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Original Research Paper

Modelling of Grey Differential Model of River Water Pollution and its Application

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ABSTRACT

Based on the grey theory, grey characters of river environment system were analyzed. The velocity and dispersion coefficient and attenuation in river were considered as uncertainty parameters and expressed as grey parameters. A grey differential equation of contaminant diffusion in river was built. And the equation has special structure. The truncation error of finite differential method in solving the model was corrected. According to the model, distribution values of pollutant concentration under sudden pollutant discharge can be obtained directly, which can provide abundant and useful water quality information for the plan and control of water pollution. It is shown that the calculated results obtained from the grey model are reliable and reasonable.

INTRODUCTION

The Grey systematic theory is proposed by Chinese professor Deng (1982). In the theory, there is not only a large amount of known information called white system, but also much unknown and uncertain information called black system. The system including white system and black system is called grey system. Contaminant transport in natural river system usually occurs in varied flow fields and in anisotropic and heterogenous media. Because the applicability of analytical solutions is extremely limited for such conditions, numerical techniques are essential for underground pollution simulation. Mecarthy (1989), Li & Wang (2004), Li et al. (2005) and Basha & El-Habel (1999) made much work about the uncertain issues. Among the numerical techniques, the grey numerical method has become very popular and is recognized as a powerful numerical tool. The distribution and transport of pollutants mentioned by Liu et al. (1999), Chen & Wagenet (1995), Xu et al. (2002) in groundwater are controlled by physical chemistry and biology functions, which include advection, diffusion, dispersion, sorption, decay and biodegradation. In the courses, there is not only the known information but also uncertain information. Therefore, it can be seen as one grey system. Considering the above mechanism synthetically, two-dimensional grey model about river water pollution is built in this paper. It has the significant practical value for the research of grey simulation of river water pollution.

ESTABLISHMENT OF THE FINITE DIFFERENTIAL EQUATION OF ATMOSPHERIC POLLUTION

Grey characters in water environment system: Water environment can be seen as an open system of large-scale systems. Flow rate, pollutant concentration, diffusion coefficient and attenuation coefficient parameter information in river system exist uncertainty. In these uncertainties, some information is an objective existence, and some are not entirely caused from the measured data, and some are caused by unclear inherent mechanism and unclear understanding of the changing law. But no matter what reasons the uncertainty is brought, would lead to decision-makers on water environmental systems on the subjective perception of uncertainty, that is unascertained. So, velocity and dispersion coefficient and attenuation in river are considered as uncertainty parameters and expressed as grey parameters. And the advection-dispersion equation is studied based on grey theory.

Grey numerical model for one-dimensional water quality: The mathematic model of solute transport equation can be written as follows:

$$\frac{\partial(\otimes c)}{\partial t}=(\otimes E)\frac{\partial^2(\otimes c)}{\partial x^2}-(\otimes u)\frac{\partial(\otimes c)}{\partial x}-(\otimes k)(\otimes c) \quad ...(1)$$

Where, $\otimes c$ is grey concentration of pollutant in section, mg/l; $\otimes E$ is the grey diffusion coefficients in the landscape orientation, m^2/s; $\otimes u$ is grey velocity in section; t is time,

s ; and x is distance, *m*.

To any differential equation, its solution can only be solved in special initial condition and boundary condition. In this paper, the constraint condition can be described as follows:

$$\begin{aligned} &\otimes c(x,0)=0 && x>0 \\ &\otimes c(0,t)=c_0 && t\geq 0 \\ &\otimes c(L,t)=0 && t=0 \end{aligned} \quad ...(2)$$

Finite difference equation can replace differential equation as follows:

$$\frac{\partial(\otimes c)}{\partial t}=\frac{(\otimes c)_i^{n+1}-(\otimes c)_i^n}{\Delta t}$$

$$\frac{\partial^2(\otimes c)}{\partial x^2}=\frac{(\otimes c)_{i+1}-2(\otimes c)_i+(\otimes c)_{i-1}}{(\Delta x)^2}$$

$$\frac{\partial(\otimes c)}{\partial x}=\frac{(\otimes c)_{i+1}-(\otimes c)_i}{\Delta x}$$

Because the finite difference approach uses limited developments of derivatives, it is only an approximation of partial differential equations leading to truncation errors. Truncation errors affect the accuracy of numerical simulations. A Taylor series expansion of *c* about any grid point is used to determine the form of truncation errors (Zhu et al. (2006). If terms of third and higher orders are neglected, then:

$$(\otimes c)_{i,j}^{n+1}\approx(\otimes c)_{i,j}^n+\Delta t\frac{\partial(\otimes c)}{\partial t}+\frac{\Delta t^2}{2}\frac{\partial^2(\otimes c)}{\partial t^2} \quad ...(3)$$

$$(\otimes c)_{i\pm1,j}^n\approx(\otimes c)_{i,j}^n\pm\Delta x\frac{\partial(\otimes c)}{\partial x}+\frac{\Delta x^2}{2}\frac{\partial^2(\otimes c)}{\partial x^2}+0(\Delta x^3) \quad ...(4)$$

$$(\otimes c)_{i,j\pm1}^n\approx(\otimes c)_{i,j}^n\pm\Delta y\frac{\partial(\otimes c)}{\partial y}+\frac{\Delta y^2}{2}\frac{\partial^2(\otimes c)}{\partial y^2}+0(\Delta y^3) \quad ...(5)$$

The second-order temporal derivative of *c* is written in terms of spatial derivatives using the differentiated form of eq. [11]. The transport parameters are assumed to be constant within each combination of time and space increments in the finite difference calculations. Thus, to second order accuracy:

$$\begin{aligned}\frac{\partial^2(\otimes C)}{\partial t^2}&=[(\otimes u)^2-2(\otimes k)(\otimes D_{xx})]\frac{\partial^2(\otimes C)}{\partial x^2}-\\ &2(\otimes k)(\otimes D_{yy})\frac{\partial^2(\otimes C)}{\partial y^2}+\\ &2(\otimes u)(\otimes k)\frac{\partial(\otimes C)}{\partial x}+(\otimes k)^2(\otimes C)\end{aligned} \quad ...(6)$$

Eq. (6) may then be written as:

$$\begin{aligned}\frac{\partial(\otimes C)}{\partial t}&=\left\{(\otimes D_{xx})-\frac{\Delta t}{2}[(\otimes u)^2-2(\otimes k)(\otimes D_{xx})]\right\}\frac{\partial^2(\otimes C)}{\partial x^2}+\\ &[(\otimes D_{yy})+\Delta t(\otimes k)(\otimes D_{yy})]\frac{\partial^2(\otimes C)}{\partial y^2}-[(\otimes u)+\Delta t(\otimes u)(\otimes k)]\frac{\partial(\otimes C)}{\partial x}-\\ &[(\otimes k)+\frac{\Delta t}{2}(\otimes k)^2](\otimes C)+s(x,y,t)\end{aligned} \quad ...(7)$$

Namely:

$$(\otimes D_{xx})^*=(\otimes D_{xx})-\frac{\Delta t}{2}[(\otimes u)^2-2(\otimes k)(\otimes u)]$$

$$(\otimes D_{yy})^*=(\otimes D_{yy})+\Delta t(\otimes k)(\otimes D_{yy})$$

$$(\otimes u)^*=(\otimes u)+\Delta t(\otimes k)(\otimes u)$$

$$(\otimes k)^*=(\otimes k)+\frac{\Delta t}{2}(\otimes k)^2$$

Eq. (7) can be simplified as:

$$\begin{aligned}\frac{\partial(\otimes C)}{\partial t}&=(\otimes D_{xx})^*\frac{\partial^2(\otimes C)}{\partial x^2}+(\otimes D_{yy})^*\frac{\partial^2(\otimes C)}{\partial y^2}\\ &-(\otimes u)^*\frac{\partial(\otimes C)}{\partial x}-(\otimes k)^*(\otimes C)+s(x,y,t)\end{aligned} \quad ...(8)$$

To remove the induced truncation errors from the finite difference model, the model can be rewritten as:

$$\begin{aligned}&(D_{xx})^*\frac{(\otimes C)_{i-1,j}^{n+1}-2(\otimes C)_{i,j}^{n+1}+(\otimes C)_{i+1,j}^{n+1}}{(\Delta x)^2}+\\ &(D_{yy})^*\frac{(\otimes C)_{i,j-1}^{n+1}-2(\otimes C)_{i,j}^{n+1}+(\otimes C)_{i,j+1}^{n+1}}{(\Delta y)^2}\\ &-(\otimes u)^*\frac{(\otimes C)_{i+1,j}^{n+1}-(\otimes C)_{i-1,j}^{n+1}}{2\Delta x}-\\ &(\otimes k)^*(\otimes C)_{i,j}^{n+1}=\frac{(\otimes C)_{i,j}^{n+1}-(\otimes C)_{i,j}^n}{\Delta t}\end{aligned} \quad ...(9)$$

Where,

$$\frac{(\otimes E_x)^*\cdot\Delta t}{(\Delta x)^2}=\otimes A;\ \frac{(\otimes E_y)^*\cdot\Delta t}{(\Delta y)^2}=\otimes B;$$

$$\frac{(\otimes u)^*\cdot\Delta t}{2\Delta x}=\otimes M$$

$$\begin{aligned}&[2(\otimes A)+2(\otimes B)+(\otimes k)\cdot\Delta t+1](\otimes C)_{i,j}^{n+1}\\ &-[(\otimes A)+(\otimes M)](\otimes C)_{i-1,j}^{n+1}\\ &-[(\otimes A)-(\otimes M)](\otimes C)_{i+1,j}^{n+1}\\ &-(\otimes B)(\otimes C)_{i,j-1}^{n+1}-(\otimes B)(\otimes C)_{i,j+1}^{n+1}=(\otimes C)_{i,j}^n\end{aligned} \quad ...(10)$$

Adopting the same picking-number with the grey number, the two following equations can be obtained.

$$\begin{aligned}&(2[A_b]+2[B_b]+[k_b]\cdot\Delta t+1)[C_b]_{i,j}^{n+1}-([A_a]+[M_a])[C_a]_{i-1,j}^{n+1}\\&-([A_a]-[M_b])[C_a]_{i+1,j}^{n+1}-[B_a][C_a]_{i,j-1}^{n+1}-[B_a][C_a]_{i,j+1}^{n+1}=[C_a]_{i,j}^{n}\end{aligned} \quad ...(11)$$

$$\begin{aligned}&(2[A_a]+2[B_a]+[k_a]\cdot\Delta t+1)[C_a]_{i,j}^{n+1}-([A_b]+[M_b])[C_b]_{i-1,j}^{n+1}\\&-([A_b]-[M_a])[C_b]_{i+1,j}^{n+1}-[B_b][C_b]_{i,j-1}^{n+1}-[B_b][C_b]_{i,j+1}^{n+1}=[C_b]_{i,j}^{n}\end{aligned} \quad ...(12)$$

The equation has the special structure, which can be solved by the special method [3][11].

$$\begin{bmatrix} a_{11}C_{1b} & a_{12}C_{2a} & a_{13}C_{3a} & \cdots & a_{1l}C_{la} \\ a_{21}C_{1a} & a_{22}C_{2b} & a_{23}C_{3a} & \cdots & a_{2l}C_{la} \\ a_{31}C_{1a} & a_{32}C_{2a} & a_{33}C_{3b} & \cdots & a_{3l}C_{la} \\ & \cdots & & \cdots & \\ a_{l1}C_{1a} & a_{l2}C_{2a} & a_{l3}C_{3a} & \cdots & a_{ll}C_{lb} \end{bmatrix} = \begin{bmatrix} f_{1a} \\ f_{2a} \\ f_{3a} \\ \cdots \\ f_{la} \end{bmatrix} \quad ...(13\text{-}1)$$

$$\begin{bmatrix} b_{11}C_{1a} & b_{12}C_{2b} & b_{13}C_{3b} & \cdots & b_{1l}C_{lb} \\ b_{21}C_{1b} & b_{22}C_{2a} & b_{23}C_{3b} & \cdots & b_{2l}C_{lb} \\ b_{31}C_{1b} & b_{32}C_{2b} & b_{33}C_{3a} & \cdots & b_{3l}C_{lb} \\ & \cdots & & \cdots & \\ b_{l1}C_{1b} & b_{l2}C_{2b} & b_{l3}C_{3b} & \cdots & b_{ll}C_{la} \end{bmatrix} = \begin{bmatrix} f_{1b} \\ f_{2b} \\ f_{3b} \\ \cdots \\ f_{lb} \end{bmatrix} \quad ...(13\text{-}2)$$

Where, $l = m \times n$

$$a_b^{i,j,n+1} = 1 + \frac{\Delta t\cdot k_b}{\Delta x} + 2\frac{\Delta t\cdot E_{xb}}{(\Delta x)^2} + 2\frac{\Delta t\cdot E_{yb}}{(\Delta y)^2}\Delta t$$

$$a_a^{i,j+1,n+1} = -\frac{\Delta t\cdot E_a}{(\Delta y)^2}\ \text{ÿ}\ a_a^{i,j-1,n+1} = -\frac{\Delta t\cdot E_{ya}}{(\Delta y)^2}$$

$$a_a^{i-1,j,n+1} = -\left(\frac{\Delta t\cdot E_a}{\Delta x^2} + \frac{u_a\Delta t}{2\Delta x}\right)$$

$$b_a^{i,j,k+1} = 1 + \frac{\Delta t\cdot k_a}{\Delta x} + 2\frac{\Delta t\cdot E_{xa}}{(\Delta x)^2} + \frac{\Delta t\cdot E_{ya}}{(\Delta y)^2}$$

$$b_b^{i,j+1,k+1} = -\frac{\Delta t\cdot E_b}{(\Delta y)^2};\quad b_b^{i,j-1,k+1} = -\frac{\Delta t\cdot E_{yb}}{(\Delta y)^2}$$

$$b_b^{i-1,j,k+1} = -\frac{\Delta t\cdot u_b}{\Delta x} - \frac{\Delta t\cdot u_b}{2\Delta x}$$

$$f_a^{i,j,k} = c_a^{i,j,k} + \Delta t\cdot s_a;\quad f_b^{i,j,k} = c_b^{i,j,k} + \Delta t\cdot s_b$$

The two equations can be solved by turns as following, and the grey concentration of groundwater quality (c_{ai} c_{bi}) can be obtained.

$$\begin{aligned}&c_{ai}^0 \xrightarrow{(13\text{-}2)} c_{bi}^1 \xrightarrow{(13\text{-}1)} c_{ai}^2 \xrightarrow{(13\text{-}2)} c_{bi}^3\ \mathbf{L\,L}\\&c_{bi}^0 \xrightarrow{(13\text{-}1)} c_{ai}^1 \xrightarrow{(13\text{-}2)} c_{bi}^2 \xrightarrow{(13\text{-}1)} c_{ai}^3\ \mathbf{L\,L}\end{aligned} \quad ...(14)$$

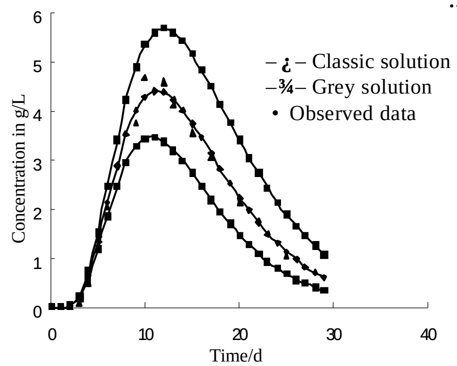

Fig. 1: Impact of grey diffusion coefficient on migration of pollutant.

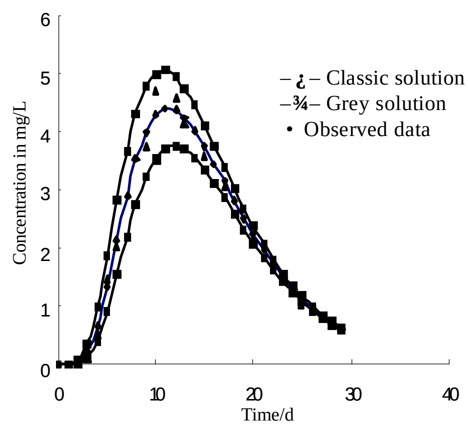

Fig. 2: Impact of grey velocity on migration of pollutant.

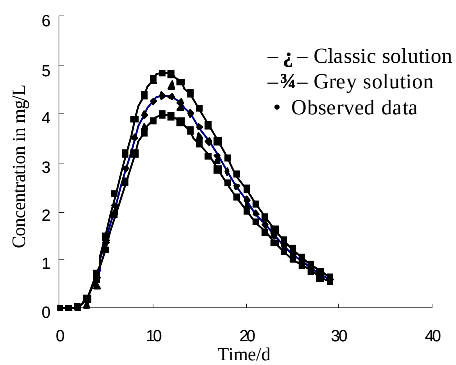

Fig. 3: Impact of grey decay coefficient on migration of pollutant.

APPLICATION

To one-dimensional river water pollution problem, the governed equation and constraint condition can be described as equation1 and equation 2. In order to verify the model, the grey result will be compared with classic numerical solution. For information input, relationship of decay coefficient k and (k_a, k_b) with pollutant concentration c and (c_a, c_b), and velocity u and (u_a, u_b) with pollutant concentration are needed to be considered. In order to analyse the sensitivity, when analyzing one parameter's influence on pollutant concentration, other parameters remains unchanged, and grey parameter can float its lower and upper value 10%. The parameters are as follows:

$k = 0.2$, $k_a = 0.18$, $k_b = 0.22$, $u = 4m/s$, $u_a = 3.6m/s$,

$u_b = 4.4m/s$, $E = 400$, $E_a = 360$, $E_b = 440$

The calculated results can be seen from Figs. 1 to 3. We can see that the curve of contaminant transport by grey numerical model is one "grey strip". That is to say the value of grey numerical model changes in some ranges, but not one certain value. While the analytical solution is within the ranges, this reveals that the method is reliable. In present study, the data of hydraulic and water quality in river water system is absent, so the grey mathematic model can be applied to the fields. Influence scope of decay coefficient is lager than other parameters.

CONCLUSIONS

1. It is reasonable and reliable that simulation and prediction of groundwater quality with uncertain information is made by grey mathematic, which provides one new method to simulate and predict the groundwater quality.
2. Compared with analytical solution, some uncertain parameters in grey model such as dispersion coefficient and seepage velocity can be given grey ranges. The result is one grey strip which has great advantages for the application of model and decision-making.
3. The numerical model in this paper has the common applicability to the surface water pollution and convection-diffusion equation.

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