summer. This clustering indicates that the four seasons are entirely different. The highest dissimilarity was reported between summer and the other seasons. CA also classified all parameters into five statistically different clusters; cluster 1: PM_{10}, $PM_{2.5}$ and CO; cluster 2: SO_2, NO_X and NO_2; cluster 3: humidity; cluster 4: temperature and radiation and cluster 5: wind speed. This study illustrates the benefits of using multivariate techniques for the evaluation and interpretation of the total variation to get a better picture of the pollution sources/factors and understand the behaviors of the parameters in the air.

KEYWORDS: Air quality, Cluster analysis, Factor analysis, Particulate matter, NO_x, SO_2.

INTRODUCTION

Air pollution is accepted to be liable for over 7 million lives passing away every year (İçağa and Sabah, 2009; Ibe et al., 2020; WHO, 2018). Air pollution has become a severe global threat to public health and human welfare (Guo et al., 2019; Li et al., 2018). A major percentage of air-pollution problems belongs to traffic, industrial installations and climatological conditions affecting the temporal and spatial distributions of contamination (Wu and Kuo, 2013). Predominantly, air contamination arises during the unsustainable combustion of fossil fuels in energy-conversion machines, human activities, rapid industrialization and urbanization, such as biomass combustion, leakages from incinerators, flare stacks, sets of electric-power generators and vehicular traffic (Njoku et al., 2016).

The most common air pollutants are particulate matter (PM_{10} and $PM_{2.5}$), sulfur dioxide (SO_2), nitrogen oxides (NO_X), nitrogen dioxide (NO_2) and carbon monoxide (CO). These gases are formed and emitted into the air when fossil fuel is burnt at high temperatures (Njoku et al., 2016). This family of contaminants consists of reactive poisoning gases that can lead to harmful effects on living organisms. A study reported that a statistical correlation was found between the air

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contamination factors; sulfur dioxide, nitrogen dioxide, ozone and particulate matter ≤10 μm in aerodynamic diameter (PM_{10}) and cardiovascular, natural-cause and respiratory mortality (Chit-Ming et al., 2008). Gui et al. found that loong-term exposures to O_3, SO_2, PM_{10} and $PM_{2.5}$ were associated with behavioral regulation, inhibitory control, metacognition and poorer performance in primary-school children's working memory (Gui et al., 2020). The outcomes presented by Ma et al.'s study indicated that air-contamination exposure leads to an increase in respiratory diseases among younger children, especially during cold seasons (Ma et al., 2020).

Several studies were conducted to investigate the relationship between air-pollution factors and climatic variables. According to Liu et al. (2016), the magnitude of air contaminants (SO_2, NO_2, PM_{10}, CO and Ozone) correlated with climatic variables and mortality rate in Chinese states. Liu et al. (2020) reported that the values of the main air contamination factors (SO_2, $PM_{2.5}$, PM_{10}, NO_2 and CO) were influenced by climatological variables. The air-pollutant concentrations were outstandingly negatively associated with relative humidity, precipitation and wind speed, while air-contaminant concentration was positively associated with atmospheric pressure. Abusalem at el. (2019) analyzed air-pollutant concentrations resulting from road traffic in an urban area. Kheyari and Dalui (2014) estimated the wind load in high buildings using computational fluid dynamics.

Among the former literature, bivariate correlation and multiple linear regression were the most employed methods to investigate the relationship between air-pollutant variables and climatological variables (Çeli̇k and Kadı, 2010; Liu et al., 2020; Oji and Adamu, 2020). Formerly, few studies employed advanced methods, such as factor analysis and cluster analysis, to evaluate air-contamination data and its relationship with climatological variables (Uygur et al., 2010; Jorquera and Villalobos, 2020; Qin et al., 2020).

For comparison and other objectives that need multiple variables to be assessed from each sample, various multivariate statistical methods were employed to assess various environmental challenges (Alkarkhi et al., 2019; Yusup et al., 2011; Keerthi et al., 2018). In order to examine the principles of interaction of environmental components in life sciences and their integration, factor analysis and cluster analysis have become significant and suitable statistical techniques (Kaplunovsky, 2005). The system's data is organized into groups called clusters using cluster analysis, which is a multivariate technique that uses similarities between different observations as a criterion for group membership (Kazancia and Ma, 2015). Recent research has reported the use of multivariate analysis for the evaluation of the quality of natural water and air. Factor analysis was utilized by Yusup et al. (2016) to evaluate the metal content and particulate matter (PM10). To evaluate the impact of micro-climate variables on carbon-dioxide flux in the tropical coastal ocean in the China Sea, Yusup et al. (2018) used multivariate analysis. Alkarkhi et al. (2009) used multivariate analysis for the assessment of heavy metals in sediments of particular Malaysian estuaries. However, there hasn't been enough research on the use of multivariate analysis to determine how metrological data affects the behavior of air pollutants. The objective of this study is to: 1) investigate the behavior of selected parameters during various seasons, 2) evaluate and identify the sources of differences in the concentrations of the selected air parameters during the four seasons and 3) investigate the similarities and dissimilarities between different air-quality parameters and between different seasons.

This article aims to statistically analyze the temporal characteristics of and the influencing climatological variables on air-pollution variables in Zonguldak, northwest of Turkey. The contribution of this article appears in using factor analysis and cluster analysis to evaluate air-pollution data in a complex environment. The factor analysis method is used to identify the sources of variation in the parameters over the four seasons (autumn, winter, spring and summer), while cluster analysis is utilized to identify the sources of differences based on the similarities of the selected parameters during the various seasons.

MATERIALS AND METHODS

Study Area

Zonguldak is a Turkish province located along the western region of the Black Sea coast (Fig. 1). The population of Zonguldak is 619,703 and the area is 3.481 km^2. Zonguldak has an undulating ground and a rough topography, where 56% of the land is covered with mountains. The altitude changes between 0 and 1000 m and 52 % of the area is covered by forest (Alkan et al., 2010). Besides, precipitation occurs primarily in autumn and winter and the mean percentage of humidity is 70%. The Zonguldak area consisted of the biggest coal mines and became the major production center in Turkey. Three thermal-power plants, an iron factory and a steel factory (ERDEMIR) are running in Zonguldak. ERDEMIR is one of the largest steel and iron plants in Europe and the thermal-power plants are some of the important ones in Turkey (Abdikan et al., 2012). Zonguldak Black Sea coastal area consist of a sea-port traffic area, the main transportation road, the industrial and the mining area. These elements negatively affected the air quality in Zonguldak and led to progressive severe impacts on air quality.

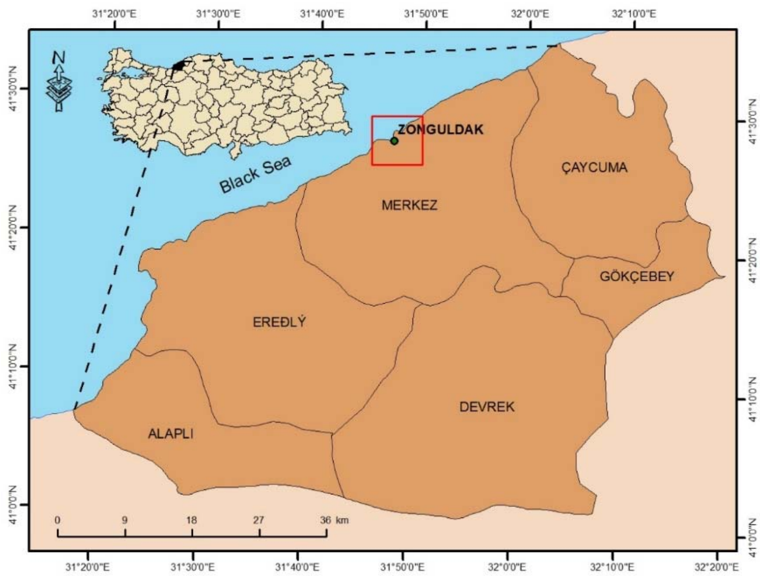

Figure (1): **The location of Zonguldak study area**

Data Collection

Climatological data, such as temperature, wind speed, humidity and net radiation flux, was collected from the Global Land Data Assimilation System (GLDAS). GLDAS data is stored in datasets provided by Google Earth Engine (GEE). GLDAS integrates ground-based observational data and satellite data products to construct optimal fields of land-surface states and fluxes using advanced data-assimilation and land-surface modeling algorithms. The land-surface climatological data is stored as gridded images in GEE. Based on the geographical location of the air-observation station in Zonguldak, the climatological data was downloaded using Javascript language (Rodell et al., 2004).

Air-pollution data was obtained from the Ministry of Environment and Urbanization's Air Quality Monitoring Station (AQMN) in Zonguldak. For air pollutants, such as sulfur dioxide (SO_2), nitrogen dioxide (NO_2) and carbon monoxide (CO), hourly measurements were taken of particulate matter (PM) having an aerodynamic diameter of less than or equal to 10 µm (PM_{10}) and less than or equal to 2.5 µm ($PM_{2.5}$). Daily, seasonal and annual values of pollutant parameters were determined with the help of hourly measurements (measured by the research team or taken from monitoring agencies) of air-pollutant data during the period between September 2019 and August 2020.

Statistical Analysis

Statistical analyses, such as descriptive statistics, factor analysis and cluster analysis, were used to analyze the climatological data and inorganic-element concentrations in Zonguldak (NW of Turkey).

Factor Analysis (FA)

The multivariate approach of factor analysis (FA) is used to depict the relationships between numerous variables. When the variables are highly correlated, FA works well and produces a lower number of new uncorrelated variables known as factors. The principal-component technique is usually employed for the extraction of the various factors. The axis defined by PCA is rotated to reduce the contribution of less significant variables. A small number of factors will be provided by this technique, such that the same amount of information will be gained from these factors as the original group of factors (Alkarkhi and Alqaraghuli, 2019; Yusup et al., 2016). FA can be expressed as a linear combination as given in Eq. (1):

$$F_i = b_1X_{1.j} + b_2X_{2.j} + b_3X_{3.j} + \cdots + b_mX_{m.j} \quad (1)$$

where Fi is defined as the factor, b represents the loading, X represents the measured value of the variable, i is the factor number, j is the sample number and m is the total number of variables.

In this work, FA is applied to identify the sources of variation in the measured data for climatological and inorganic parameters and as a result to identify the contribution of variables (parameters) in explaining the total variance and to identify the responsibility of each factor for the differences between seasons. SPSS Version 16 software was used for carrying out the factor analysis of the data.

Cluster Analysis

To find an appropriate classification where the observations or objects within each cluster are the same and where the clusters differ from one another, cluster analysis (CA), a multivariate technique, divides the recorded observations into groups called clusters using Mahalanobis distance as a measure of similarity (Yusup and Alkarkhi, 2011). The most common technique for sequentially creating clusters is hierarchical clustering. Climate data and inorganic parameters from air samples were subjected to carry out CA. The output of a hierarchical-clustering technique can be graphically displayed, similar to how the results of CA are typically given in a dendrogram, which shows all the steps in the hierarchical process (Shah and Shaheen, 2008). At each step, the distance was found for every pair of clusters and the two clusters with the smallest distance (largest similarity) were merged. The distances or similarities between two clusters A and B are defined as the minimum distance between a point in A and a point in B, as given in Eq. (2).

$$D(A,B) = min\{d(x_i, x_j), for\ x_i\ in\ A\ and\ x_j\ in\ B\} \quad (2)$$

After two clusters were merged, the procedure was repeated for the next step: the distances between all pairs of clusters were calculated again and the pair with the minimum distance was merged into a single cluster. The result of a hierarchical-clustering procedure can be displayed graphically using a tree diagram, also known as a dendrogram, which shows all the steps in the hierarchical procedure. SPSS Version 16 software was used for carrying out cluster analysis of the data.

RESULTS AND DISCUSSION

Descriptive Statistics

The means and standard deviations for the selected parameters (PM_{10}, SO_2, NO_2, NO_x, $PM_{2.5}$, air temperature, wind speed, humidity and net short-wave radiation flux) are presented in Table 1. The mean concentrations of most selected parameters were the highest in winter, except for NO_2 (in autumn) and the lowest concentrations were observed in summer, except for NO_2 and NO_X (in spring). Temperatures and net short-wave radiation flux peaked in winter and peaked in summer, as expected. Wind speed showed the lowest level in autumn and the highest level in spring, while humidity remained at the same level. These differences in the lowest and highest levels of the selected parameters are attributed to the fluctuation of ambient air temperature in winter and summer seasons. In general, low concentrations of the selected parameters were seen during the summer season compared to the other seasons. Most inorganic compounds experienced their highest concentration levels in winter compared to the other seasons (Bozkurt et al., 2018; Sari et al., 2019).

In addition to various reasons, such as the use of coal in industrial activities in the region, the use of coal in houses during the winter months and unfavorable meteorological conditions (lower mixing heights and precipitation) may cause pollutant concentrations to increase during the winter period. A high concentration of NO_x was observed at low humidity and low temperature (Sari et al., 2019; de Foy, 2018). It can be said that high pollution levels in winter could be due to the primary source of heating. The pollution level was high during the winter period, which could be due to the prevailing wind from the southeast direction as well as the effect of local coal used in the near and distant residences located in the southeast of the air-quality monitoring station. Besides, in the city center, coal mines, Zonguldak port and traffic density contribute significantly to the increase in air-pollution emissions, especially with the effect of adverse meteorological conditions. The topography is also an important factor in terms of air pollution, especially for Zonguldak. The city is in a position open to the sea winds, as the north and west directions are open to the sea. The fluctuations in the selected parameters during each season are exhibited by the standard deviation (SD) for each parameter (Table 1). The highest standard deviation for all parameters was exhibited in autumn, except for NO_2 being exhibited in spring, whilst the lowest level was recorded in summer-instance PM_{10}, SO_2, NO_x, $PM_{2.5}$, except for CO and NO_2 being exhibited in winter. Wind speed and net short-wave radiation flux showed the lowest levels in autumn and summer, respectively. The high value of the standard deviation indicates that the level of the selected pollutant parameter fluctuates from low to high, which means that it is not maintained at the same level. High fluctuations in the parameters can be explained by the adverse effects of meteorological and topographical factors on the dispersion of inorganic pollutants emitted from residential heating, traffic and industrial activities in Zonguldak. In this area, there are three thermal-power plants, an iron factory and a steel factory, noting that the thermal-power plants are running daily. Moreover, the area consists of seaport traffic, the main transportation road and coal-mining activities, which may directly contribute to the high levels of air-pollution parameters in this area. More explanation is presented in the study-area section.

Table 1. Means and standard deviations for the selected parameters like SO_2, CO, … etc… ppm)

Season		PM_{10}	SO_2	CO	NO_2	NO_x	$PM_{2.5}$	Temperature	Wind Speed	Humidity	Radiation Flux
Autumn	**Mean**	45.967	11.100	569.333	43.333	86.133	23.933	297.733	3.500	0.005	142.100
	SD	24.327	7.754	120.362	8.381	24.939	20.497	6.721	0.100	0.001	36.957
Winter	**Mean**	62.333	17.633	618.033	40.967	94.467	29.300	284.333	4.333	0.004	107.567
	SD	14.351	7.572	53.086	1.966	12.973	10.489	1.550	0.404	0.001	16.638
Spring	**Mean**	59.367	4.667	513.767	29.500	50.500	23.267	295.500	4.933	0.005	187.600
	SD	20.720	2.928	66.461	9.283	20.825	8.823	5.603	0.208	0.001	27.193
Summer	**Mean**	34.567	3.100	332.567	32.200	52.867	7.767	306.200	4.533	0.005	212.733
	SD	1.518	0.200	91.532	2.211	2.470	1.701	2.330	0.451	0.001	9.504
Annual	**Mean**	**50.558**	**9.125**	**508.425**	**36.5**	**71**	**21.067**	**295.95**	**4.325**	**4.75**	**162.5**

Factor Analysis

The data for twelve months covering the four seasons (autumn, winter, spring and summer) was analyzed using factor analysis to identify the sources of variation in the data which includes the parameters (PM_{10}, SO_2, CO, NO_2, NO_x, $PM_{2.5}$, air temperature, wind speed, humidity and net short-wave radiation flux). Factor analysis extracted ten factors explaining 100% of the total variance. Factor analysis was actually performed on the correlation matrix between different parameters followed by Varimax rotation. As a measure of the contributions of various parameters, two factors with eigen-values greater than 1 can be chosen (the first eigen-value is 2.508 and the second eigen-value is 1.395, while subsequent eigen-values are less than 1). An eigen-value gives a measure of the significance of a certain factor; the factors with the highest eigen-values are most significant and responsible for explaining large variations in the data. More than 82% of the total variance is explained by the two components (based on the highest two eigen-values). The parameter loadings for the two factors are presented as given in Eqs. (3-4).

$$F_1 = 0.83\ PM_{10} + 0.89\ SO_2 + 0.87\ CO + 0.74\ NO_2 + 0.84\ NO_X + 0.91\ PM_{2.5} - 0.94\ Air\ Temperature - 0.17\ Wind\ Speed - 0.08\ Specific\ Humidity - 0.94\ Net\ Short - wave\ Radiation\ Flux \quad (3)$$

$$F_2 = -0.22\ PM_{10} + 0.27\ SO_2 + 0.07\ CO + 0.49\ NO_2 + 0.43\ NO_X + 0.03\ PM_{2.5} + 0.21\ Air\ Temperature - 0.93\ Wind\ Speed + 0.81\ Specific\ Humidity - 0.29\ Net\ Short - wave\ Radiation\ Flux \quad (4)$$

The first factor (F_1) explained 62.90% (corresponding to the first eigen-value) of the total variance and was highly positively correlated (Eq.3) with PM_{10}, SO_2, CO, NO_2, NO_X, $PM_{2.5}$ and air temperature, while being highly negatively correlated with net short-wave radiation flux. Furthermore, the first element had a very modest connection with wind speed and humidity. The relationship between temperature and other specified characteristics might be referred to as a result of this factor. This variable describes the state of the air masses flowing between the two points. The second element, which could be linked to the local geographical circumstances of the two locations, was influenced by wind speed and humidity. The second factor accounted just for 19.47% (corresponding to the second eigen-value) of the overall variation in the data and was substantially negatively correlated with wind speed and positively correlated with humidity, while other measures had extremely minimal correlations with the second factor. This factor may be termed as the difference between humidity and wind speed.

The relationship between the months and factor values was studied to show the behavior of the selected parameters during different months. The contributions of the selected parameters to different months are presented in Fig. 2, showing the effects of different parameters on different months. It can be seen that the contributions of the parameters to the first two months in autumn (September and October) were negative, while being positive to the third month (November). Those contributions were positive to winter and negative to summer, while being negative to the first two months of spring (April and May) and positive to March.

Positive contributions could be due to the high values of PM_{10}, SO_2, CO, NO_2, NO_X and $PM_{2.5}$ while negative contributions could be due to the high values of air temperature and net short-wave radiation flux. Positive contributions of the parameters in winter may be due to the use of poor-quality coal for heating (Ulutaş et al., 2019).

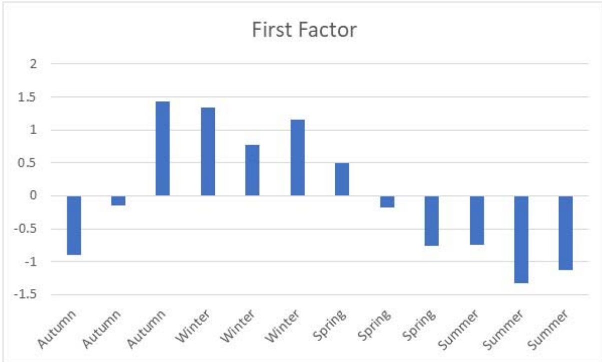

Figure (2): Factor values for the first factor for the four seasons

The values for the second factor are presented in Fig. 3, showing the effects of different parameters on different months. Positive contributions could be due to the high value of humidity, while negative contributions could be due to the high value of wind speed. The positive and negative behaviors may be due to the fluctuation in the industrial activities in the studied area (the magnitude of the values (positive or negative) is due to the level of the selected parameter in each month).

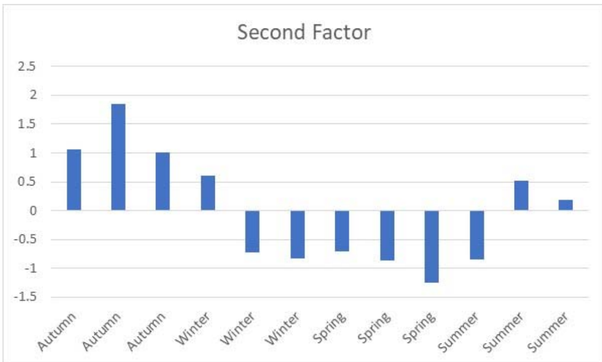

Figure (3): Factor values for the second factor for the four seasons

The values of both factors are presented in Fig. 4, showing the contribution of each factor to various months. The third month of fall (November) is similar to the first month of winter (December), whereas the first month is similar to summer. This could be due to the high values of PM_{10}, SO_2, CO, NO_2, NO_X and $PM_{2.5}$ in December, compared to October and November. Humidity is usually high in all months of autumn and the wind speed is low compared to other months. The first month of other seasons showed values close to those of the previous season; for example, the first month of spring (March) is close to winter and the first month of summer (June) is close to spring. It can be clearly seen that the behavior of various parameters of the last month for each season is close to the behavior of the first month of the next season; for instance, autumn represents September, October and November and the behavior of various parameters in November is close to the behavior of winter in December, while the last month of winter (February) is close to spring in March and the same is valid for other seasons. This indicates the changes in the behavior of the selected parameters from season to another.

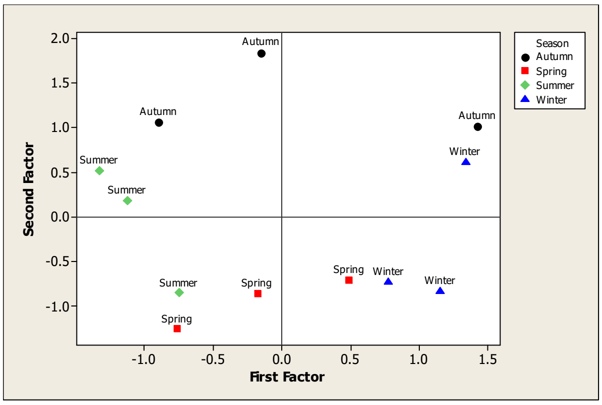

Figure (4): Factor values for the first and second factors

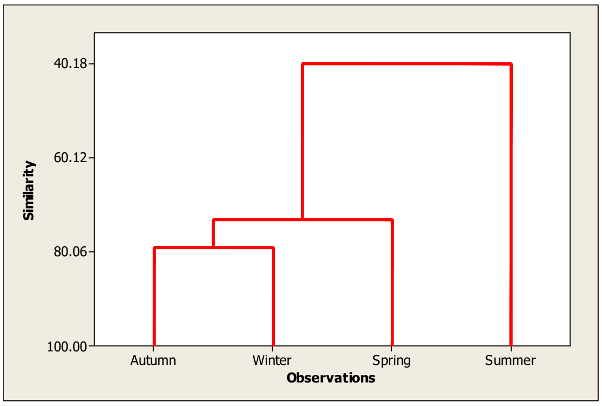

Figure (5): Dendrogram showing the clustering of the selected air parameters in the various seasons

Cluster Analysis

The data for climatological factors was further analyzed using cluster analysis (CA) to identify the sources of differences based on the similarities of the selected parameters during various seasons. CA provides information about the behaviors of the selected parameters and groups them under a specific category (season). CA for climatological data produced a dendrogram as presented in Fig. 5, clustering the data into four statistically different groups (seasons), cluster 1: autumn, cluster 2: winter, cluster 3: spring and cluster 4: summer.

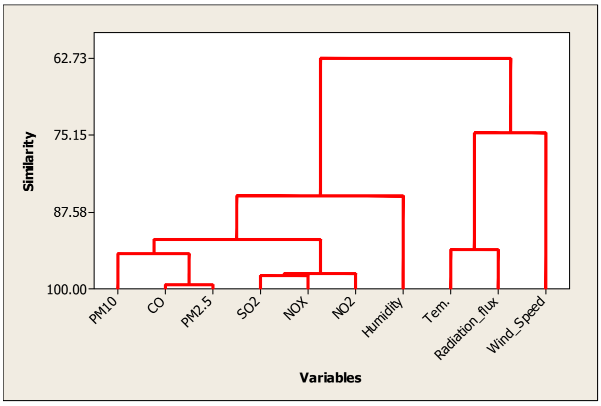

Figure (6): Dendrogram showing the clustering of all air parameters monthly during 2019 - 2020

This clustering indicates that the four seasons are different in general. The highest dissimilarity is reported between summer and the other seasons, which may be due to meteorological differences between summer and other seasons. Moreover, the highest levels of inorganic pollutants, such as NO_2 and SO_2, were reported in winter compared to summer (Artun et al., 2017). CA for all parameters throughout the year is also investigated to identify the difference between the parameter groups, as shown in Fig.6, grouping the parameters into five statistically different clusters; cluster 1: PM_{10}, $PM_{2.5}$ and CO; cluster 2: SO_2, NO_X and NO_2; cluster 3: humidity alone; cluster 4: temperature and radiation and cluster 5: wind speed alone. The dissimilarity between the groups revealed that some parameters have different behaviors during the seasons (Yusup and Alkarkhi, 2011). However, CO and $PM_{2.5}$ in cluster 1 and SO_2, NO_X and NO_2 in cluster 2 have the same behavior in both clusters 1 and 2. This similarity could indicate that these parameters are affected by or belong to the same source, which is mainly due to the emissions from nearby industries. Moreover, the dissimilarity for humidity, temperature and wind speed in clusters 3, 4 and 5 could be due to the natural fluctuation of these metrological parameters between the seasons.

CONCLUSIONS

The average concentrations of air parameters were recorded to be higher than the Turkish air-quality standard, except for SO_2. Even so, there were lower concentrations of some parameters in the spring and summer seasons compared to the standard. The concentrations of all selected parameters determined (positive correlation with temperature) were higher in winter than in summer. Based on the analysis, it can be concluded that the high concentrations of the selected parameters were due to the adverse effects of meteorological and topographical factors on the dispersion of inorganic pollutants emitted from residential heating especially in winter, traffic and industrial activities in Zonguldak rather than from crustal/natural sources. The mean concentrations of most selected parameters were the highest in winter, except for NO_2 (in autumn) and the lowest in summer, except for NO_2 and NO_X (in spring). Factor analysis (FA) showed that more than 80% of the total variation belongs to two factors: 19.47% of the variation is due to wind speed and humidity, while other parameters are responsible for 62.90% of the total variance. The dissimilarity of parameter groups between the seasons revealed the contributions of climatological parameters (temperature, wind speed, humidity and radiation) on the selected air-quality parameters. Moreover, the similarity between some selected parameters revealed the same source of these parameters, while the dissimilarity between the other parameters revealed the contribution of some other sources or factors for changes in the behavior of these parameters.

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