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Point Propagation Model of Pollution Sources of Heavy Metals in the Surface Soil

Hai-ming Zhang[1], *Hong-gui Deng*[1*], *Gu Teng-feng*[1] , *Fang Yang*[1], *Yi Sun*[1], *Ji-an Duan*[2]

1.School of Physics and Electronics, Central South University, Changsha 410083, China
2.State Key Laboratory of High Performance Complex Manufacturing, School of Mechanical and Elec trical Engineering, Central South University, Changsha 410083, China)
[*] Corresponding author E-mail: denghonggui@163.com

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The soil pollution caused by heavy metal is difficult to treat. Many scientists and researchers are focusing on solving the problem in recently years. By probing into the law of diffusion and the law of conservation of mass, we establish the point propagation model of pollution sources of heavy metals and come to the distribution characteristics function of the local area the concentration of heavy metals in soil. Finally, the proposed point propagation model is utilized to establish a method for determining the point pollution sources.

Keywords: Law of Diffusion, Law of Conservation of Mass, Point Propagation Model

1. INTRODUCTION

With the fast growth of economy and the rapid advance of urbanization and industrialization in the world, the environmental issues have become increasingly prominent. With the growing awareness of environment protection, many researchers have shown great interests on the mechanism of heavy metals pollution, and they have made great efforts to find solutions to mitigate this problem. In recent decades, many of the great achievements of the world were accomplished on the propagation characteristics of the heavy metal pollutants. The propagation characteristics are mainly characterized by the propagation models, which includes analytical models of deterministic solutions (e.g. the convection-diffusion-adsorption model [1], WASP4 water quality model [2], migration transformation model [3]) and empirical models of uncertain solutions, (e.g. the stochastic model [4]).

In the analytical models, the distribution regularity and characteristics of the concentration of heavy metal element over time and space can be determined by rigorous derivation and proof.

However, because these models are just conceptual models [5-9], they are generally employed only for theoretical analysis without any practical value. With those necessary parameters such as the permeability of the heavy metal elements, the migration performance, the soil permeability, and the diffusion coefficient [10] are measured accurately. Theoretically these models can be precisely solved. However, these parameters are different in different regions, even for the different soils in the same region, they may vary greatly. In addition, the measurements are too complex and tedious to be applied for engineering application.

In the stochastic model, the input parameters are treated as random variables, normal distribution or lognormal distribution is employed to estimate the randomness of the output variables. Because the influencing factors are loosely treated as random variables in this model, the essential characteristics of the heavy metal pollution cannot be reflected, and the error is large. This model can only perform general estimation and analysis.

In this paper, the propagation characteristic of solid waste pollution is modeled. Mainly by the soluble metal compound being dissolved in water, the contamination caused by the accumulation and burying of heavy metal contained wastes enter into the soil and spread to the surrounding areas with the water in the soil [11]. Based on the Law of Diffusion and the Law of Conservation of Mass, the point propagation model of pollution sources of heavy metals is built under strict deducing and reasonable assumption. With this model, we can more accurately determine the pollution sources through sampling points, meanwhile, the shortness of analytical model and random model, which are not practical and accurate, will not appear in the proposed model.

2. PROPAGATION MODEL OF POINT SOURCES OF HEAVY METAL POLLUTANTS

In the research of the diffusion of solute， we use the function N(x, y, z, t) to indicate the solute concentration of substance G in the location (x, y, z) and at the time t.

According to the Law of Diffusion and the Law of Conservation of Mass, in the infinitesimal period dt, the mass dm which flows through the infinitesimal area dS along the normal direction n is proportional to the derivative $\frac{\partial N}{\partial n}$ of the concentration along the normal direction of the curved surface ds, which can be expressed as:

$$dm = -D(x,y,z)\frac{\partial N}{\partial n}dSdt \qquad (1)$$

Where D(x, y, z) is called the diffusion coefficient of substance G at the point (x, y, z) in the solution.

For an arbitrary closed curved surface Γ in the solution, the region enclosed by it is referred as Ω. The entire mass of G which flows into this closed curved surface from time t_1 to t_2 is defined as

$$m = \int_{t_1}^{t_2} \iint_{\Gamma} D(x,y,z) \frac{\partial N}{\partial n} dSdt \qquad (2)$$

Where $\frac{\partial N}{\partial n}$ represents the directional derivative of N along the unit normal direction n of the surface Γ.

The mass of the inflow indicates that the concentration of the substance G in the Ω has changed. In the time interval (t_1, t_2), the concentration has changed from N(x, y, z, t_1) to N(x, y, z, t_2), while the mass of G corresponding to the changed concentration is defined as

$$\iiint_{\Omega} [N(x,y,z,t_2) - N(x,y,z,t_1)] dxdydz$$

From the Law of Conservation of Mass, we can determine

$$\int_{t_1}^{t_2} \iint_{\Gamma} D \frac{\partial N}{\partial n} dSdt = \iiint_{\Omega} [N(x,y,z,t_2) - N(x,y,z,t_1)] dxdydz \qquad (3)$$

Suppose that the element N has second-order continuous partial derivatives about (x, y, z) and a first-order continuous partial derivatives about t. According to Green's Formula, we can put equation (3) into

$$\int_{t_1}^{t_2} \iiint_{\Omega} \left[\frac{\partial}{\partial x}(D\frac{\partial N}{\partial x}) + \frac{\partial}{\partial y}(D\frac{\partial N}{\partial y}) + \frac{\partial}{\partial z}(D\frac{\partial N}{\partial z}) \right] dt = \iiint_{\Omega} \left(\int_{t_1}^{t_2} \frac{\partial N}{\partial t} dt \right) dxdydz$$

Exchanging the integral order to determine

$$\int_{t_1}^{t_2} \iiint_{\Omega} \left[\frac{\partial N}{\partial t} - \frac{\partial}{\partial x}(D\frac{\partial N}{\partial x}) - \frac{\partial}{\partial y}(D\frac{\partial N}{\partial y}) - \frac{\partial}{\partial z}(D\frac{\partial N}{\partial z}) \right] dt = 0 \qquad (4)$$

As t_1, t_2 and the region Ω are arbitrary, we can determine

$$\frac{\partial N}{\partial t} = \frac{\partial}{\partial x}(D\frac{\partial N}{\partial x}) + \frac{\partial}{\partial y}(D\frac{\partial N}{\partial y}) + \frac{\partial}{\partial z}(D\frac{\partial N}{\partial z}) \qquad (5)$$

If the solution is uniform, then D is a constant, that is,

$$\frac{\partial N}{\partial t} = D(\frac{\partial^2 N}{\partial x^2} + \frac{\partial^2 N}{\partial y^2} + \frac{\partial^2 N}{\partial z^2}) \qquad (6)$$

If the diffusion occurs in an enclosed thin layer, the diffusion equation is dimension-decreased to be two-dimensional equation, which is expressed as

$$\frac{\partial N}{\partial t} = D(\frac{\partial^2 N}{\partial x^2} + \frac{\partial^2 N}{\partial y^2}) \qquad (7)$$

In the moisture-containing porous unsaturated soil, the main migration form of heavy metal pollution is the diffusion in the soil and the migration of soluble heavy with soil moisture[11]("Improvement model of coupled transmission process in unsaturated porous media"). In the soil, the diffusion capacity of the non-soluble heavy metal compound and the heavy metal dust particles is very weak, so the impact can be ignored. With the soil layer is deeper, the pore size of soil will be smaller and the soil is mostly clay, which has a strong block to heavy metals [12]("The study of the accommodate block ability of clay to heavy metal pollutant "), that will greatly hindered the diffusion of heavy metal. When certain depth is reached, the vertical proliferation can be ignored. Relative to the entire region, the thickness is so small that the entire area can be regarded as a thin slice. With soluble heavy metal compound treated as the solute, the concentration distribution of the heavy metal pollutant satisfies equation (7) approximately.

To solve the equation (7), the initial and boundary conditions are necessary, which are

$$\begin{cases} \frac{\partial N}{\partial t} = D(\frac{\partial^2 N}{\partial x^2} + \frac{\partial^2 N}{\partial y^2}), \\ N(x,y,0) = \varphi(x,y), \\ N\Big|_{x^2+y^2=R^2} = 0. \end{cases}$$

Where the initial condition $\varphi(x,y)$ denotes the initial distribution of pollutant concentration and the boundary condition denotes when R large enough, the region outside is almost free from contamination, that is, the pollutant concentration is 0.

We use the method of variables separation to solve the partial differential equations. Taking $N(x,y,t) = T(t)V(x,y)$ into the above equation first, we can determine

$$\frac{T^{'}(t)}{DT(t)} = \frac{\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2}}{V(x,y)} = -\lambda,$$

Where λ is a non-zero constant.

Processing separation to get

$$T^{'}(t) + \lambda DT(t) = 0 \qquad (8)$$

$$\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} + \lambda V = 0 \qquad (9)$$

From the above, we can determine

$$T(t) = Ae^{-D\lambda t}$$

The equation (9) can be rewritten into polar form, which is

$$\frac{\partial^2 V}{\partial r^2} + \frac{1}{r}\frac{\partial V}{\partial r} + \frac{1}{r^2}\frac{\partial^2 V}{\partial \theta^2} + \lambda V = 0 \qquad (10)$$

Continues using the method of variables separation and taking $V(r,\theta) = R(r)\Theta(\theta)$ into equation (10), we can determine

$$\frac{\partial^2 R(r)}{\partial r^2}\Theta(\theta) + \frac{1}{r}\frac{\partial R(r)}{\partial r}\Theta(\theta) + \frac{1}{r^2}R(r)\frac{\partial^2 \Theta(\theta)}{\partial \theta^2} + \lambda\Theta(\theta)R(r) = 0 \qquad (11)$$

The moisture-containing porous unsaturated soil can be seen as the solution of heavy metal pollutant. With the soil properties are similar and the water content is basically the same in some areas, it can be regarded as the homogeneous solution with isotropic. Thus, $\Theta(\theta)$ and θ are not associated. With only one variable θ contained in $\Theta(\theta)$, $\Theta(\theta)$ is a constant. Then the equation (11) can be defused as

$$\frac{\partial^2 R(r)}{\partial r^2} + \frac{1}{r}\frac{\partial R(r)}{\partial r} + \lambda R(r) = 0 \qquad (12)$$

Taking $\rho = r\sqrt{\lambda}$ as a replacement, equation (11) can be expressed as

$$\rho^2 \frac{\partial^2 R(\rho)}{\partial \rho^2} + \rho\frac{\partial R(\rho)}{\partial \rho} + \rho^2 R(\rho) = 0 \qquad (13)$$

The solution of the equation (13) is the zero-order Bessel function, that is,

$$R(\rho) = J_0(\rho) = \sum_{m=0}^{\infty} \frac{(-1)^m \cdot a_0}{2^{2m}(m!)^2}\rho^{2m}$$

Taking $r = \rho / \sqrt{\lambda}$ as a replacement contrary to above, it can be expressed as

$$R(r) = \sum_{m=0}^{\infty} \frac{(-1)^m \cdot a_0}{2^{2m}(m!)^2 \lambda^m} r^{2m}$$

Thus the results can be determined as

$$N(r,\theta,t) = Ae^{-D\lambda t} \cdot \Theta(\theta) \cdot \sum_{m=0}^{\infty} \frac{(-1)^m \cdot a_0}{2^{2m}(m!)^2 \lambda^m} r^{2m}$$

Where $A, \Theta(\theta), a_0$ are non-zero constants, therefore the final results can be expressed as

$$N(r,t) = Ae^{-D\lambda t} \cdot \sum_{m=0}^{\infty} \frac{(-1)^m}{2^{2m}(m!)^2 \lambda^m} r^{2m} \qquad (14)$$

According to the boundary and initial conditions, the constants λ and A can be determined respectively to obtain the propagation equation of the heavy metal pollutant completely.

3. APPLICATION OF THE MODEL

In equation (14), the time variable t is included. However, in general, when a certain region is to be sampled, the sampling interval is so short that we can ignore the difference of sampling moment of the respective sampling points, that is, the time variable t and $e^{-D\lambda t}$ in the natural equation are both constants. Thus the equation (14) can be expressed as

$$N(r,t) = A \cdot \sum_{m=0}^{\infty} \frac{(-1)^m}{2^{2m}(m!)^2 \lambda^m} r^{2m} \qquad (15)$$

Assuming that there is only one source of pollution in the sampled region and the form of pollution is point pollution, prior to the pollution, this region has not been contaminated, or the time interval between this pollution and the last contaminated is long enough to avoid affecting the current pollution dispersion. Thus, the pollution dispersion form in this region greatly conforms to the propagation model proposed in this paper. If the boundary and initial conditions are determined, we can solve equation (15) to draw the unknown variables. In fact, for the time factor is eliminated, the statement of the initial conditions no longer exists. Meanwhile, the initial conditions cannot be obtained because the initial condition is the description of the pollutant concentration of the whole region. The boundary conditions also cannot be determined according to the information of the sampling points because the pollution source is unknown in advance, so the radius R of the region in the equation $N\big|_{x^2+y^2=R^2} = N_0$ cannot be determined. Although it is impossible to solve this equation, we can get the revelation: we can assume a point (x_0, y_0) as the pollution source and N_0 as the concentration, then, A in the equation (15) is equal to N_0. The boundary conditions can be determined by treating those sampling points which are close to the background value of heavy metal elements as the boundary, thereby variable λ in the formula and the spatial distribution function of the concentration are also determined. We know that the concentration of pollution sources is the largest, which provides reference range when we determine the value of N_0. N_0 should be larger than the maximum value of the sampling points, and the upper limit can be assumed based on experience, or it can also be set great sufficiently. For each value of N_0, we can get a different distribution function, which corresponds to the theoretical value of this function according to the coordinates of the sampling points and then calculate the variance of the theoretical value and the actual value. According to the preset scope and the required accuracy, N_0 is traversed to get a minimum variance for the point (x_0, y_0). Then, we can identify the minimum variance points, that is, the pollution sources by point traversal. In conclusion, we establish a method to find the pollution sources by the information of sampling points. It should be noted that the above work can be carried out by Matlab.

4. CONCLUSION

In the paper, we propose a point propagation model of heavy metals in the soil based on the Diffusion Law and the Law of Conservation of Mass. Three-dimensional point source propagation model is established on the basis of the assumption that soil is isotropic, and then based on the dynamic balance of the elements in the vertical direction, the model is transformed to two-dimensional point source propagation model by dimension reduction. It can be further simplified as two-dimensional harmonic equation by the assumption that the concentration change rate is constant or the rate is very slow, thus the distribution law of heavy metals in the soil is obtained. All this extend a method to determine the pollution sources by the information of sampling points. The method is simple and flexible, and is suitable in engineering application. In addition, the accuracy is relatively high by experimental verification.

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