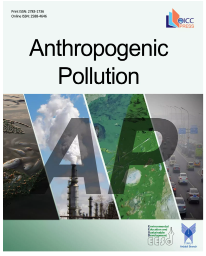

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Dispersion modelling of potentially toxic elements and particulate matter concentrations from the stack of Shahid Rajaei power plant using the AERMOD method

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Abstract:

This study was conducted with the aim of evaluating the dispersion of suspended particles and potentially toxic elements in the air and soil around Shahid Rajaei Thermal Power Plant. For this purpose, soil sampling was carried out in a regular network with a radius of 10 km to measure the concentration of potentially toxic elements, and separately, the distribution model of particles and potentially toxic elements released from the power plant chimney was determined using AERMOD software up to a distance of 25 km. Results showed that the concentration of potentially toxic elements in the soil around the power plant has a direct relationship with the particles coming out of the power plant chimney and their deposition in the soil, and the trend of soil pollution up to a distance of 8 to 10 km from the power plant shows the highest concentration of the studied elements, and with increasing distance from the power plant, pollution levels are reduced. In the affected areas, the concentrations of vanadium, nickel, zinc, and copper exceeded the standard with values of 237, 88,210 and 112 ppm, respectively, and the four elements cobalt, chromium, molybdenum, and lead with values 21, 115, 4.7 and 42 ppm showed lower levels of pollution which are also related to the type of fuel consumed by the power plant. Modeling of particle dispersion in the air by AERMOD method with the trend of dispersion and concentration of the above elements is consistent with the analysis of soil pollution and shows an acceptable level of accuracy between the two evaluation methods.

Keywords: Air and soil pollution; Thermal power plant; Fossil fuel

1. Introduction

Population growth, rapid development, and industrialization have significantly increased pollutant levels (Mostofie et al., 2014). One of the societal impacts of air pollution is the rise in mortality rates (Moghadam et al., 2021). Research indicates a direct correlation between daily concentrations of suspended particles in the air and daily mortality rates (Schwartz and Dockery, 1999). According to the World Health Organization (WHO), air pollution is the fourth leading cause of death globally, after smoking, diet, and obesity, with suspended particles causing approximately 5 million premature deaths annually (WHO, 2016). Studies in the United States have demonstrated that elevated levels of suspended particles contribute to mortality from cancer, respiratory diseases, and cardiovascular diseases (Pope et al., 1995). A study conducted in Ohio investigated the dispersion and inhalation of manganese over a year using the AERMOD method, revealing that adult residents are exposed to this metal (Rosemarie et al., 2016; Fard and Khoramnejadian, 2020). One major source of pollution and environmental damage from power plants is the emission of dust and heavy metal particles. Research on suspended particles in the textile industry in Isfahan Province has shown that high concentrations pose a significant risk factor for chronic respiratory diseases in occupational settings (Barjoee and Azimzadeh, 2020).

Additionally, a study on dust from the Sepahan Cement Factory in Isfahan revealed that concentrations of SO2 and NOx exceeded Iran's clean air standards, potentially harming local populations and vegetation. While suspended particles smaller than 2.5 microns were below the permissible limit, those smaller than 10 microns exceeded the limit at all monitoring stations (Rahmani and Hatefi, 2023). Mishra et al. (2024) conducted research in the Dhanbad region of India, highlighting that coal extraction and use release significant amounts of air pollutants and potentially toxic elements such as Cd, Cr, Cu, Mn, Ni, Pb, and Zn. They employed multiple linear regression models to assess the impact of atmospheric metals on plants' ability to tolerate air pollution. Eslamidoost et al. (2023) investigated pollutant emission sources near a gas refinery in Iran, demonstrating that due to chimney heights and wind effects, pollutant concentrations were low at the base of the stacks and decreased with distance.

The AERMOD model is also utilized to compare pollutant concentrations from sources with global standards. For example, results from the Ramin Power Plant in Ahvaz indicated that sulfur dioxide concentrations were below global environmental standards (Momeni et al., 2011). Among airborne pollutants, PM2.5 is particularly hazardous. Numerous studies suggest that PM2.5 can damage human lung tissue and exacerbate chronic respiratory and cardiovascular diseases, with every 10 $\mu g/m^3$ increase leading to a 1.29% rise in hospital visits for cardiovascular and respiratory issues. The International Agency for Research on Cancer has classified PM2.5 as a carcinogen (Wang et al., 2019; Vinikoor-Imler et al., 2011). In industrial parks and special economic zones with multiple active factories, pollution from these sources increases the density and concentration of pollutants. For instance, in the Pasir Gudang Industrial Park in Johor, Malaysia, concentrations of nitrogen dioxide, sulfur dioxide, and particulate matter less than 10 microns were simulated using the AERMOD model. The results demonstrated that AERMOD effectively predicted pollutant concentrations at 36.20, 8.59, and 5.40 $\mu g/m^3$, respectively (Afzali et al., 2017).

Furthermore, AERMOD has been applied to model the dispersion of mercury in residential areas, revealing that meteorological characteristics, stack height, and topography significantly influence air pollution distribution. However, AERMOD may underestimate PM concentration during summer due to its limitations in representing vertical dispersion. An inverse relationship was observed between mercury concentration and stack height, with communities at higher elevations near industrial sources experiencing greater exposure to air pollution compared to flatter areas (Heckel and LeMasters, 2011).

The AERMOD model predicts the concentration of each pollutant emitted from industrial stacks within a radius of up to 50 km, using the physical characteristics of the stacks, land use, meteorological data at both the surface and aloft, topography, and the number of stacks. By modeling air pollution with AERMOD, it is possible to forecast the concentration and distribution of pollutants in the study area, which can inform managerial and engineering solutions for controlling suspended particles such as PM2.5 and PM10 (Fard et al., 2024). The elements investigated in the health threat, especially have risks such as reduced growth of children, kidney diseases, carcinogenic factors and many adverse effects on the health of citizens (Sadigh et al., 2021). Some toxic metals such as cadmium and lead are unnecessary and carcinogenic elements. Some other metals such as nickel, zinc and copper are necessary for the growth of the body, but they have toxic effects in high concentrations. In past studies, focusing on the way air pollution is spread, or whether the concentration of elements in the soil has been investigated independently, and how the relationship between them has been given less attention, and there is a research gap in this regard. One of the features and innovations of this research is establishing a connection between the model of pollution in the air and the rate and trend of increasing the concentration of metals in the soil around the power plant. Therefore, this study aims to predict the dispersion of pollutants from the Shahid Rajai Power Plant's stack, with a particular focus on the dispersion of potentially toxic elements.

2. Materials and methods

2.1 Study area

The Shahid Rajaei Power Plant is situated 25 km from the Qazvin-Karaj highway, covering an area of 290 hectares at an elevation of 1280 m above sea level (figure 1, Table 1). This facility includes both combined cycle and thermal power generation units. In the combined cycle sector, there are 9 units with a total capacity of 1042 MW, while the average operational power of the plant is 900 MW (JICA, 2018).

2.2 Data collection

To determine the required values, the study area must be divided into appropriate sectors based on land use types and vegetation cover in a clockwise manner. These parameters are then introduced on a monthly, seasonal, and annual basis. In this project, we utilized coefficients specified by the U.S. Environmental Protection Agency (EPA) for land surface characteristics such as albedo, Bowen ratio, and surface roughness height as outlined in the AERMET preprocessor guide. These coefficients are essential for assessing thermal flux and atmospheric stability in the study area.

The AERMOD model is an advanced Gaussian model used for permanent forecasting, specifically designed to model the dispersion of air pollutants from point, volume, and surface sources within distances of less than 50 km from the emission source. Meteorological characteristics, chimney height, and topography significantly affect the spatial distribution of pollution and the release of particles into the air. Upland areas close to point sources may experience two to three times more pollution exposure than flat regions. The variation in pollutant exposure depends on the height of the point source chimneys and the ambient concentrations, with AERMOD illustrating the differences in concentrations received by high ground relative to flat land. In estimating

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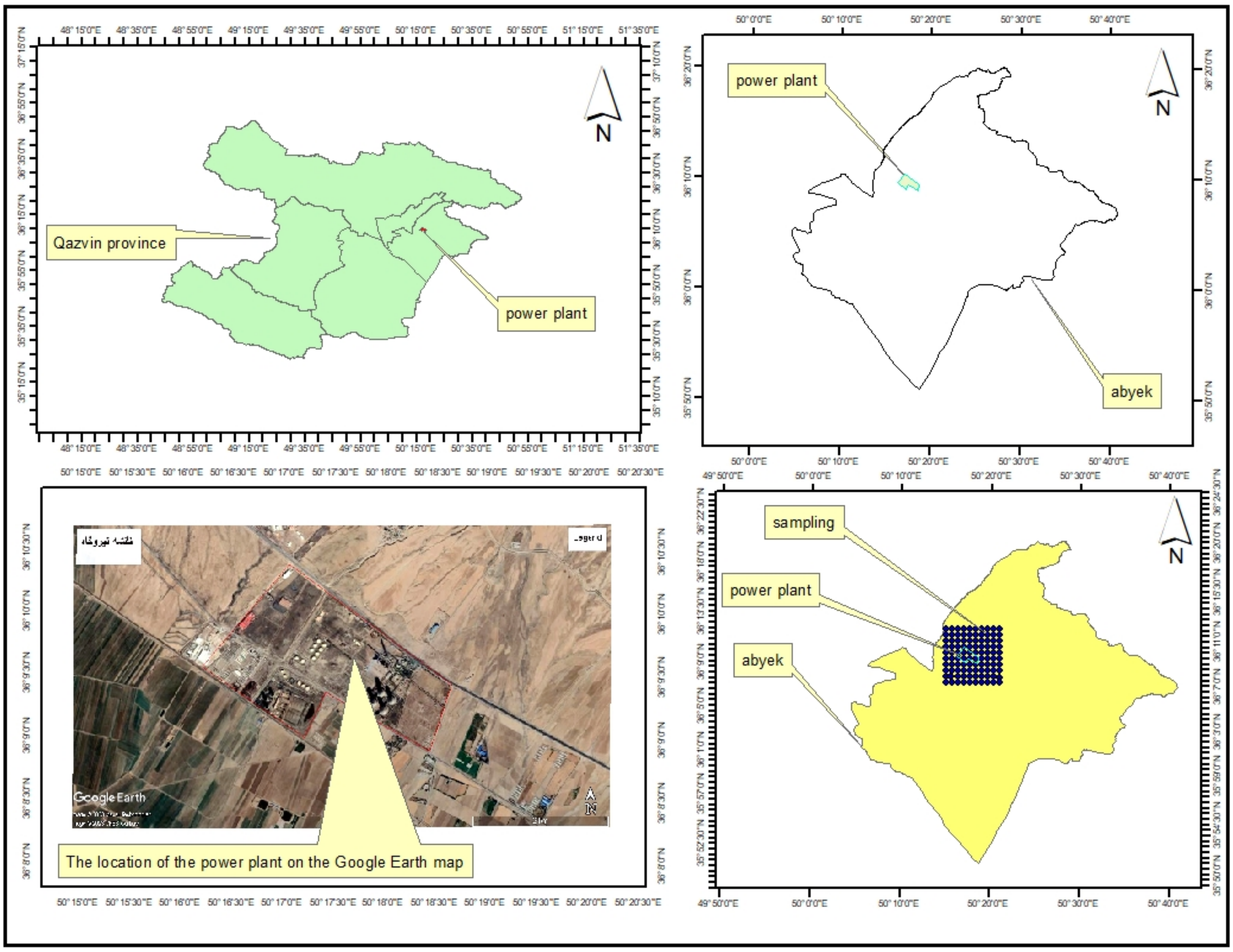

Figure 1. Location of the studied area in Qazvin province.

emissions from industrial chimneys, it was found that the surface roughness length parameter significantly influences the concentrations received by each receptor. The height of the receptors, as determined by the AERMOD preprocessor, is typically greater than the height of the surface beneath the chimney or source. If the receptor is at a higher altitude, the wind flow may not effectively disperse the pollutants, resulting in higher concentrations at those receptors. Conversely, if the receptors are lower than the chimney height, the wind can disperse the pollutants more efficiently, leading to lower concentrations of polluting particles. (Figure 2)

2.3 Data processing

After running AERMOD and preparing the necessary meteorological files for the model, project data were introduced into the model via the input file for processing. The dispersion modeling of suspended particulate pollutants was conducted for 1-hour, 8-hour, and annual averaging periods. AERMOD requires specific information for each type of pollutant source. For the sources considered in this research, which are classified as point sources, details such as pollutant emission rates, release height above ground level, temperature and velocity of the gases exiting the source, and the internal diameter at the emission point were defined. In this study, receptors were positioned within a Cartesian grid covering a 25×25 km area. The AERMAP preprocessor was employed to process the topographic data of the area. Finally, the maximum concentrations simulated by the model for each scenario were compared with global soil standards, which are presented in Table 2.
In the stable boundary layer (SBL), the concentration distribution is assumed to be Gaussian in both the vertical

Table 1. Coefficients and surface characteristics of the studied area.

Sector number	Beginning of sector (grade)	Beginning of sector (grade)	Application type of vegetation	Surface roughness (m)	Bouan's ratio (dimensionless)	Albedo coefficient (dimensionless)
1	0	180	Mountainous or wasteland	0.04	0.925	0.29
2	180	360	Agriculture	0.0725	0.75	0.28

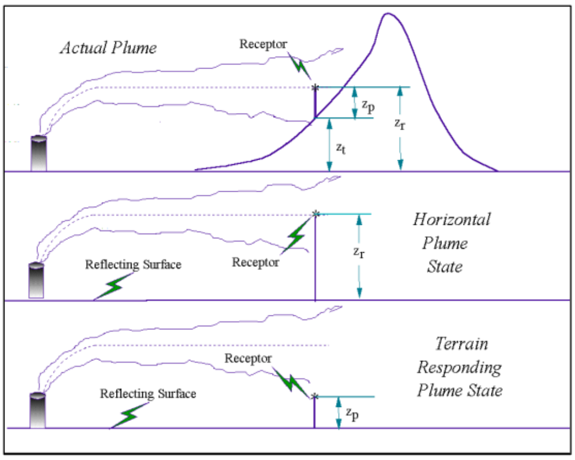

Figure 2. AERMOD two state approach. The total concentration predicted and weighted sum of the two extreme possible plume states (EPA, 2023b).

Table 2. Comparison of toxic elements Concentration Standards with Regional Soil (ppm).

Elements	Co	Cr	Cu	Mo	Ni	Pb	V	Zn
Global shale (Turekian and Wedepohl, 1961)	19	90	45	2.6	68	20	130	95
Global soil (Kabata-Pendias and Mukherjee, 2007)	6.9	42	14	1.8	18	25	60	62
The average concentration of elements in the study area	15	79	46	3.9	59	12	105	63

and horizontal. In the convective boundary layer (CBL), the horizontal distribution is assumed to be Gaussian, but the vertical distribution is described with a bi-Gaussian Probability Density Function (PDF). This behavior of the concentration distributions in the CBL was demonstrated by Willisand and Deardorff (1981) and Briggs (1993). Additionally, in the CBL, AERMOD treats "plume lofting" whereby a portion of plume mass, released from a buoyant source, rises to and remains near the top of the boundary layer before becoming vertically mixed throughout the CBL. The model also tracks any plume mass that penetrates into an elevated stable layer, and then allows it to re-enter the boundary layer when and if appropriate. (Figure 3)

2.4 Sampling design

To evaluate the concentration of potentially toxic elements specifically lead, vanadium, zinc, cobalt, chromium, copper, molybdenum, and nickel in the soils surrounding the Shahid Rajai Power Plant, a comparative analysis of the dispersion of suspended particles was conducted. A total of 63 sampling stations were established within a 5-10 km radius of the plant's chimney. At each station, a 1 kg soil sample was collected from a depth of 0-20 cm. Due to obstacles such as highways, old roads, the Qazvin-Karaj railway, military barracks, the main water canal, secondary canals, the Caspian 1 industrial park, and scattered industrial units, some samples were located several meters away from the

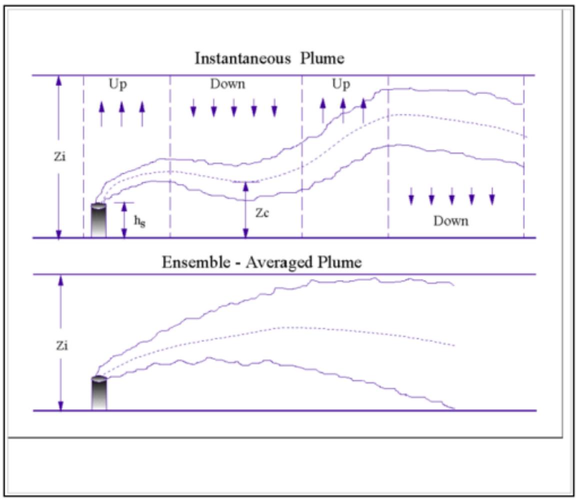

Figure 3. Instantaneous and corresponding ensemble-averaged plume in the CBL (EPA, 2023a).

central grid. Figures 4 illustrate the sampling locations, grid layout, and wind rose diagram within the power plant area.

2.5 Sample preparation and analysis method

Soil samples were initially prepared following standard protocols to ensure homogenization. The samples were dried in an oven and then sieved through a 2 mm mesh to obtain 200 g portions. Acid digestion was performed by adding specified amounts of hydrochloric, perchloric, and nitric acids to the samples. The samples were then placed in a Hot Box at 220 °C for four hours to complete the digestion process. After cooling to ambient temperature, the samples were diluted with distilled water to prepare them for analysis using ICP-OES and ICP-MS devices, specifically the Agilent Series 4500 ICP-MS model. The concentrations of heavy metals were then measured, converted, and processed. Table 3 presents the results of the ICP-OES analysis of soil samples collected around the power plant (ppm).

2.6 Stack emission data

The technical specifications of the chimney indicate the emission of suspended particles into the air, and these specifications were entered into the software. The required parameter values are provided in Table 4.

2.7 Meteorological data

The dispersion and concentration of airborne pollutants at the surface are influenced by various meteorological parameters, including wind speed, wind direction, ambient temperature, turbulence, and mixing height. The AERMOD dispersion model requires preprocessed meteorological data, consisting of both surface and profile files, and estimates boundary layer parameters using AERMET. AERMET requires hourly surface meteorological data, which includes wind speed, wind direction, temperature, and cloud cover, as well as upper atmospheric data. For this research, surface meteorological data were sourced from 10-minute intervals provided by the Shahid Rajai Power Plant's meteorological station. Figure 4 displays the grid layout and sampling lo-

Table 3. Results of ICP-OES Analysis of Soil Samples around the Power Plant (ppm).

Number	Cu	Cr	Co	Pb	Ni	Mo	V	Zn
Sum	2873	4971	944	734	3688	245.3	6644	5833
Average	45.604	78.905	14.984	11.651	58.54	3.8937	105.46	92.587
Max	112	115	21	42	88	4.7	237	210
Min	27	60	11	7	36	3	59	67

Table 4. Values and parameters of Power plant chimney used in AERMOD model.

Diffusion coefficient ($\mu g/m^3$)		Output speed (m/s)	Outlet temperature (K)	External diameter (m)	Inner diameter (m)	Chimney height (m)	Latitude (UTM)	Longitude (UTM)
PM2.5	PM10	11	432	4	5.6	220	4001996	437057
0.28	1.12							

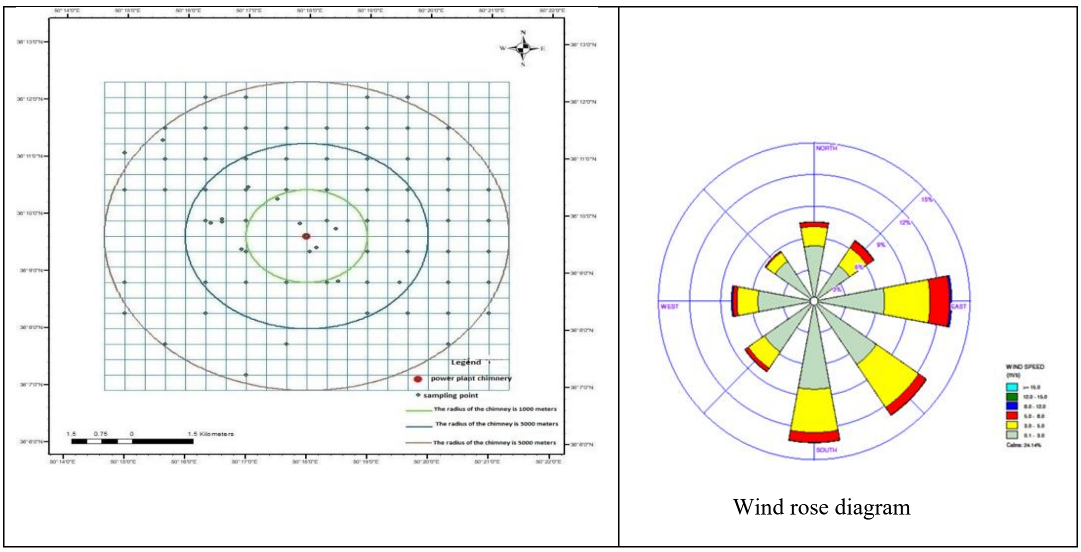

Figure 4. Grid Network Method and Sampling Point Locations (on the left) and wind rose diagram of the Region (on the right).

Table 5. Average meteorological data specifications.

X(UTM)	**Y**(UTM)	**Rain for 6 hours**	**Wind speed**	**Wind direction**
437808	4001423	0.128	1.981	158.348
Cloudy	**Humidity**	**Station surface pressure**	**Temperature**	**H**
2.334	51.776	872.073	15.389	1300

cations (left) alongside the wind rose diagram for the area (right).

In this study, meteorological data were obtained from the Qazvin Provincial Meteorological Organization and entered into the model. Table 5 presents the average meteorological data specifications used in this research.

As shown in figure 4 and Table 6, the wind directions of the area is illustrated in 8 directions. At this station, the predominant wind directions are as follows: 24.15% of winds are from the dominant southern direction, 13.37% from the eastern direction, and 13.10% from the southeast direction. These three wind directions account for the majority of the winds. Other wind directions are present throughout the region, with the least frequent being from the northwest, which accounts for 5.72% of the total winds. Table 6 displays the classification of wind speeds and predominant winds in the study area.

3. Results and discussion

AERMOD is one of the most efficient software tools for modeling average pollutant concentrations, and it was utilized in this study. Based on the evaluations and predictions made, the performance of AERMOD in forecasting pollutant concentrations is considered satisfactory. Studies by Momeni et al. (2011), Rahmani and Hatefi (2023), and Rosemarie et al. (2016), and Heckel and LeMasters (2011) have confirmed AERMOD's results, validating its application. Thus, AERMOD is deemed a suitable scientific tool for analyzing control strategies and policies aimed at reducing and preventing air pollution.

After running the model, results are generated for different time intervals. Predictions of average concentrations for 1-hour, 8-hour, and annual periods, as shown in figures 5 and 6, indicate that the average concentrations of PM2.5

Table 6. Classification of wind speeds and predominant winds in the study area.

Wind directions	**Wind speed (m/s)**	**Wind speed class (m/s)** 0.1-3.0	3.0-5.0	5.0-8.0	8.0-12.0	12.0-15.0	**Total (%)**	**Dominant winds**
Northern	337.5 - 22.5	5.22518	1.8219	0.42691	0.03608	0	7.51	-
Northeast Eastern	22.5 - 67.5	4.07071	2.01431	0.77566	0.06614	0.00601	6.93	-
Eastern	67.5 - 112.5	6.75245	4.37135	1.87601	0.19842	0.01203	13.21	second
Southeast	112.5 - 157.5	7.21544	4.92454	0.87788	0.0481	0	13.06	third
South	157.5 - 202.5	8.30978	4.10078	0.93199	0.03006	0	13.37	first
Southwest	202.5 - 247.5	5.77837	1.87601	0.3728	0.0481	0	8.075	-
western	247.5 - 292.5	5.41158	2.0083	0.39685	0.14431	0.00601	7.96	-
Northwest	292.5 - 337.5	4.54573	1.03421	0.12026	0.01203	0.01203	5.72	-
Sum of directions	Sub-Total	47.3092	22.1514	5.77837	0.58325	0.03608	75.85	-

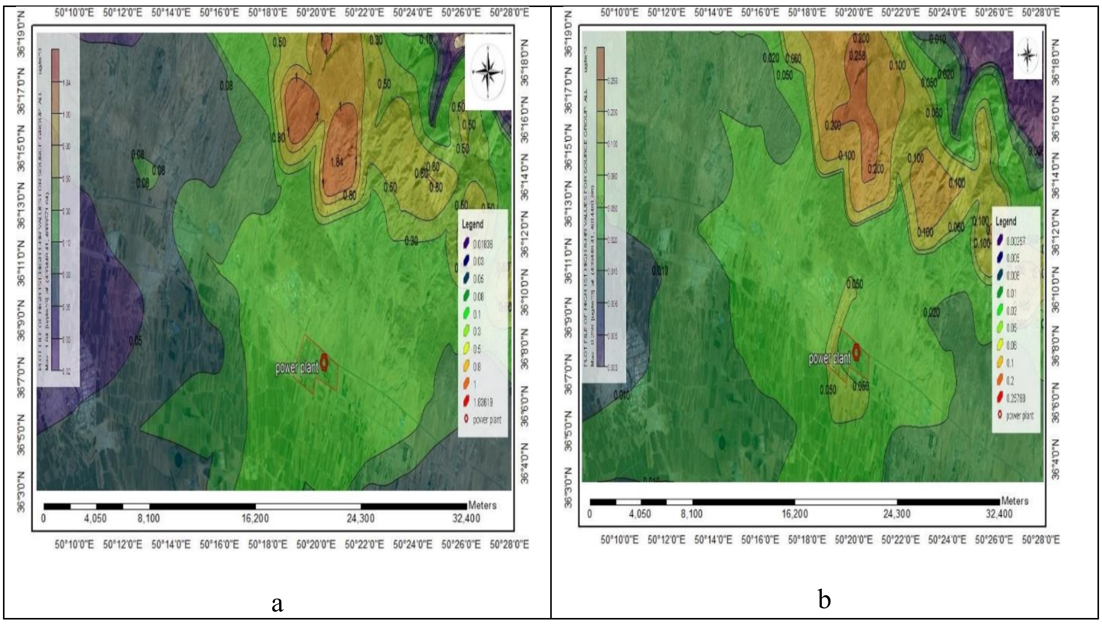

Figure 5. Illustrates the dispersion of PM2.5 particle concentrations over different time periods: a- 1-hour, b- 8-hour.

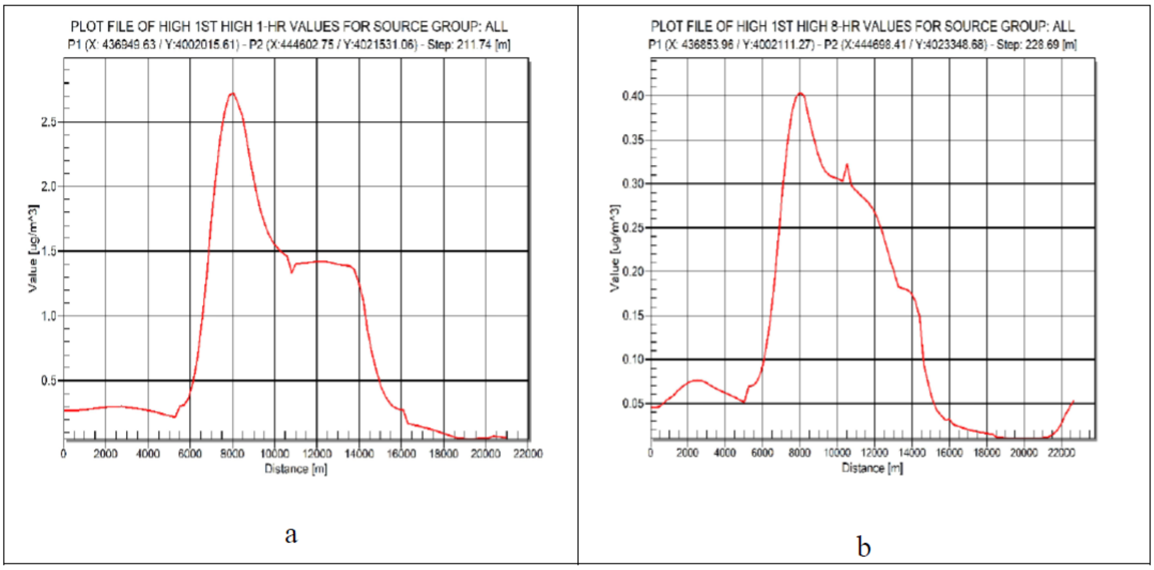

Figure 6. Diagram illustrates the variations in PM2.5 particle concentrations relative to the distance from the power plant's chimney: (a) 1-hour, (b) 8-hour.

and PM10 particles in the study area are measured in μg/m^3. The coordinates for these predictions in the study area are X=437808 and Y=4001423.

Based on figure 7, the dispersion of PM2.5 particles from the power plant's chimney, extending up to a 25-km radius as modeled using AERMOD, reveals the following key findings:

a. **1-Hour PM2.5 Concentrations:** The minimum concentration within approximately 6 km from the chimney is less than 0.5 μg/m^3, while the maximum concentration, observed at a distance of approximately 8 km from the chimney, is 0.40 μg/m^3.

b. **8-Hour PM2.5 Concentrations:** The minimum concentration within about 1 km from the chimney is 0.5 μg/m^3, whereas the maximum concentration, found at a distance of approximately 8 km from the chimney, exceeds 2.5 μg/m^3.

c. **Annual PM2.5 Concentrations:** The minimum concentration, recorded around 6 km from the chimney, is less than 0.002 μg/m^3. The maximum concentration, found at approximately 13 km from the chimney, exceeds 0.020 μg/m^3.

Based on figure 8 the dispersion of PM10 particles from the power plant's chimney, extending up to a 25-km radius, as modeled using AERMOD, reveals the following findings:

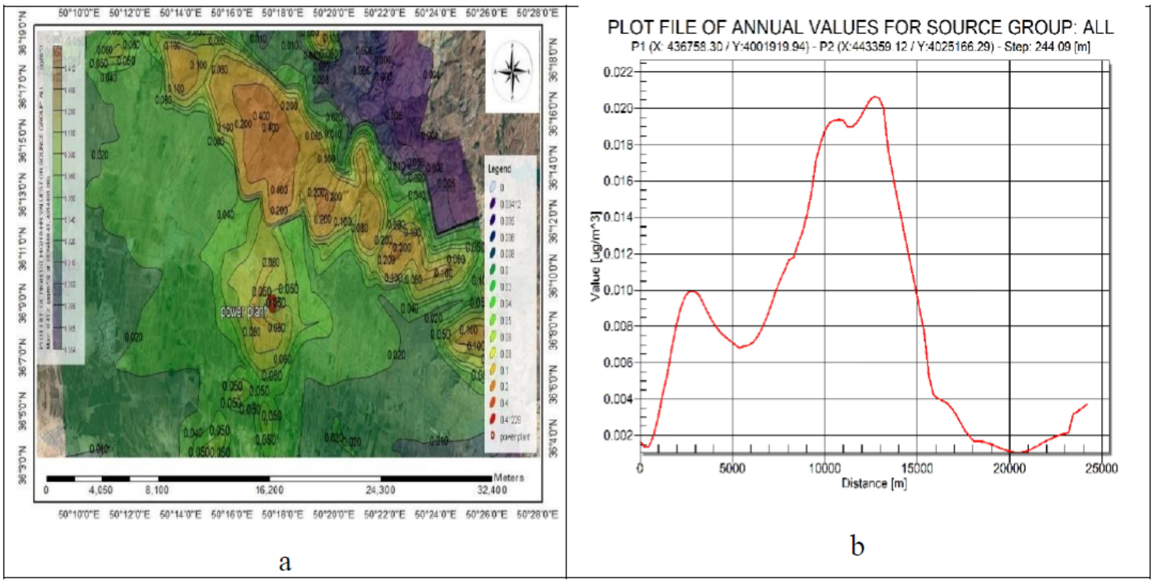

Figure 7. a: Illustrates the dispersion of PM 2.5 particle concentrations annual averages, b: Diagram illustrates the variations in PM 2.5 particle concentrations relative to the distance from the power plant's chimney annual averages.

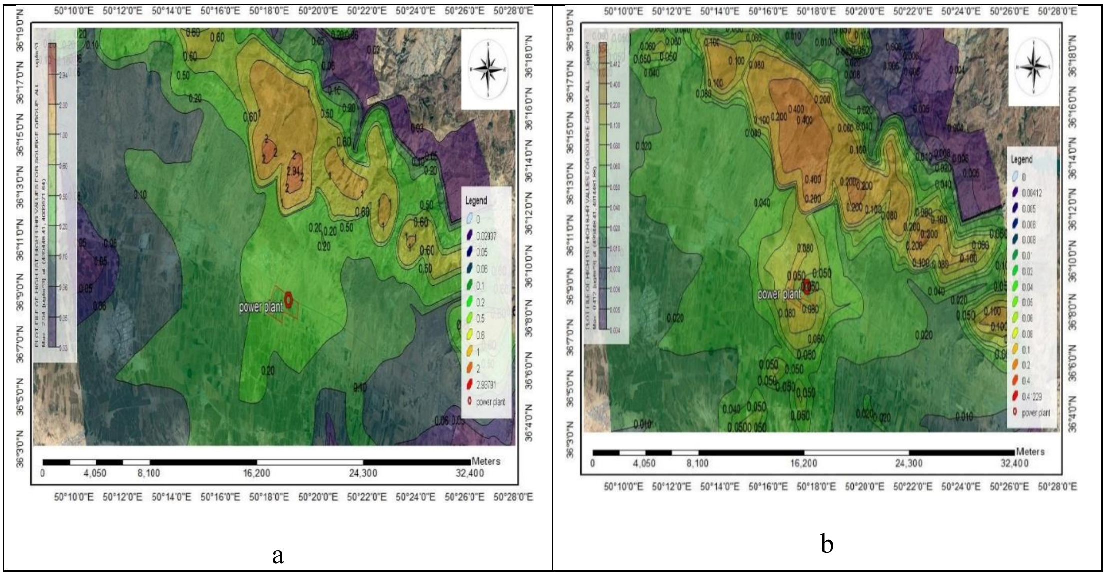

Figure 8. Shows the dispersion patterns of PM10 particle concentrations over different time periods: (a) 1-hour, (b) 8-hour, and (c) annual averages.

a. **1-Hour PM10 Concentrations:** The minimum concentration, observed at approximately 5 km from the chimney, is less than 0.2 μg/m^3. The maximum concentration, found about 9 km from the chimney, exceeds 1.1 μg/m^3.

b. **8-Hour PM10 Concentrations:** The minimum concentration, observed at less than 5 km from the chimney, is greater than 0.20 μg/m^3. The maximum concentration, found about 13 km from the chimney, exceeds 0.22 μg/m^3.

c. **Annual PM10 Concentrations:** The minimum concentration, observed at approximately 5 km from the chimney, is less than 0.004 μg/m^3. The maximum concentration, found about 13 km from the chimney, exceeds 0.014 μg/m^3.

The concentration of PM 2.5 particles shows the correlation between predicted values and actual soil measurements. The concentration of PM 2.5 was compared at different sampling points up to a radius of 25 km from the power plant and areas with higher or lower levels of suspended particles were highlighted. PM10 particle concentrations similar to PM 2.5, validation results for PM10 provide insights into the accuracy of dispersion modeling relative to actual soil pollution levels. This information helps to evaluate the effectiveness of emission control measures and identify high-impact areas. Determining the dispersion and emission of particles throughout the year provides a comprehensive view of long-term exposure and environmental effects. By comparing the annual data in this study, the seasonal changes and the long-term trend of pollution were determined in the area with the highest density of the pollution load. This pattern in the research conducted by Kholodovetal (2020) shows a suitable match in comparing the soil pollution around the power plant with the state of air pollution at similar distances. Significance is obtained figure 7 and Table 6 provide a detailed view of how soil pollution is related to the dispersion of airborne particles, which helps to evaluate and control methods of pollution and reduce environmental effects. Based on figures 5 and 6 as well as Tables 2, 3 and 6, the comparison of the obtained results with the permissible limits of particle pollution showed that the maximum concentration for 1-hour, 8-hour and annual averages is more than the standard and within the range and distances 8 to 14 km from the power plant, the concentration of elements in the soil is higher than the international standard and the soil sample. And in the areas where the prevailing wind is in that direction, the concentration of pollution increases, and the north and northeast areas are affected by this issue.

4. Conclusions

This study was conducted in order to identify the distribution model of suspended particles and potentially toxic elements around the power plant and how the pollution spreads in the surrounding lands. The following are the main results of the research:

1. The pattern of pollution in the air is directly related to the type of fuel, the compounds coming out of the power plant, the height of the chimney, and the weather conditions are influential in the distribution model, and therefore, the concentration of pollution is more based on the prevailing wind in the region in the north and northeast of the power plant.

2. Within the distance of 25 km from the emission source of the power plant, the trend of increasing pollution with the distance from the power plant is not decreasing, but within the limit of 8 to 14 km, based on the graphs obtained from the AERMOD model, the concentration of compounds and elements increases and

shows the most pollution. This model can follow this model in other power plants according to the prevailing wind condition and chimney height. The maximum concentration of 1-hour, 8-hour and annual suspended particles in the above intervals is more than the standard.

3. Sampling of the surface soil (20 cm deep) based on a regular grid and its analysis shows that the concentration of toxic elements such as zinc, vanadium, nickel and copper is higher than the international standards and ground soil. And molybdenum, cobalt, lead and chromium elements have less acoustic risk. And in general, the type of soil pollution also indicates the man-made factors related to the power plant activity.
4. The comparison of the results obtained from AERMOD model in the air and the deposition of suspended particles and compounds in the soil confirms the trend of increasing the concentration of elements in the soil and the range of increasing air pollution, and the pollution zoning obtained in the lands around the power plant has a significant similarity with the concentration There is pollution in the air, and therefore, to identify areas with pollution from man-made sources, such as power plants and chimneys of large industrial units, the mixture used in this research will have favorable validity.
5. One of the limitations of the research is topographical conditions and neighboring mountains and other polluting sources such as agricultural industries and road transportation, which in most cases should be determined and corrected.

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Authors Contributions

Authors have contributed equally to prepare the paper.

Availability of Data and Materials

All data generated or analysed during this study are available from the corresponding author upon reasonable request.

Conflict of Interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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