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Pollution of Heavy Metal in Soils by Fuzzy Analytic Method and Determine the Location of Pollution Sources

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Abstract With the city's rapid economic development and increasing of the population, urban environmental quality has been greatly affected. In this article, all the data are from 2011 National Mathematical Modeling Competition. Two problems are researching in this article, such as: 1) treat the data, draw spatial distribution of the eight heavy metal pollution and define the pollution levels of each heavy metal; 2) use fuzzy analytic method to analyze the data, define the membership functions to calculate the fuzzy relationship matrix of each area, combine the concentration of heavy metal pollution with the toxicity index. According to the evaluation model, the results are: living area' pollution is the most seriously, industrial area pollute seriously, mountain area pollute slightly, transportation district pollute seriously, park green area pollute seriously; 3) convection, spread and mechanical dispersion are considered in the soil environment system. Transport mechanism and transport equations in soil about the heavy mental are given. Then analysis the boundary conditions and construct two-dimensional transport model in order to determine the location of pollution sources. Finally, eight pollution sources of the five regions are identified by difference method.

Keywords Heavy metal; Pollution levels; Toxicity index; Fuzzy analytic method; Fuzzy relationship matrix; Soil Solute; Convection; Spread; Mechanical dispersion

1. Introduction

The rapid development of urban economy and the increasing population have an increasing impact on the quality of urban environment. Due to the abnormality of urban soil geological environment, people are paying more and more attention to how to apply the data obtained by verification to carry out urban environmental quality assessment and the evolution pattern of urban geological environment under the influence of human activities. Because different regional environments are affected by human activities, the urban area are divided into living area, industrial area, mountainous area, transportation area and park green area according to different functions. The soil geological environment of a certain urban area is investigated. The area is divided into grid sub-area with a distance of about 1 km. The topsoil is sampled and numbered according to one sampling point per square kilometer, and the position of the sampling points is recorded by GPS. Specialized instrument test analysis is used to obtain concentration data of various chemical elements contained in each sample. The key issues to be solved in this paper are: 1) give the spatial distribution map of 8 major heavy metal elements in the urban area, define the pollution level; 2) analyze relevant data, analyze the problems related to heavy metal pollution; 3) consider the soil environmental system, The migration mechanism and migration equation of heavy metals in soil are given, and the two-dimensional transport model is constructed. The numerical method is used to determine the pollution source.

2. Heavy metal pollution degree distribution map and grade definition

2.1. Spatial distribution map of 8 heavy metals

In order to obtain the spatial distribution of eight heavy metal elements in this region, we analyzed the data in Annex 1 and Annex 2, using the data given in Annex 3 as a standard by Matlab, we we analyze the pollution degree of each heavy metal and draw a map of the pollution degree of heavy metals in the urban area, as shown as figure 1 to 8 (the ordinate is the altitude of the altitude).

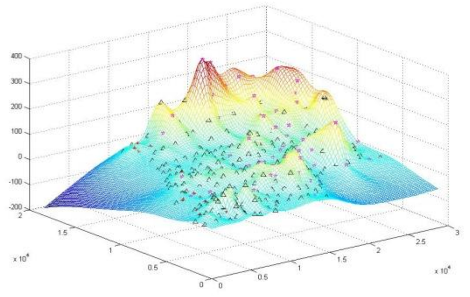

Figure 1: Spatial distribution of As in the city

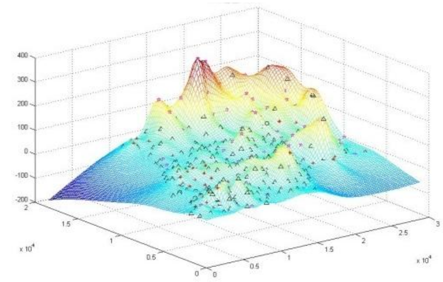

Figure 2: Spatial distribution of Cd in the city

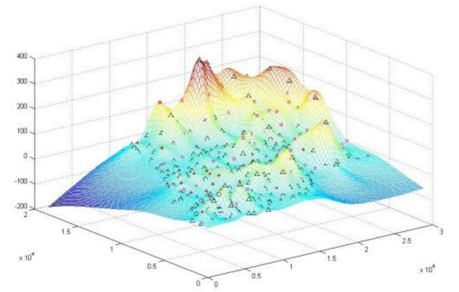

Figure 3: Spatial distribution of Cr in the city

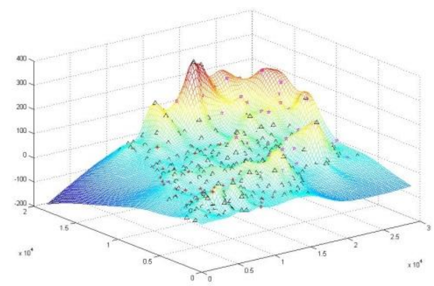

Figure 4: Spatial distribution of Cu in the city

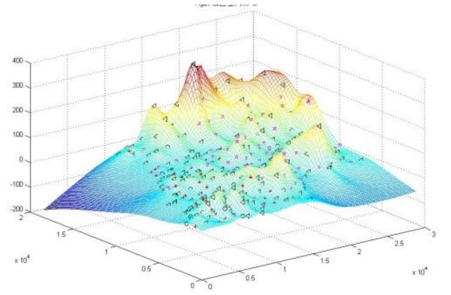

Figure 5: Spatial distribution of Hg in the city

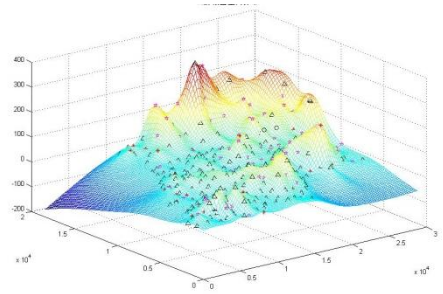

Figure 6: Spatial distribution of Ni in the city

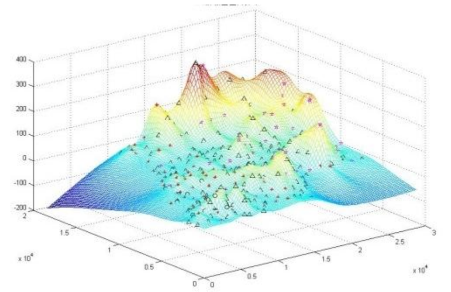

Figure 7: Spatial distribution of Pb in the city

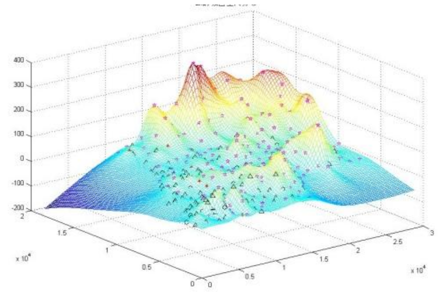

Figure 8: Spatial distribution of Zn in the city

2.2. Definition of pollution levels for 8 heavy metals

The classification of 8 heavy metal elements is based on the ratio of the concentration of 8 heavy metal elements in the urban area to the background value, the level definition is shown in Table 1:

Table 1: Pollution levels of 8 heavy metals

As	Range	[0, 1]	(1, 2.5]	(2.5, 4]	(4, $+\infty$)
	Grade	normal	primary pollution	secondary pollution	tertiary pollution
Cd	Range	[0, 1]	(1, 2]	(2, 4]	(4, $+\infty$)
	Grade	normal	primary pollution	secondary pollution	tertiary pollution

Cr	Range	[0, 1]	(1, 3]	(3, 5]	(5, +∞)
	Grade	normal	primary pollution	secondary pollution	tertiary pollution
Cu	Range	[0, 1]	(1, 5]	(5, 10]	(10, +∞)
	Grade	normal	primary pollution	secondary pollution	tertiary pollution
Hg	Range	[0, 1]	(1, 4]	(4, 10]	(10, +∞)
	Grade	normal	primary pollution	secondary pollution	tertiary pollution
Ni	Range	[0, 1]	(1, 2]	(2, 3]	(3, +∞)
	Grade	normal	primary pollution	secondary pollution	tertiary pollution
Pb	Range	[0, 1]	(1, 2]	(2, 4]	(4, +∞)
	Grade	normal	primary pollution	secondary pollution	tertiary pollution
Zn	Range	[0, 1]	(1, 4]	(4, 10]	(10, +∞)
	Grade	normal	primary pollution	secondary pollution	tertiary pollution

2.3. Pollution levels of 8 heavy metals in five categories

According to the definition of Section 1.2, the pollution levels of eight heavy metals in five regions are shown in Table 2 to 6(unit $\mu g / g$):

Table 2: Pollution level of heavy metals in living area

Elements	**As**	**Cd**	**Cr**	**Cu**	**Hg**	**Ni**	**Pb**	**Zn**
Background values	3.60	0.13	31	13.20	0.04	12.30	31	69
Average value	6.44	0.35	162.44	79.99	0.22	18.94	109.43	627.90
Pollution level	primary	secondary	tertiary	secondary	secondary	primary	secondary	secondary

Table 3: Pollution level of heavy metals in industrial area

Elements	**As**	**Cd**	**Cr**	**Cu**	**Hg**	**Ni**	**Pb**	**Zn**
Background values	3.60	0.13	31	13.20	0.04	12.30	31	69
Average value	9.86	0.38	88.97	280.63	0.72	24.72	130.51	490.59
Pollution level	secondary	secondary	primary	secondary	tertiary	secondary	tertiary	secondary

Table 4: Pollution level of heavy metals in mountainous area

Elements	**As**	**Cd**	**Cr**	**Cu**	**Hg**	**Ni**	**Pb**	**Zn**
Background values	3.60	0.13	31	13.20	0.04	12.30	31	69
Average value	6.01	200.20	82.46	33.79	0.09	28.66	57.04	75.21
Pollution level	primary	primary	primary	primary	primary	secondary	primary	primary

Table 5: Pollution level of heavy metals in traffic area

Elements	**As**	**Cd**	**Cr**	**Cu**	**Hg**	**Ni**	**Pb**	**Zn**
Background values	3.60	0.13	31	13.20	0.04	12.30	31	69
Average value	8.86	0.35	146.32	113.52	1.67	49.32	78.74	555.45
Pollution level	primary	secondary	secondary	secondary	tertiary	tertiary	secondary	secondary

Table 6: Pollution level of heavy metals in park area

Elements	**As**	**Cd**	**Cr**	**Cu**	**Hg**	**Ni**	**Pb**	**Zn**
Background values	3.60	0.13	31	13.20	0.04	12.30	31	69
Average value	6.66	0.38	52.39	62.70	0.41	17.59	80.91	494.04
Pollution level	primary	secondary	primary	primary	tertiary	primary	secondary	secondary

3. Analysis of heavy metal pollution by fuzzy analysis

The fuzzy analytic hierarchy process (F-AHP) is a kind of modeling method that can be easily realized by programming. It has good practicability, can solve the qualitative and quantitative abstraction in the device selection problem well, it can also avoid the difficulty of matrix consistency and the difference between established matrix and human thinking.

The fuzzy mathematics method [1-4] adopted in this paper describes the gradual and fuzzy nature of heavy metal pollution in soil by membership degree, makes the evaluation result more accurate and reliable. The key issue in applying fuzzy mathematics to pollution assessment is how to determine the weight of each indicator. The dual weighting factor combines the concentration of pollution with the toxicity index to find the optimal weight for each indicator. This method can increase the resolution and accuracy of the evaluation results.

3.1. Evaluation model

The fuzzy comprehensive method uses the membership to describe the fuzzy pollution classification boundary. The membership of each evaluation level is corrected by the weight of each evaluation factor, and the membership of the evaluation sample to the evaluation level is obtained. Let A be the membership degree of each evaluation factor to the evaluation level, R be the weight vector of each evaluation factor, and B be the membership degree of the evaluation sample to the evaluation level. The mathematical model is:

$$B = R \bullet A \tag{1}$$

3.2. Establishment of evaluation factor membership function and fuzzy relation matrix

In order to perform the fuzzy operation, membership function should be determined, and describe the fuzzy boundary of soil pollution status by membership degree. If the soil environmental quality is divided into m levels, then $V = (1, 2, ..., m)$. In this paper, the membership degree is characterized by a semi-trapezoidal distribution:

$$X_{ij} = \begin{cases} 1 & X \le S_{ij} \\ (S_{ij+1} - X)/(S_{ij+1} - S_{ij}) & S_{ij} \le X \le S_{ij+1} \\ 0 & X \ge S_{ij+1} \end{cases} \tag{2}$$

In the formula X_{ij} ------ the membership of the pollution factor;

S_{ij} ------ a sample pollution factor i in the $j-level$ indicator;

X ------ the measured concentration of the pollution factor.

Then the evaluation factor, that is membership matrix of index i for level j is:

$$A = \begin{bmatrix} X_{11} & \dots & X_{1m} \\ \dots & & \dots \\ X_{n1} & \dots & X_{nm} \end{bmatrix} \tag{3}$$

3.3. Determination of evaluation factor weight vector R

The current heavy metal pollution assessment method often uses **the pollutant concentration exceeding the standard weighting methods.** For different heavy metals, because the pollutants have different levels of toxicity, the pollutant concentration exceeding the standard weighting method may mask the toxicity of some low-concentration organic components. Therefore, it is necessary to consider the toxicity level of heavy metals as a weight to reflect the combined effects of heavy metal concentration and toxicity. Weighted and superimposed the contaminant concentration and toxicity level index, and normalized. The weight formula is as follows:

$$r_i = \frac{C_i}{f_i} / \sum_{i=1}^{n} \frac{C_i}{f_i}$$

$$C_i = \frac{x_{ij}}{\sum_{j=1}^{m} S_{ij}} / \sum_{i=1}^{n} \frac{x_{ij}}{\sum_{j=1}^{m} S_{ij}} \tag{4}$$

In the formula x_i ------ the measured concentration of the $i-th$ pollution factor of the sample, ng/g or $\mu g/g$;

f_i ------ the toxicity level index of the $i-th$ pollution factor;

R_i ------ the weight value of the $i-th$ pollution factor of the sample, and $\sum_{i=1}^{n} C_i = 1, \sum_{i=1}^{n} r_i = 1$。

Substituting the measured concentration values, toxicity indices and selected evaluation criteria of each pollution factor into the formula (4), the weight value of each pollution factor can be calculated, thus, the weight vector r of each participating factor of a sample is obtained: $R = [r_1, r_2, \cdots, r_n]$, Similarly, weight vectors for each of the participating factors of other samples are available.

3.4. Establishment and evaluation of fuzzy comprehensive evaluation model

Substituting the weight vector R and the membership vector A into the formula (1), according to the principle of maximum membership, the pollution level of the sample can be determined.

3.5. Determination of fuzzy relation matrix

living area: $A_1 = \begin{bmatrix} 0 & 0.974 & 0.026 & 0 \\ 0 & 0.205 & 0.795 & 0 \\ 0 & 0 & 0 & 1.00 \\ 0 & 0.320 & 0.680 & 0 \\ 0 & 0.159 & 0.841 & 0 \\ 0 & 0.960 & 0.040 & 0 \\ 0 & 0 & 0.470 & 0.530 \\ 0 & 0 & 0.300 & 0.700 \end{bmatrix}$; industrial area: $A_2 = \begin{bmatrix} 0 & 0.341 & 0.659 & 0 \\ 0 & 0.051 & 0.949 & 0 \\ 0 & 0.565 & 0.435 & 0 \\ 0 & 0 & 0 & 1.000 \\ 0 & 0 & 0 & 1.000 \\ 0 & 0.490 & 0.510 & 0 \\ 0 & 0 & 0 & 1.000 \\ 0 & 0 & 0.963 & 0.037 \end{bmatrix}$

mountain area: $A_3 = \begin{bmatrix} 0.107 & 0.893 & 0 & 0 \\ 0 & 0.974 & 0.026 & 0 \\ 0 & 0.670 & 0.330 & 0 \\ 0.220 & 0.780 & 0 & 0 \\ 0 & 0.984 & 0.016 & 0 \\ 0 & 0.170 & 0.830 & 0 \\ 0 & 0.773 & 0.227 & 0 \\ 0.940 & 0.060 & 0 & 0 \end{bmatrix}$; traffic area: $A_4 = \begin{bmatrix} 0 & 0.526 & 0.474 & 0 \\ 0 & 0.205 & 0.795 & 0 \\ 0 & 0 & 0.280 & 0.720 \\ 0 & 0 & 0.560 & 0.440 \\ 0 & 0 & 0 & 1.000 \\ 0 & 0 & 0 & 1.000 \\ 0 & 0.307 & 0.793 & 0 \\ 0 & 0 & 0.650 & 0.350 \end{bmatrix}$

park area: $A_5 = \begin{bmatrix} 0 & 0.933 & 0.067 & 0 \\ 0 & 0.051 & 0.949 & 0 \\ 0.310 & 0.690 & 0 & 0 \\ 0 & 0.611 & 0.389 & 0 \\ 0 & 0 & 0 & 1.000 \\ 0.140 & 0.860 & 0 & 0 \\ 0 & 0.260 & 0.740 & 0 \\ 0 & 0 & 0.947 & 0.053 \end{bmatrix}$

3.6. Weight of the participating factors

According to Hakanson's standardized heavy metal toxicity response coefficient, the toxicity index of eight heavy metal organisms was assigned (Table 8). The smaller the index, means the greater the toxicity.

Substituting the data of Tables 7 and 8 into the formula (4), the weight values of the heavy metal participating factors in different regions are obtained (see Table 9).

Table 7: The measured values of 8 elements in various areas of the city (mg/kg)

Elements	As	Cd	Cr	Cu	Hg	Ni	Pb	Zn
Area 1	6.44	0.35	162.44	79.99	0.22	18.94	109.43	627.90
Area 2	9.86	0.38	88.97	280.63	0.72	24.72	130.51	490.59
Area 3	6.01	0.20	82.46	33.79	0.09	28.66	57.04	75.21
Area 4	8.86	0.35	146.32	113.52	0.17	49.32	78.74	555.45
Area 5	6.66	0.38	52.39	62.70	0.41	17.59	80.91	494.04

Table 8: Classification criteria and biological toxicity index of 8 kinds of elements

Elements	Normal	Slightly	Seriously	More seriously	Toxicity index
As	3.60	6.3	11.70	14.40	3
Cd	0.13	0.20	0.39	0.52	2
Cr	31	62	124	155	5
Cu	13.20	39.60	99	132	4
Hg	0.04	0.09	0.25	0.35	1
Ni	12.30	18.45	30.75	36.90	4
Pb	31	46.50	93	124	2
Zn	69	172.50	483	690	6

Table 9: Weight values R_i of each heavy metal assessment factor

Areas	As	Cd	Cr	Cu	Hg	Ni	Pb	Zn
Living area	0.0064	0.0003	0.1615	0.0797	0.0002	0.0188	0.1088	0.6243
Industrial area	0.0096	0.0003	0.0866	0.2734	0.0007	0.0242	0.1272	0.478
Mountain area	0.0212	0.0007	0.2909	0.1192	0.0003	0.1011	0.2013	0.2653
Traffic area	0.0093	0.0004	0.1534	0.1189	0.0018	0.0517	0.0825	0.582
Park area	0.0093	0.0005	0.0733	0.0877	0.0006	0.0246	0.1131	0.6909

3.7. Fuzzy comprehensive evaluation results

According to the fuzzy relation matrix of the five types of zones and the weights of the participating factors, the evaluation results calculated by the fuzzy comprehensive evaluation model are:

Table 10: Fuzzy comprehensive evaluation results of five types of districts

Areas	Normal	Primary pollution	Secondary pollution	Tertiary pollution
Living area	0	0.050	0.293	0.657
Industrial area	0	0.064	0.517	0.419
Mountain area	0.278	0.500	0.232	0
Traffic area	0	0.030	0.558	0.412
Park area	0.026	0.163	0.773	0.038

3.8. Analysis of Results

It can be seen from Table 10 that the living area belongs to the tertiary pollution area; the industrial area belongs to the secondary pollution area; the mountain area belongs to the primary pollution area; the transportation area belongs to the secondary pollution area; the park green area belongs to the secondary pollution area.

In the living area, there is a large variety of domestic garbage, and heavy metal elements in the garbage enter the atmosphere or directly enter the soil, resulting in three levels of pollution in the living area; in the industrial zone, there are a large number of heavy metal-containing wastes and the content of Cd, Hg, Cr, Cu, Zn, Ni, Pb and As in the waste is high, with the discharge of wastewater and rainfall, it is brought into rivers and lakes directly or indirectly into the soil, causing secondary pollution in industrial areas; the mountain area is sparsely populated, the transportation is inconvenient, and it is far away from the industrial area, however, due to farmers applying pesticides containing heavy metals and unreasonable application of chemical fertilizers, causing pollution in mountainous areas; in the traffic area, automobile exhaust emissions and automobile tire wear generate a large amount of harmful gases and dusts containing heavy metals, which are naturally settled and rain-sinked into the soil, causing secondary pollution of heavy metals in the traffic area; due to sewage irrigation and sludge fertilization of vegetation in the park area, the land contains a large amount of organic matter and nutrients such as nitrogen, phosphorus and potassium, in addition, a large amount of heavy metals enter the park green space with municipal sludge, so that the heavy metal content in the park area is constantly increasing, resulting in secondary pollution.

4. Determination of soil heavy metal pollution sources

4.1. Basic theory and mathematical model of soil solute transport

Soil solute moves along the soil moisture in the soil. During the migration process, the soil solute is also affected by the soil matrix, the Physical and chemical properties of the soil solute and other chemical components in the soil. The physical mechanism of soil solute transport mainly includes convection, diffusion and mechanical dispersion [5-6].

4.1.1. Convection

Convection refers to the relative displacement between the various parts of the fluid due to the macroscopic movement of the fluid. The convection of heavy metals in the soil refers to the movement process of the solute as the soil moisture migrates. The mass of solute passing through the unit soil cross-sectional area per unit time is called the solute flux. The solute flux of solute in soil is related to soil water flux and solute concentration. The relationship between them is:

$$J_c = J_w c \tag{5}$$

J_c ------ Soil solute flux;

J_w ------ Soil moisture flux;

c ------ Soil solute concentration.

4.1.2. Diffusion

Diffusion is a phenomenon in which molecules enter each other. It is caused by the thermal motion of solute molecules and has a tendency to migrate from a high concentration to a low concentration in order to achieve equal concentrations. In soil solutions, the diffusion of soil solute molecules follows Fick's first law, and its mathematical expression is:

$$J_{ds} = -\theta D_s \frac{\partial c}{\partial z} \tag{6}$$

θ ------ Volumetric water content of soil;

J_{ds} ------ The flux of solute molecules in the soil;

D_s ------ The diffusion coefficient of solute molecules in the soil.

The diffusion coefficient of the general solute in the soil is only expressed as a function of water content, and regardless of the concentration of the solute, the commonly used empirical formula is:

$$D_s = D_0 \tau \tag{7}$$

In equation (7), $D_s < D_0$, τ means dimensionless bending factor.

4.1.3. Mechanical dispersion

Mechanical dispersion is due to the fact that the pores in the soil vary in size and shape. When the aqueous solution migrates in these pores, the flow velocity in each pore differs in size and direction, causing the solute molecules to diffuse and increasing the migration range.

The mechanical diffusion flux produced by soil solute during transport can be mathematically expressed as:

$$J_h = -\theta D_h \frac{\partial c}{\partial z} \tag{8}$$

J_h ------ Mechanical diffusion flux of solute;

D_h ------ The mechanical diffusion coefficient of the solute.

D_h can usually be expressed as:

$$D_h = \lambda |v|^n \tag{9}$$

λ ------ Dispersion, related to the texture and structure of the soil;
v ------ The average flow rate of the pores;
n ------ Usually the value is 1.

Under two-dimensional conditions, λ consists of a longitudinal dispersion λ_L parallel to the direction of the water flow and a transverse dispersion λ_T perpendicular to the flow direction. In the two-dimensional Cartesian coordinate system, D_h in equation (9) consists of D_{xx}, D_{xy}, D_{yy} and D_{yx} , and the calculation formula is:

$$\begin{cases} D_{xx} = \dfrac{\lambda_L v_x{}^2}{v} + \dfrac{\lambda_T v_y{}^2}{v} \\ D_{xy} = D_{yx} = \dfrac{(\lambda_L - \lambda_T) v_x v_y}{v} \\ D_{yy} = \dfrac{\lambda_T v_x{}^2}{v} + \dfrac{\lambda_L v_y{}^2}{v} \end{cases} \tag{10}$$

In the formula, v_x and v_y respectively represent the average pore flow in the direction x and y, and v is the average pore flow velocity, and λ_L is generally 3 to 20 times larger than λ_T.

Molecular diffusion and mechanical dispersion of solutes can cause migration of solutes in the soil. However, in the actual migration process, these two effects are difficult to distinguish, and the solute transport flux caused by these two factors has the same mathematical form. Therefore, in the actual measurement calculation process, these two factors are often considered together. The joint form of the two factors is called hydrodynamic dispersion, and the solute flux caused by it can be expressed by mathematical expression:

$$J_{dh} = -\theta D \frac{\partial c}{\partial y} \tag{11}$$

J_{dh} ------ Solute transport flux caused by hydrodynamic dispersion;

D ------ Effective hydrodynamic dispersion coefficient.

4.2. Mathematical model of heavy metal transport in soil

4.2.1 Basic equations for heavy metal migration in soil

In summary, the total flux of solute transport in the soil is the sum of flux and hydrodynamic diffusion flux, and its expression is:

$$J = J_c + J_{dh} = J_w c - D \frac{\partial c}{\partial y} \tag{12}$$

According to the principle of conservation of mass, the rate of change of solute in the soil volume studied should be equal to the difference between the flux of solute flowing in and out, similar to the continuous equation for deriving soil moisture, the continuous equation for soil solute transport in two-dimensional conditions is:

$$\frac{\partial(\theta c)}{\partial t} = \frac{\partial}{\partial x}\left(\theta D_{xx}\frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial x}\left(\theta D_{xy}\frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(\theta D_{yy}\frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial y}\left(\theta D_{yx}\frac{\partial c}{\partial y}\right) - \frac{\partial(J_{wx}c)}{\partial x} - \frac{\partial(J_{wy}c)}{\partial y} \tag{13}$$

Further, the convection-diffusion equation for Jordan can be summed as:

$$\frac{\partial(\theta c)}{\partial t}=\frac{\partial}{\partial x_i}\left(\theta D_{ij}\frac{\partial c}{\partial x_j}\right)-\frac{\partial(J_{wj}c)}{\partial x_j}, \quad (i,j=x,y) \tag{14}$$

Equation (14) is the basic equation for soil solute transport.

When the water content in the soil is saturated, divide by θ on both sides of (14) will get:

$$\frac{\partial c}{\partial t}=\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial c}{\partial x_j}\right)-\frac{\partial(v_j c)}{\partial x_j} \tag{15}$$

When the solute flux in the soil does not change with time, equation (15) can be rewritten as:

$$\frac{\partial c}{\partial t}=D_{ij}\frac{\partial}{\partial x_i}\left(\frac{\partial c}{\partial x_i}\right)-\frac{\partial(v_j c)}{\partial x_j} \tag{16}$$

4.2.2. Determining conditions for mathematical model of soil solute transport

When the mathematical model of soil solute transport is a partial differential equation, to solve these partial differential equations, we must know their conditions for the solution: initial conditions, boundary conditions.

1) Initial conditions

Initial concentration distribution in the study area

$$c(x,y,z,0)=c_0(x,y,z) \tag{17}$$

2) Boundary conditions

The boundary conditions in soil solute transport generally include the following three categories:

The first type (known concentration), the mathematical expression is:

$$c(x,y,z,t)\Big|_{L_1}=c_1(x,y,z,t) \quad x,y,z\in L_1 \tag{18}$$

In the equation, $c_1(x,y,z,t)$ is a known.

The second type (known diffusion flux), the mathematical expression is:

$$\theta(D_{ij}\frac{\partial c}{\partial x_j})_{n_i}\Big|_{L_2}=-J(x,y,z,t) \quad x,y,z\in L_2 \tag{19}$$

The third type (known solute flux), the mathematical expression is:

$$\theta(cv_i-D_{ij}\frac{\partial c}{\partial x_j})_{n_i}\Big|_{L_3}=-J(x,y,z,t) \quad x,y,z\in L_3 \tag{20}$$

In the equations (19) and (20), $J(x,y,z,t)$ is known.

4.3. Simulation realization of two-dimensional transport of heavy metal pollutants in soil

4.3.1 Numerical solution of two-dimensional transport of heavy metal pollutants in soil

The basic equation for the transport of heavy metal pollutants in saturated, isotropic soils is:

$$R_d\frac{\partial c}{\partial t}=D_x\frac{\partial^2 c}{\partial x^2}+D_y\frac{\partial^2 c}{\partial y^2}-v_x\frac{\partial c}{\partial x}-v_y\frac{\partial c}{\partial y} \tag{21}$$

In the above formula, D_x and D_y respectively represent the diffusion coefficients in the direction x and y, v_x and v_y respectively represent the convection velocities in the direction x and y, and the rest are as described above.

For equation (21), the finite difference method is used to find the numerical solution. [8–9] The commonly used finite difference schemes for two-dimensional partial differential equations are explicit, implicit, Crank-Nicolson, and alternating direction implicit (ADI). In order to solve such two-dimensional partial differential equations, Peaceman and Rachford introduce an alternating direction implicit format, also known as the P-R format difference method, it has second-order precision and it is unconditionally stable, therefore it has been widely used. The essence of this difference format is to introduce the layer $k+1/2$ of the intermediate layer between the layer k and the layer $k+1$, that is, it is carried out in two steps in one time step. The implicit difference format is used for the direction x in the first 1/2 time step, and the explicit difference format is used for the direction y; In the latter 1/2 time step, that is, the explicit difference format is used for the direction x, and the implicit difference format is used for the direction y.

Using Δx and Δy to denote the spatial step size in the directions x and y respectively, and Δt denotes the time step, then expand the equation (21) according to the alternating implicit difference method to establish the difference equation as equations (22) and (23):

$$R_d \frac{c_{i,j}^{k+1/2} - c_{i,j}^{k}}{\frac{\Delta t}{2}} = \frac{D_x}{(\Delta x)^2}(c_{i+1,j}^{k+1/2} - 2c_{i,j}^{k+1/2} + c_{i-1,j}^{k+1/2}) + \frac{D_y}{(\Delta y)^2}(c_{i,j+1}^{k} - 2c_{i,j}^{k} + c_{i,j-1}^{k}) - \frac{v_x}{2\Delta x}(c_{i+1,j}^{k+1/2} - c_{i-1,j}^{k+1/2}) - \frac{v_y}{2\Delta y}(c_{i,j+1}^{k} - c_{i,j-1}^{k}) \quad (22)$$

$$R_d \frac{c_{i,j}^{k+1} - c_{i,j}^{k+1/2}}{\frac{\Delta t}{2}} = \frac{D_x}{(\Delta x)^2}(c_{i+1,j}^{k+1/2} - 2c_{i,j}^{k+1/2} + c_{i-1,j}^{k+1/2}) + \frac{D_y}{(\Delta y)^2}(c_{i,j+1}^{k+1} - 2c_{i,j}^{k+1} + c_{i,j-1}^{k+1}) - \frac{v_x}{2\Delta x}(c_{i+1,j}^{k+1/2} - c_{i-1,j}^{k+1/2}) - \frac{v_y}{2\Delta y}(c_{i,j+1}^{k+1} - c_{i,j-1}^{k+1}) \quad (23)$$

Formula (22) can be obtained as:

$$\left[1+\frac{D_x\Delta t}{R_d(\Delta x)^2}\right]c_{i,j}^{k+1/2} + \left[\frac{v_x\Delta t}{4R_d\Delta x} - \frac{D_x\Delta t}{2R_d(\Delta x)^2}\right]c_{i+1,j}^{k+1/2} - \left[\frac{v_x\Delta t}{4R_d\Delta x} + \frac{D_x\Delta t}{2R_d(\Delta x)^2}\right]c_{i-1,j}^{k+1/2} = \left[1-\frac{D_y\Delta t}{R_d(\Delta y)^2}\right]c_{i,j}^{k} + \left[\frac{D_y\Delta t}{2R_d(\Delta y)^2} - \frac{v_y\Delta t}{4R_d\Delta y}\right]c_{i,j+1}^{k} + \left[\frac{v_y\Delta t}{4R_d\Delta y} + \frac{D_y\Delta t}{2R_d(\Delta y)^2}\right]c_{i,j-1}^{k} \quad (24)$$

Formula (23) can be obtained as:

$$\left[1+\frac{D_y\Delta t}{R_d(\Delta y)^2}\right]c_{i,j}^{k+1} + \left[\frac{v_y\Delta t}{4R_d\Delta y} - \frac{D_y\Delta t}{2R_d(\Delta y)^2}\right]c_{i+1,j}^{k+1} - \left[\frac{v_y\Delta t}{4R_d\Delta y} + \frac{D_y\Delta t}{2R_d(\Delta y)^2}\right]c_{i,j-1}^{k+1} = \left[1-\frac{D_x\Delta t}{R_d(\Delta x)^2}\right]c_{i,j}^{k+1/2} + \left[\frac{D_x\Delta t}{2R_d(\Delta x)^2} - \frac{v_x\Delta t}{4R_d\Delta x}\right]c_{i,j+1}^{k+1/2} + \left[\frac{v_x\Delta t}{4R_d\Delta x} + \frac{D_x\Delta t}{2R_d(\Delta x)^2}\right]c_{i,j-1}^{k+1/2} \quad (25)$$

The equations composed of equations (24) and (25) are the difference equations of the alternating direction implicit format of equation (21). Calculated from the initial condition, that is, at time $k=0$, the concentration value at time 1/2, that is $c_{i,j}^{1/2}$, can be calculated by the equation (24). At this time, the formulas on the right side of (24) are known, so this paper adopts the method of fixing j on the left side, and uses the chasing method in the direction i. This step only calculates the direction i, so it can be called chasing in the direction x ;Then, the concentration $c_{i,j}^{1}$ of a time step Δt can be calculated from the formula (25), then substituting $c_{i,j}^{1}$ into equation (24) to calculate the concentration value $c_{i,j}^{1+1/2}$ at $(1+1/2)\Delta t$. This calculation process is essentially the same as the calculation method in direction x, except that it needs to fix i at this time, and uses the chasing method in the direction j, so this calculation process is also called chasing in the direction j. Then substituting the value just obtained into the equation (25), the concentration value $c_{i,j}^{2}$ at $2\Delta t$ can be obtained.

Repeating the iteration until the termination condition is satisfied, that is, the value of the concentration $c_{i,j}^{k}$ is obtained.

4.3.2. The solution of the model

The data in this paper is derived from the investigation of the soil geological environment in a certain urban area, and the area is divided into grid sub-areas with a distance of 1 km, the topsoil is sampled and numbered according to one sampling point per square kilometer, and the position of the sampling points is recorded by GPS, applying special instrument test analysis to obtain concentration data of various chemical elements contained in each sample. Using the two-dimensional convection diffusion model constructed in the paper, doing dynamic simulation experiments on 319 sampling points, eight pollution source points in five regions can be obtained. The specific geographical locations of each pollution source are as follows:

Table 11: Location of the source of pollution

Urban area	**Source of pollution**	**Location of the source of pollution**		
		x (m)	y (m)	**Elevation** (m)
Living area	source of pollution 1	4592	4603	6
	source of pollution 2	9328	4311	24
Industrial area	source of pollution 3	2383	3692	7
	source of pollution 4	4948	7293	6
Mountain area	—	—	—	—
Traffic area	source of pollution 5	3299	6018	4
	source of pollution 6	13797	9621	18
	source of pollution 7	12696	3024	27
Park area	source of pollution 8	4153	2299	73

5. Conclusions

With the continuous development of the city, the impact of heavy metal pollution on people's lives is growing. This paper takes the data provided by the 2011 Chinese College Students Mathematical Contest in Modeling (MCM) Undergraduate Group A as a case to analyze the heavy metal pollution in the soil. Using the fuzzy analysis method to evaluate the heavy metal pollution in various regions and obtained the pollution situation in each region. Considering the convection, diffusion and mechanical dispersion of heavy metals in the soil environment system, this paper gives the migration mechanism and equations of heavy metals in the soil, and the differential model is established, it embodies the dynamic characteristics of heavy metal concentration changes at each sampling point; establishing a two-dimensional model, when considering the propagation of heavy metals in the surface layer of the soil, according to the horizontal and vertical coordinates of the taken points, combined with the altitude given in the appendix, the actual location of the relevant points can be spatially located, which is conducive to the further determination of the location of the pollution source. But there are also some shortcomings: 1) this paper assumed that the soil is homogenous in all directions, ignoring the influence of different soil geological environments on the propagation rate; 2) this paper didn’t consider the seepage adsorption of heavy metals in the vertical direction of the soil, the absorption or discharge of plant roots accompanied by unsteady state of soil solution, the effect of soil density and water content on the migration of heavy metals in soil; 3) this paper ignored the possibility of heavy metal propagation caused by other pathways on the macro scale. In order to further study the evolution of urban geological environment, the future work is to comprehensively consider the modes of heavy metal’s transmission caused by atmospheric deposition, agricultural sludge and fertilization; urban crop coverage and its absorption of heavy metals, soil adsorption; heavy metal seepage conditions.

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Background

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