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Calculation model based on the Gaussian diffusion of heavy metal pollution sources

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ABSTRACT

The analysis on urban topsoil heavy metal pollution is the important foundation of urban management and urban planning. The topsoil in the city proper was uniformly sampled to measure the concentration data of 8 kinds of heavy metals at each sampling point. The evaluating method of the single factor index and the Nemerow comprehensive pollution index method were adopted to analyze the degree of heavy metal pollution in different areas in the city. Through analyzing the propagation characteristics of heavy metal contamination in the air, solids and the liquid, a mathematical model was constructed utilizing the Gauss equation to confirm the location of the polluter and eight kinds of heavy metal polluters were accurately calculated utilizing the sampled data. To be more realistic, considering the influence of factors like wind speed, gravity deposit, raindrop deposit and others on heavy metal contamination concentration's distribution, optimized Gaussian Model after reasonable correction is built.

KEYWORDS

Heavy metal pollution; The Nemerow pollution index; Propagation characteristics; Gauss diffusion; Difference method.

INSTRODUCTION

With the rapid development of the urban economy and the ever-growing urban population, human activities have an increasingly prominent influence on the quality of the urban environment. Investigation and verification of the abnormal urban soil geological environment, and how to carry out city environment quality evaluation applying the acquired mass data, and studying the evolution mode of city geological environment under the influence of human activities seem to be pretty important.

According to the functions, cities can be divided into 5 areas, such as living areas, industrial areas, mountainous areas, main roads areas and park green spaces. Environments of different areas are affected by the influence of human activities at different levels. For studying and analyzing the evolutionary patterns of the urban geological environments, the target cities will be divided into grid regions with gaps between the left sides and right sides. Sampling for topsoil (0~10 cm for depth) will be done according to 1 sampling site per square kilometer. Also GPS will be applied to record the locations of sampling sites. Concentration data of 8 major heavy metal elements contained by each sample will be tested and analyzed. According to the data of the sampling sites, reasonably analyze the pollution degree of every kind of heavy metal in every area of the city, and utilize Gauss diffusion model to work out the polluter of every kind of heavy metal[1].

ANALYSIS FOR THE POLLUTION DEGREE

According to the sample data, first, use matlab to analyze the topographic map of elevation and the special distribution diagram of eight heavy metal elements, which can relatively intuitively analyze the order of the pollution level of each heavy metal in different areas.

As for different areas, in order to get a clear pollution level of the heavy metals, it needs to use more precise assessment methods. Currently, there are many assessment methods on soil heavy metal pollution at home and abroad, such as the factor index assessment method, Nemerow comprehensive pollution index method, land accumulation index method, ecological damage index method, fuzzy comprehensive assessment method produced with the combination of the fuzzy mathematics theory and modified grey clustering method. Taking the operability into consideration, when evaluating the degree of pollution for various elements of heavy metals in soil, comprehensive pollution index method of Nemerow, which is used more widely, is applied[2][3].

The calculation formula of comprehensive pollution index method (Nemerow pollution index) is:

$$P = \sqrt{\frac{(P_{iave})^2 + (P_{i\max})^2}{2}} \qquad (1\text{-}1)$$

P_{iave} refers to the average value of all the single pollution indexes of the heavy metal, and $P_{i\max}$ refers to the maximal value among the single pollution indexes of the heavy metal.

The comprehensive pollution assessment result of the heavy metal element obtained by using software calculation program, is shown in Table 1.

Table 1 : The comprehensive pollution assessment result of the heavy metal element

Area	pollutant element degree							
	As	Cd	Cr	Cu	Hg	Ni	Pb	Zn
living areas	serious	mild	serious	mild	moderate	serious	serious	moderate
industrial areas	safe	moderate	serious	moderate	heavy	safe	serious	moderate
mountainous areas	safe	serious	serious	safe	safe	safe	safe	safe
main roads	safe	moderate	serious	mild	heavy	serious	mild	moderate
park green spaces	safe	mild	safe	safe	moderate	safe	serious	mild

ESTABLISHMENT OF POLLUTION SOURCE MODEL

Propagation characteristics of heavy metals in soil

(a) Sedimentation in the atmosphere

The heavy metals in the atmosphere mainly come from the industrial production in industrial areas, the emission of automobile exhaust, the abrasion of vehicle tyres, the burning of household fuel gas etc. Most of the heavy metals in the air generally enter the soil by the natural sedimentation and the rain settlement, and then cause the pollution of heavy metals in soil. They are mostly distributed in the industrial areas and both sides of main roads, as well as above the living areas in the air. The strength of the pollution of heavy metals gradually decreases in the axle of the main roads to the both sides.

Pollutions of Cd, Hg and Zn resulted from the industrial production in industrial areas are heavy, so various kinds of heavy metals spread from the industrial areas as the centers.

(b) Propagation in solids

Using the farm chemicals which contain Pb, Hg, Cd, As and other heavy metals and unreasonably using the fertilizers could lead to the heavy metal pollution in the soil. Generally, super phosphate contains more heavy metals such as Hg, Cd, As, Zn, Pb and nitrogen fertilizers contain more Pb, and As and Cd can cause serious pollution. The green areas of the garden need to be fertilized and sprayed insecticide, which leads to the increase of the concentrations of Cd, Hg and Zn. Thus because the garden areas are often watered, it causes that the heavy metal elements spread out along with the water flow.

(c) Propagation in the liquid

Due to the rapid development of urban industrialization, a large amount of industrial wastewater flows into the watercourse, and the heavy metal elements spread out with the water current, which is also a primary route of transmission of the heavy metal.

(d) The accumulation of waste containing heavy metals

There are a wide range of wastes containing heavy metals, and the damaging methods and pollution levels are determined by the types of wastes. The range of pollution is generally centered by the discard pile and diffuses around. The content and form distribution characteristics of heavy metals in soil are influenced by release rate from waste, and the content of heavy metals decreases with the distance increasing. The different kinds of waste lead to different pollution levels of heavy metals. For example, Cd, Hg and Pb from the stockpiling pile of chromium slag are in high pollution; Zn, middle level pollution; Cr and Cu, mild concentration.

By the analysis, heavy metals are mainly spread through diffusion, and the Gauss diffusion equation could be adopted and established to solve the polluter positions.

Establishment of the Gauss diffusion equation

Suppose the location of the source of heavy metal pollutions is , the horizontal direction is axis, the vertical direction is another axis, and the horizon perpendicular to the axis of horizontal direction (axis) is Y direction to create a space coordinates system. And remember the concentration of heavy metal pollutants at any point in the space is at a certain time . According to the hypothesis, suppose that the pollution amount crossing the unit normal area is positively correlated with the concentration gradient, and then there are:

$$\vec{q} = -\delta_i \cdot gradC \qquad (2\text{-}1)$$

$\delta_i(i = x - x_0, y - y_0, z - z_0)$ is diffusion coefficient, a minus indicates moving from the more concentrated areas to the less concentrated ones.

Investigate the spatial domain Ω, the volume is V, the curved surface of encircle Ω is S, because the spread of pollutants is radioactive, so the S is a regular spherical, the outer normal vector of S is:

$$\vec{n} = \left(-\frac{x - x_0}{z - z_0}, -\frac{y - y_0}{z - z_0}, 1 \right)$$

then in $(t, t + \Delta t)$ the flux of the heavy metal contamination through Ω is:

$$Q_1 = \int_t^{t+\Delta t} \iint_s \vec{q} \cdot \vec{n} d\sigma dt \qquad (2\text{-}2)$$

In spatial domain Ω the increment of the heavy metal contamination is:

$$Q_2 = \iiint_v [C(x - x_0, y - y_0, z - z_0, t + \Delta t) - C(x - x_0, y - y_0, z - z_0, t)] dv \qquad (2\text{-}3)$$

the total contamination from spreading by heavy metal pollution sources is:

$$Q_0 = \int_t^{t+\Delta t} \iiint_\Omega p_0 dV dt \qquad (2\text{-}4)$$

According to the law of conservation of mass and the contamination of heavy metal diffusion the principle of continuity, in the meantime Through the curved surface S out diffusion of increment of heavy metal pollutants and heavy metal pollutants in the surface is equal to the out diffusion of pollutant sources of pollution within this period of time. It is:

$$Q_0 = Q_1 + Q_2 \qquad (2\text{-}5)$$

$$\iiint_v [C(x-x_0, y-y_0, z-z_0, t+\Delta t) - C(x-x_0, y-y_0, z-z_0, t)] dv + \int_t^{t+\Delta t} \iint_s \vec{q} \cdot \vec{n} d\sigma dt = \int_t^{t+\Delta t} \iiint_\Omega p_0 dV dt$$

According to curvilinear intergral's Gauss Fromula (where div is divergence insignia):

$$\iint_s \vec{q} \cdot \vec{n} d\sigma = \iiint_V div\vec{q} dV \qquad (2\text{-}6)$$

$$\therefore \iiint_v \left[\frac{C(x-x_0, y-y_0, z-z\ , t+\Delta t) - C(x-x_0, y-y\ , z-z_0, t)}{\Delta t} \Delta t \right] dv + \int_t^{t+\Delta t} \iiint_v div\vec{q} dV dt = \int_t^{t+\Delta t} \iiint_\Omega p_0 dV dt$$

$$\therefore \frac{\partial C}{\partial t} = \lim_{\Delta t \to 0} \frac{C(x-x_0, y-y_0, z-z_0, t+\Delta t) - C(x-x_0, y-y_0, z-z_0, t)}{\Delta t} = \lim_{\Delta t \to 0} \frac{\int_t^{t+\Delta t} kdiv(gradC) dt}{\Delta t}$$

from the above two formula: $\iiint_V [\frac{\partial C}{\partial t}] dV \cdot \Delta t + \iiint_V div\vec{q} dV \cdot \Delta t = \iiint_\Omega p_0 dV \cdot \Delta t$

It is:

$$\iiint_V [\frac{\partial C}{\partial t}] dV + \iiint_V div\vec{q} dV = p_0 \qquad (2\text{-}7)$$

According to the reference literature[4]:

$$\frac{\partial c}{\partial t} = \delta_{x-x_0} \cdot \frac{\partial^2 c}{\partial (x-x_0)^2} + \delta_{y-y_0} \cdot \frac{\partial^2 c}{\partial (y-y_0)^2} + \delta_{z-z_0} \cdot \frac{\partial^2 c}{\partial (z-z_0)^2} + p_0 \qquad (2\text{-}8)$$

the result is:

$$C(x-x_0, y-y_0, z-z_0, t) = \frac{p_0}{(4\pi t)^{3/2} \left(\delta_{x-x_0} \delta_{y-y_0} \delta_{z-z_0}\right)^{1/2}} \exp\left\{ -\frac{(x-x_0)^2}{4\delta_{x-x_0} t} - \frac{(y-y_0)^2}{4\delta_{y-y_0} t} - \frac{(z-z_0)^2}{4\delta_{z-z_0} t} \right\}$$

After the analysis and calculation, City mountain elevation is higher than other area. According to the sampling data , only mountain is not polluted. The other four regional's elevation is the same, so we can ignore the elevation. Pollution source model can be simplified to:

$$C(x-x_0, y-y_0, t) = \frac{p_0}{(4\pi t)^{3/2} \left(\delta_{x-x_0} \delta_{y-y_0}\right)^{1/2}} \exp\left\{ -\frac{(x-x_0)^2}{4\delta_{x-x_0} t} - \frac{(y-y_0)^2}{4\delta_{y-y_0} t} \right\}$$

According to the sampling data, the location of the source of 8 heavy metal pollutions is shown in Table 2.

TABLE 2: The location of the source of 8 heavy metal pollutions

heavy metal element	X-axis（x/m）	Y-axis (y/m)	area
As	17945	9984	main roads
Cd	2811	2356	main roads
Cr	3006	5845	main roads
Cu	2388	3695	industrial areas
Hg	2388	3695	industrial areas
Ni	3321	6110	main roads
Pb	4797	4854	living areas
Zn	13845	9675	main roads

According to the Table 2, we can conclude that Cu and Hg which are heavy metal elements have the same coordinate, and both of them are located in the industrial district, so they have the same pollutant source. Therefore, there are 8 heavy metal elements and 7 pollutant sources, and most of them are distributed in main road areas and industrial districts, which indicates that heavy metal pollutions and industrial pollutions brought about by transportation are the main accumulation areas of pollutant sources.

THE IMPROVEMENT AND PERFECTION OF THE MODEL

The advantages and disadvantages of the model built

The built model shows good stability and the position of the source of pollution can be solved through this model more accurately. Gauss diffusion equation, which can reflect the characteristics of heavy metal pollution clearly, can be used to solve the source of pollution. However, since the impact of factors such as rainfall and wind speed on the spread of heavy metals is not taken into consideration, it may affect the results of the model.

The impact of rainfall on heavy metal contamination concentration

Rainfalls have the effect of cleaning on the heavy metal particles and aerosols in the air, and the gas and steam of the soluble heavy metal pollutants can also dissolve in the rain, and then, the heavy metal pollutants carried by the rain will penetrate into the soil and cause the soil heavy metal pollution. Such wet deposition caused by the rainfall process is another important mechanism that leads to the deposition of the heavy metal pollutants to the ground. Cleaning coefficient is usually used to describe the magnitude of cleaning effect of rainfall on the pollutant in the air, and then cleaning coefficient can indicate the coefficient of the deposit pollutant in soil because of the rainfall.

The relationship of clean coefficient φ and rain intensity I can be expressed as (a, b refers to the empirical coefficient):

$$\varphi = aI^b \qquad (3\text{-}1)$$

For the depletion of heavy metal pollutants in the air and the increase of soil heavy metal pollution, which are caused by the wet deposition, the wet deposition reduction factor can be adopted to conduct a modification on the source strength Q, which obtains

$$Q(x) = Q\exp(-\frac{\varphi x}{\bar{u}}) \qquad (3\text{-}2)$$

The impact of wind speed on the concentration of heavy metals

When analyzing the impact of wind speed on heavy metal contamination concentration, it should be analyzed under different conditions based on wind speed. If the diameter of heavy metal pollutant particles is more than 10 microns, the particle will have obvious gravity sedimentation. The sedimentation velocity of heavy metal pollutant particle depends on the air resistance and gravitational balance, which can be formulated by Stokes formula:

$$Vs = \frac{\rho g D^2}{18\mu} \qquad (3\text{-}3)$$

Because at the same time of the diffusion process, there is a displacement of gravity settling superposition to the center line of the plume, the center line will slope down, and all heavy metal pollutant particles correspond to diffusing on the declinate center line. The superposition of diffusion and sedimentation of this type of heavy metal pollutant particle could be thought as in the plume moving process, the speed of moving downstream divided by the height of moving downstream which means that the source height drops by . In fact, because of airflow and other exogenic action, the ground is not the surface which absorbs completely. It's necessary to multiply by a reflection coefficient to the reflection term, and its design formula of consistency after dry deposition is:

$$c(x,y,z,H)=\frac{Q}{2\pi k\sigma_y\sigma_z}\exp(-\frac{y^2}{2\sigma_y^2})\{\exp[-\frac{(z-H+\frac{V_s x}{\bar{u}})^2}{2\sigma_z^2}]+\exp[-\frac{(z+H-\frac{V_s x}{\bar{u}})^2}{2\sigma_z^2}]\}$$

CONCLUSION

Three reasonable hypotheses derived from the analysis of the characteristics of heavy metal diffusion are as follows: supposing that all the sources of heavy metal pollutants are point sources, they are also sources of pollution within a specific range of deviation; under the presumption that the pollutant levels are the highest at source, and the concentration will decrease with the increasing of time and the distance from the source; suppose that heavy metal pollutants outspread through homogeneous diffusion from the pollutant source. According to the Gauss diffusion equation, construct the polluter model and accurately calculate 8 heavy metals' polluter positions.

There is only one spreading source for each heavy metal based on the solution of this model, because of the complexity of the influence of human activities, two different heavy metals have the possibility of existing in the same polluter or it is also possible that each heavy metal has multiple polluters, and these factors should be considered in the practical applications. The different cities should consider the influences of rainfall level and climate and improve the model properly according to the local features to raise further the accuracy of the model.

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