ANALYSIS OF POLLUTION DUE TO HEAVY METALS: MATHEMATICAL MODELLING TO FIND THE SOURCE OF POLLUTION

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Abstract:

This study investigates heavy metal pollution in urban soils using mathematical modelling to identify sources of contamination. Soil samples from five functional regions—industrial, residential, traffic, forest, and mountain—were analysed for eight heavy metals. Spatial distribution was assessed using biharmonic spline interpolation, while pollution levels were evaluated through the Geo-accumulation index. Pearson correlation analysis identified relationships among metals, and the Gaussian diffusion model was applied to trace pollution sources. Results show that industrial and traffic areas exhibit the highest contamination, with mercury, copper, and zinc being the major contributors. The findings highlight the role of industrial emissions and vehicular activities in heavy metal pollution, offering a scientific basis for urban environmental management.

Keywords:

Heavy metal pollution, Soil contamination, Geo-accumulation index, Biharmonic spline interpolation, Gaussian diffusion model, Pearson correlation, Urban environment, Source identification

1. Introduction:

Urbanization and industrialization have intensified due to the rapid rise of the urban economy and population. Humans are willing to sacrifice the environment for better advancements. These days, human activity significantly degrades the quality of the urban environment, particularly the topsoil. According to studies on inorganic soil pollution, one of the most important elements affecting human survival is heavy metal poisoning. More precisely, India's gross area of land with excessive levels of heavy metals has risen to over 50 million acres and continues to rise. Human health is harmed by heavy metal pollution, which is hard to control. These pollutants in soil can be broken down into methyl compounds by microorganisms. The breakdown products have considerable toxicity that inhibits cells division. It will enter the food chain after being absorbed by crops. In the end, people's health will be at risk due to the metallic elements they consume. Therefore, determining the cause of metal pollution in various urban areas can be aided by evaluating the level of heavy metal pollution and locating the source of pollution. Additionally, the survey's findings will draw in more residents and serve as the foundation for the governance plan.

The amount of soil has a big influence on industrial, agricultural, and human health. A precise measurement of the pollution level can offer a logical guideline for maximizing land use efficiency. The Nemerov index and the single factor index are currently widely used techniques for dividing contamination levels and calculating environmental pollution indices. The significance of extreme value may be emphasized using the Nemerov index, which is an expansion of the single factor index. Several environmental impact elements are weighted using this strategy without affecting individuals. This technique evaluated the overall soil nutrients in the eucalyptus plantation of the state-owned Gir Forest Farm in Gujrat in 2021. There are various elements that contribute to the nutrient demand of trees. The overall fertility level of forest soil is assessed using these impact parameters. Additionally, the negative effect of trees' nutrient requirement is avoided with this strategy. The outcome has turned into a standard for applying fertilizer in forest production. The comprehensive pollution status of heavy metals can be obtained by evaluating soil pollution using the Nemerov index. However, the Nemerov Index ignores the variations in the effects of various pollutants, even if it takes into account the effects of the most serious pollution variables.

The single factor index and the Nemerov index approaches do not appear to be suitable for determining the level of pollution in various locations since the toxicity of metals in the soil is also correlated with the species and attributes. The accumulation index approach was used to determine the level of heavy metal contamination in the soil. This technique was developed by Muller in the 1960s to quantitatively evaluate the amount of heavy metal contamination in sediments and the related pollution state categorization criteria. The accumulation index is a suitable method for classifying and evaluating the level of heavy metal contamination in soil.

The source of pollution can be identified in a variety of ways. In recent years, scientists have combined statistics and mathematics to study environmental issues. Spearman introduced the factor analysis approach, which is a very effective way to confirm the source of contaminants.

To quantify the link between several variables, the factor analysis method was created, which simplifies data by converting different factors into a few linear independence indicators. Nevertheless, it is frequently impossible to observe the linear composite index precisely. The conventional technique for identifying the cause of heavy metal pollution is the multivariate statistic. Principal component analysis, a technique for reducing data dimensions, is one of them. A new composite indicator can be produced in this manner. Analysing the source of pollution may be based on the principal component score obtained from this indicator. Principal component analysis, however, is merely a statistical technique and cannot identify the exact source of contaminants. Furthermore, in order to get complex results, the analyst need a large amount of sample data, which is inappropriate for a quantitative assessment of source contribution.

The Gauss diffusion model can be applied to the problem of identifying the source of heavy metal pollution. The model has a number of relevant conditions. First of all, the wind direction is flat and the wind speed is constant across the tested area. Second, pollutant dispersal complies with mass conservation. Lastly, the pollutant source's source strength is consistent and constant. This approach is appropriate for identifying the origins of heavy metal pollution based on the propagation characteristics of the pollutants. Urban areas are separated into residential, commercial, mountainous, traffic, and forest zones based on the functional segmentation. The reasons of contamination can be identified by assessing the level of heavy metals in the soil in these five areas and identifying the pollution source. The contamination levels in this study are calculated using the Geo-accumulation index. Maps showing the pollution distribution of the eight main heavy metal components in each location provide a general idea of the contamination status. In order to determine the location of the pollution source, a model is finally validated based on the propagation characteristics of heavy metal pollutants.

2. Methodology

Human-caused environmental degradation is intensifying as the urban economy grows and the population grows. The geological environment of a town's soil is examined in this research. The concentration of eight metals in the sample sites will then be determined after 319 sampling sites have been chosen. Furthermore, environmental samples from remote natural places will be assessed. The measurement results can be thought of as the baseline levels of Application of Mathematical approach in The Study of Heavy Metal Ions – Soil Interactions eight heavy metals in the urban area's surface soil.

It is possible to determine the level of pollution and the source of heavy metals in various parts of the town by using mathematical models to assess the spatial distribution. Next, locate the source of the contamination.

2.2 Biharmonic Interpolation:

There is a continuous geographical distribution of metal. The metal concentration varies with the terrain's elevation. The measured samples, however, are spatially distinct. Consequently, suitable data interpolation should be carried out for the data-free position points. One technique for interpolating Application of Mathematical approach in The Study of Heavy Metal Ions – Soil Interactions the data is biharmonic spline interpolation. The influence function or point source function are other names for the green function. Differential equations with boundary conditions are solved using it. Furthermore, the procedure of solving a biharmonic equation using the green function is known as biharmonic spline interpolation.

By choosing a collection of irregular spatial data points, the cubic spline function can be used to determine the smoothest curve or surface. From a mechanical point of view, the approach is to force an elastic rod to match each data point. An elastic rod subjected to a vertical force $\delta(X — X$j) in point Xj, j = 1,2,. .. is for each elastic rod point. It is calculated how much an elastic thin rod will bend when subjected to focused force in a variety of locations. The function of displacement *g(x)* of harmonic equation is as follows:

$$\nabla^4 g(x - x_j) = 6\delta(x - x_j) \quad \text{……………………..(1)}$$

For eq. (5.1), the particular solution is:

$$g(x - x_j) = |x - x_j|^3 \quad \text{……………………….(2)}$$

On interpolating the all-data points w_j at x_j, the biharmonic eq. will be as follows:

$$\nabla^4 w(x) = \sum_{j=1}^{N} \quad 6\delta a_j(x - x_j) \quad \text{………………..(3)}$$

$$w(x_j) = w_j \quad \text{……………………………(4)}$$

$w(x)$ is the particular solution of equations (3) and (4), which can given as a linear combination of green's function of pressure at every point:

$$w(x) = \sum_{j=1}^{N} \quad \delta a_j(x - x_j) = \sum_{j=1}^{N} \quad a_j|x - x_j|^3 \quad \text{……………………(5)}$$

In this equation coefficient a_j will be procured by solving the linear equations:

$$w_j = \sum_{j=1}^{N} \quad a_j|x - x_j|^3, \; i = 1,2,3 \ldots\ldots N \quad \text{………………………..(6)}$$

Equation (5) can be used to calculate the value of the interpolation function $w(x)$ at any moment once aj has been established.

This technique can create topographic maps of the areas under study and interpolate discrete sample data. The eight heavy metals' geographical distribution characteristics can then be acquired.

2.3 Geo-accumulation index:

Muller first developed the geological accumulation index in the 1970s, based on research on heavy metal contamination in sediments. This index measures the level of heavy metal pollution in sediments or other materials and is written as Igeo, where geo is the word for geography. Later, it was used to evaluate soil heavy metal pollution by soil scientists both domestically and overseas. This approach takes into account how both natural geological processes and human activity affect the background value. Additionally, the impact of human activity on the environment and the natural variation of heavy metal distribution can be obtained.

The scope of applicability includes both single-element and multi-element comprehensive evaluations. The magnitude of I_{geo}, a quantitative indicator used to investigate heavy metal contamination in water environments, is used to quantify the level of pollution in the single element evaluation. By computing the correlation between the observed value and its reference value, it is also frequently used to determine the level of contamination of a single element. MATLAB calculates the index. The severity of soil pollution increases with I_{geo}'s size. In the entire evaluation procedure, the "from inferior to superior" approach is typically used to calculate the soil contamination grade. The comprehensive pollution grade of the sampling site is defined as the pollution grade that corresponds to the most widespread geological accumulation index of each heavy metal element. Muller provided the following formula to calculate the geological accumulation index:

$$I_{geo} = log_2^{\frac{C_i}{\propto B_i}} \text{ .... (7)}$$

Where:

C_i : is evaluated value of element i from the sample points

B_i : is the background value of element i from the sample points

$\propto$: this is an index value due to differences in rocks which eliminates the variations in the background values

It is possible to determine the sample's Person correlation coefficient by evaluating its covariance and standard deviation. This is typically shown by

$$r = \frac{\sum_{i=1}^{n}(X_i - \underline{X})(Y_i - \underline{Y})}{\sqrt{\sum_{i=1}^{n}(X_i - \underline{X})^2}\sqrt{\sum_{i=1}^{n}(Y_i - \underline{Y})^2}} \text{ ....(9)}$$

By computing the Person correlation coefficients of eight heavy metal types in various geographical locations, the correlation can be found. The likelihood that two metals are homologous increases with their degree of relatedness. In order to assess the causes of pollution, homologous metal contaminants might be grouped into a single category.

2.4 Gauss Diffusion Method:

The pollution content of spatial point sources is determined using the Gauss diffusion model, which has the following equation:

$$C(x,y,z) = \frac{Q}{2\pi\mu\sigma_y\sigma_z} exp\left[-\frac{1}{2}(\frac{y^2}{\sigma_y{}^2} + \frac{z^2}{\sigma_z{}^2})\right] \text{..........................(10)}$$

The pollution concentration (mg/m3) in the space points (x, y, z) is represented by C in formula (4). The pollutant discharge (mg/s) per unit of time is denoted by Q. The average wind speed (m/s) is denoted by μ. Flue gas diffusion coefficients are denoted by σ_y and σ_z. These two factors have to do with the horizontal distance and atmospheric stability.

This article examines the heavy metal content on the soil surface, whereas formula (5.4) indicates the pollutant concentration in the air. The following is the derivation of the formula:

$$C(x,y,z) = \frac{A}{\sigma_y\sigma_z} exp\left[-\frac{1}{2}(\frac{y^2}{\sigma_y{}^2} + \frac{z^2}{\sigma_z{}^2})\right] \text{..................................(11)}$$

Pollutant concentration transmission is not thought to be influenced by atmospheric environment factors like wind speed. Therefore, a constant coefficient A is created by combining the elements associated to this in formula (5.10). The source point is set to the origin by default in the Gaussian diffusion equation. Assume, therefore, that (x_{0i}, y_{0i}, z_{0i}) is the coordinate of the heavy metal *i* pollution source. The following formula is obtained via coordinate translation:

$$C(x - x_{0i}, y - y_{0i}, z - z_{0i})$$

$$= \frac{A}{\sigma_y\sigma_z} exp\left[-\frac{1}{2}(\frac{(y-y_{0i})^2}{\sigma_y{}^2} + \frac{(z-z_{0i})^2}{\sigma_z{}^2})\right] \text{...........................(12)}$$

Where,

$\sigma_y = 0.229x^{0.9193}$ and $\sigma_z = 0.114x^{0.9410}$

3. Discussion and result:

In this article, the measured data is interpolated using biharmonic spline interpolation. Next, create a sampling point distribution map and a three-dimensional topographic map using the interpolation data. The spatial distribution of heavy metals in different city areas is intuitively depicted by the graphs. Additionally, the Index of Geo-accumulation can be used to assess the level of heavy metal contamination in soil. Pearson correlation analysis of the data is used in the study to determine the correlation between various metals. Metals with the precise source of contamination can thus be located. This article then uses the Gauss diffusion model to analyse the location of the pollution source.

3.1 selected area with its topography and the pollution extension:

The geography and environmental circumstances of the area will affect the concentration of pollutants in the soil, which have a tendency to flow. Therefore, in order to examine the concentration of pollutants, it is important to view the topography of the study region. This is how the topographic map appears:

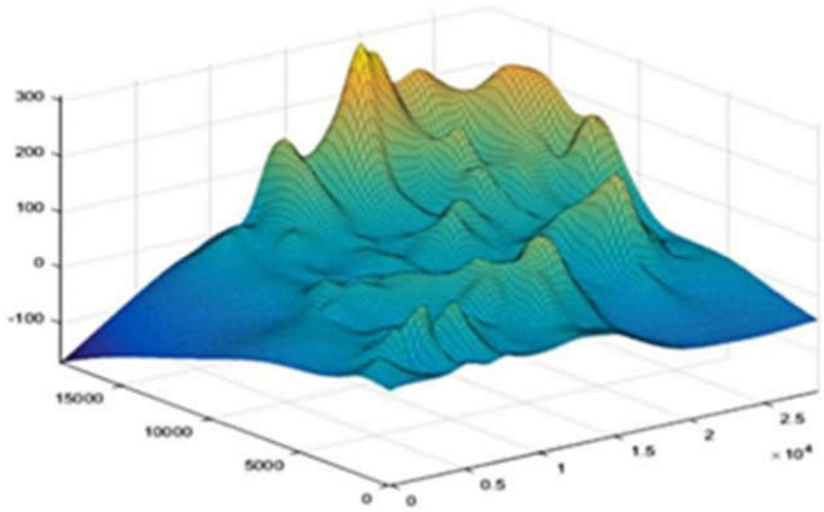

Fig. 1: Topographic map

The sample data can be interpolated using the Triangulation method using Linear Interpolation. Following that, maps will be created using the acquired data. The northeast corner of the area has higher ground, as seen in Figure (1). Additionally, the southwest corner has lower ground. As a result, metal contamination levels may move from higher to lower elevations. Because to different interpolation, the ground levels in the northwest and southeast corners are less than 0 meters above sea level.

Samples are collected from the five areas that make up the region: the dwelling area, the industrial area, the mountain area, the traffic area, and the forest area. The graphic below displays the distribution contour lines of the sampling points:

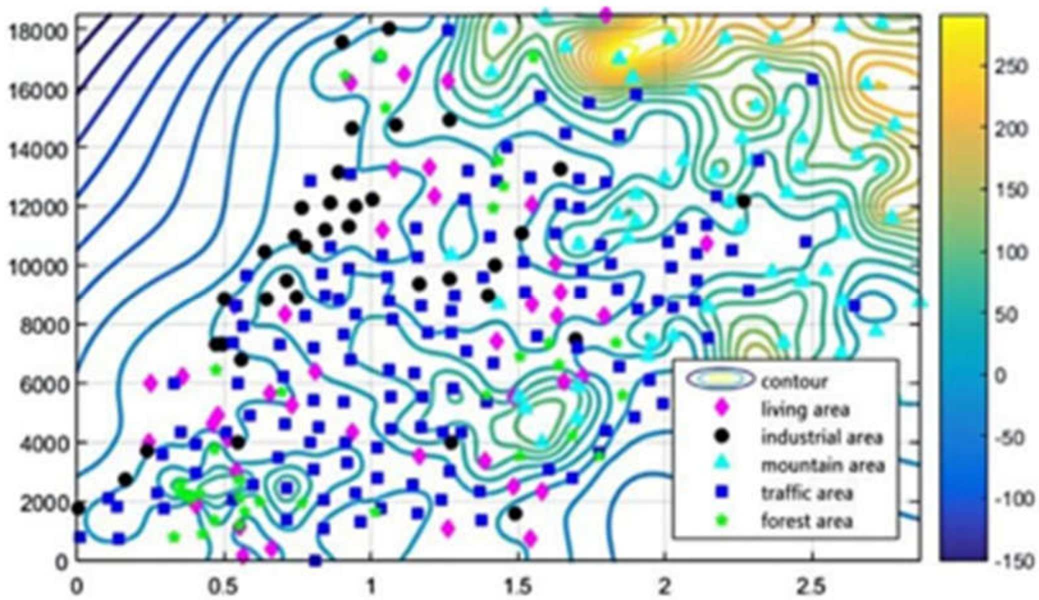

Fig. 2: Contour map

The uniform distribution of sample points in Figure (2) suggests that the experimental setup is appropriate. Additionally, the residential districts are dotted with traffic and industrial zones. The northeast corner is dominated by mountains, whereas the southwest part is dominated by forests.

Each of the eight elements' iso-concentration lines is depicted separately, and the pictures show how unevenly distributed they are.

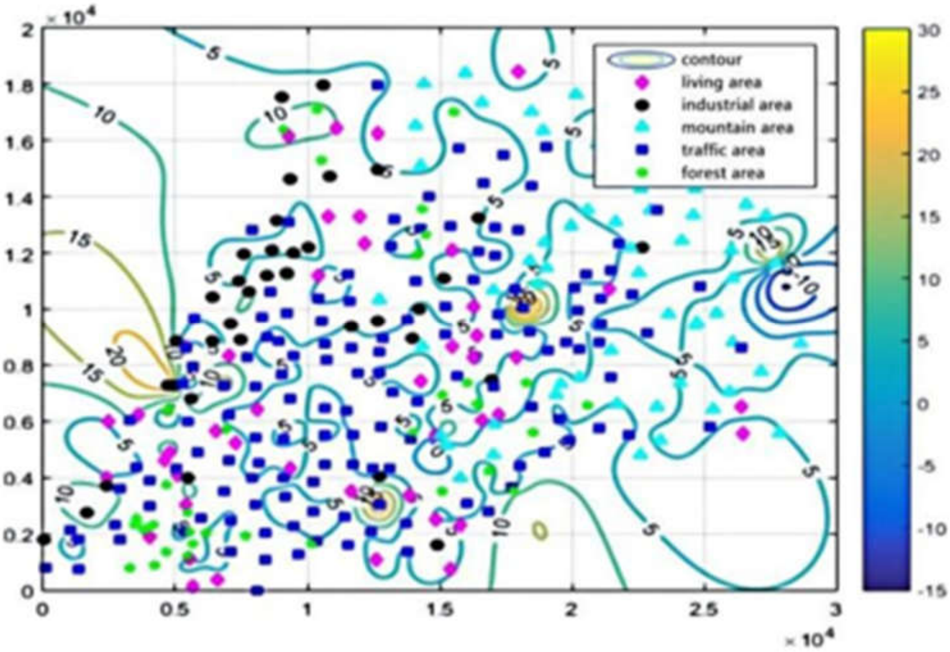

Fig. 3: ‘As’ concentration contour

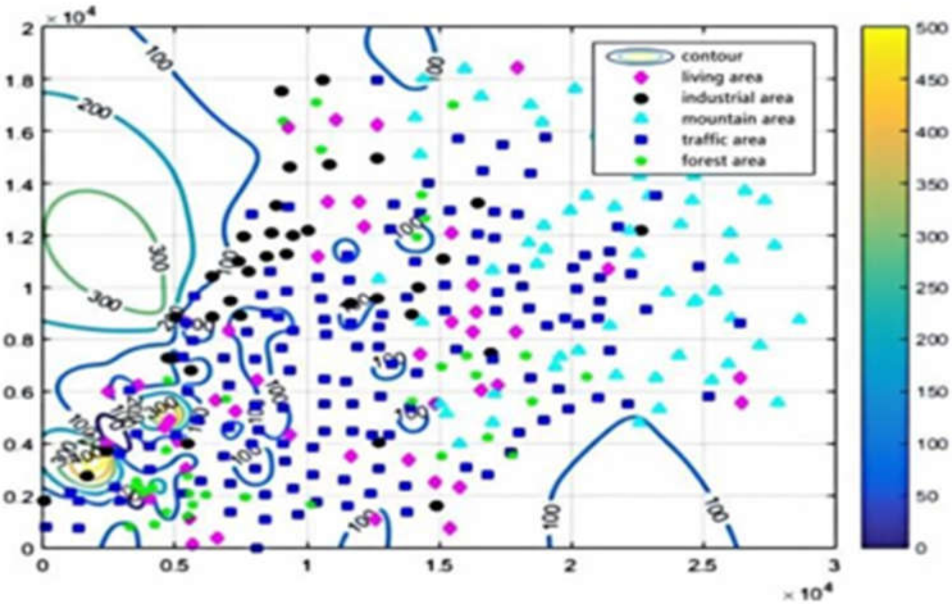

Fig. 4: ‘Pb’ concentration contour

It is evident from comparing the concentration diagrams for Figures (3) and (4) that the metal ‘As’ is most broadly distributed, with the largest concentrations of the metal ‘As’ primarily found in traffic areas. With the exception of the northeast, CD is widely disseminated around the world. Additionally, the concentration contour maps for Cr, Cu, and Ni are comparable, and their distribution range is narrow, primarily centred in the southwest. Additionally, the southwest is where the majority of Hg, Pb, and Zn are found, while the middle of the map shows the aggregation distribution of Hg and Zn.

3.2 Pollution determining degree:

In the following table, heavy metals index of land accumulation is given.

Area	Pb	Cu	Zn	Hg	Ni	Cd	As	Cr
Mountain	0.45	-0.39	-0.59	-0.59	-0.45	-0.52	0.12	0.14
Industrial	0.67	1.37	0.85	1.31	-0.03	0.79	0.21	-0.03
Living	0.23	0.87	0.46	0.19	-0.07	0.33	0.12	0.14
Forest	0.12	0.39	0.05	0.19	-0.33	0.18	0.13	-0.16
Traffic	0.28	1.07	0.62	0.43	-0.18	0.59	-0.05	0.02

Table 1

With the highest pollution index as the area's evaluation result, the five regions' respective indices are 0.876, 1.377, -0.395, 1.074, and 0.395. Table 1 indicates that there is no pollution in mountainous regions, minimal pollution in residential and woodland regions, and substantial pollution in places with traffic and industry.

According to table 3's index figure, the three elements that contribute most to pollution in this urban region are mercury, copper, and zinc. Fuel combustion, smelting, and waste incineration are the primary sources of mercury pollution. This metal also finds its way into the soil through household trash, herbicides, fertilization, and other means. The production of steel, machinery, copper and zinc ore mining and smelting, and other processes are the main causes of copper pollution. Additionally, emissions from the galvanizing and paper industries, as well as machine manufacture, contribute to zinc pollution. According to the data above, industrial and vehicle exhaust emissions are the main sources of heavy metal pollution in this urban region.

3.3 heavy metals and their correlation:

The following are the findings of the Person correlation analysis that was performed on eight heavy metal pollutants:

Metal	Pb	Cu	Zn	Hg	Ni	Cd	As	Cr
Pb	1.1	0.35	0.19	0.6	0.07	0.32	0.29	0.25
Cu	0.26	0.1	0.36	0.40	0.27	0.33	0.67	0.44
Zn	0.19	0.36	1.1	0.54	0.11	0.72	0.39	0.43
Hg	0.16	0.41	0.54	1.12	0.42	0.51	0.53	0.39
Ni	0.9	0.24	0.15	0.43	1.14	0.12	0.30	0.21
Cd	0.07	0.27	0.13	0.42	1.16	0.11	0.31	0.28
As	0.24	0.47	0.49	0.39	0.22	0.47	0.52	0.26
Cr	0.29	0.67	0.39	0.58	0.32	0.33	0.47	0.58

Table: 2

In Table 4, the Person correlation coefficient between Pb and Cd, Ni, and Cr is greater than 0.6. The two metal groups most likely originated from the same contamination source. The main anthropogenic sources of Cd and Pb have been found to include coal, fuel burning, non-ferrous metal smelting, and ore mining, all of which are most likely to occur in industrial locations. Ni and Cr buildup in soil is more likely to result from the use of inorganic phosphorus, and the sources of pollution are most likely to be found in forested areas.

3.4 Detection of pollution sources:

The following is the outcome of solving the improved Gaussian diffusion equation with the data in Formula (6):

Heavy metal	K	□□	□□	□□
As	31	-21746	1.5	17
Cr	41	-354435	3.4	41
Cd	67	-55785	5.2	3
Cu	71	-74689	-7.4	12
Hg	14	-14879	-6.1	47
Ni	41	-66214	3.4	7
Pb	47	-73741	5.1	24
Zn	79	-21497	1.8	3

Table 3: Fitting coefficients using formula (6)

The fitted equation was subsequently solved using the least-squares approach, yielding the eight metals' sources of contamination. The table below displays the findings:

Heavy metal	□□	□□	□□
As	13542	10043	80
Cr	25542	11346	6043
Cd	21123	11493	48
Cu	2443	3565	10
Hg	2880	3001	5
Ni	3394	6010	5910
Pb	1842	2973	8
Zn	9442	4322	5024

Table: 4

4. Conclusion:

The region was split up into five functional regions for this investigation, and sample points were chosen at random from each region. The sampling spots were visualized, the rough distribution rules of eight metals were derived, and the rule that the topography in this area steadily decreases from east to west was derived. Additionally, the cumulative index approach is used to evaluate the pollution level of various functional sectors, and the results show that the highest pollution levels are found in low-lying traffic and industrial regions. The location of each source of metal contamination is then determined using the least squares method once the Gaussian diffusion model has been refined. The majority of metal pollution sources are located in the low-lying middle region as a result of industrial pollution and atmospheric pollution factor precipitation.

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