Numerical Simulation of River Water Pollution Using Grey Differential Model

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***Abstract*—Based on the grey theory, grey characters of river environment system are analyzed, the velocity and dispersion coefficient and attenuation in river are considered as uncertainty parameters and expressed as gray parameters. A grey differential equation of contaminant diffusion in river is built. And the equation has special structure. The truncation error of finite differential method in solving the model is corrected. According to the model, distribution values of pollutant concentration under sudden pollutant discharged 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 gray model are reliable and reasonable.**

***Index Terms*—grey model; truncation error; finite differential**

I. Introduction

Gray systematic theory is proposed by Chinese professor Deng Jurong in 1982 [1]. 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 gray 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 [2], Li et al. [3],Li & Wang[4], Basha & El-Habel [5] made much work about the uncertain issues. Among the numerical techniques, the gray 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. [6], Chen & Wagenet [7], Xu et al. [8] 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 gray system. Considering the above mechanism synthetically, two-dimensional gray model about river water pollution is built in this paper. It has the significant practical value for the research of gray simulation of river water pollution.

II. Mechanism of Contaminant Transport

The contamination usually occurs at an isolated sites, and then infiltrates the soil and finally into groundwater. Following the groundwater flow, contaminants are transported and dispersed to the surrounding areas. Several processes are involved with this transport, including advection, diffusion, dispersion, sorption, decay and biodegradation.

A. Advection

Contaminant advection is defined as the movement of contaminants with the groundwater flow through the porous media. The gray advection flux is:

$$\otimes F_x = \otimes v \cdot \otimes c \tag{1}$$

Where $\otimes F_x$ is the gray convection flux of pollutant in x direction ($mg/(m^2 \cdot s)$); $\otimes v$ is the velocity in x direction(m/s); $\otimes c$ is the gray density of pollutant (mg/m^3).

B. Diffusion

Diffusion is the process of molecular and ionic movements. Because of the irregular moving of molecule, solutes in groundwater move from high density to low density by diffusion. This course is called molecule diffusion. Even if in the static situation, materials can be transformed to make the interface between pollutant and groundwater gradually smudgy and gradually diffuse with time. The diffusion flux can be got through the first Fick law.

$$\otimes M_1 = -\otimes D_m \frac{\partial \otimes c}{\partial x} \tag{2}$$

Where $\otimes M_1$ is the gray molecule spreading flux,($g/(m^2 \cdot s)$); $\otimes D_m$ is Coefficient of molecule spreading(m^2/s).

C. Dispersion

Dispersion is a mixing process during the computation of contaminant advection. The mean velocity and density represent the distribution value for simplicity. Generally, dispersion is recognized as an irreversible course. By analysis, the gray flux can also be described by the first Fick law, that is:

$$\otimes M_2 = -\otimes D_o \frac{\partial \otimes c}{\partial x} \tag{3}$$

Where $\otimes M_2$ is dispersion flux in x direction ($g/(m^2 \cdot s)$), $\otimes D_o$ is Coefficient of dispersion

doi:10.4304/jcp.5.9.1417-1423

(m^2/s)

D. Radioactive decay

Substances containing radioelement in the groundwater will have disintegration with time so as to reduce density. The rule of Radioactive decay can be described as follows

$$\otimes c = \otimes c_0 \exp(-\lambda_0 t) \quad (4)$$

So $$\frac{\partial(\otimes c)}{\partial t} = -\lambda_0(\otimes c) \quad (5)$$

E. Adsorption and desorption

Absorption and desorption is an appearance which occurs in the cross section between solid and liquid phase. Solute in liquid phase may be absorbed by solid phase, while, solute in solid phase can enter liquid phase by the effect of solute and ion exchange. Here, we use Henery absorption constant temperature formula to calculate:

$$\otimes s = (\otimes k)(\otimes C) \quad (6)$$

Where $\otimes s$ is gray concentration of solid when equilibrium of absorption arrives (ug/g), $\otimes k$ is experience constant, which is relevant to factors such as water temperature and nature of pollutant and so on; $\otimes c$ is gray concentration of pollutants in groundwater environment when absorption equilibrium arrives.

F. Biodegradation

Organic contaminants in groundwater system degrade into inorganic matters and synthesize new cell under the effects of microbial population gradually, which makes the concentration of organic contaminants decreased. Degradation velocity of microbes and pollutants is relevant to biochemical action. The velocity has a vital and common sense to anticipate and control of organic contaminants.

Biodegradation velocity of organic contaminants can be described as follows:

$$\frac{d(\otimes C)}{dt} = -\frac{v_m(\otimes C)}{K_c + (\otimes C)} X \quad (7)$$

Where X is concentration of microbes at present time (mg/l), K_c is constant, Concentration of organic contaminants in groundwater is generally low, that's to say, $\otimes C$ is much smaller than K_c, the formula above can be transformed to:

$$\frac{d(\otimes C)}{dt} = -\frac{v_m X}{K_c}(\otimes C) \quad (8)$$

Because microbes are short of food under the environment of low contaminant concentration, increment speed of organic contaminants is rather little, which means that concentration of microbes is turning balanced population. $\frac{v_m}{K_c} = k_1$, here, k_1 can be treated as a constant, so

$$\frac{d(\otimes C)}{dt} = -(\otimes k_1)(\otimes C) \quad (9)$$

G. Retardation

Sorption results in retardation which is the phenomenon that the contaminant solute does not move as fast as the general groundwater flow. Transportation of organic chemicals in geological medium is influenced by groundwater flow, adsorption and desorption, ion exchange, chemical precipitation/solution, mechanical filtration and many other physico-chemical reactions. The transportation way is nearly the same with the way of groundwater flow. Transportation velocity of contaminants has the relationship with the velocity of groundwater flow as follows:

$$\otimes v' = \otimes v / \otimes R_d \quad (10)$$

Where $\otimes R_d$ is the gray retardation coefficient of pollutants in porous medium.

III. Establishment of Finite Differential Equation of River Water Pollution

Assuming pollutant particles and river environment particles have the same hydromechanics characteristics. On the basis of discussing parameters and variables, the finite differential equation of air pollution is educed according to the principles of mass conservation and energy conservation. The process is as follows.

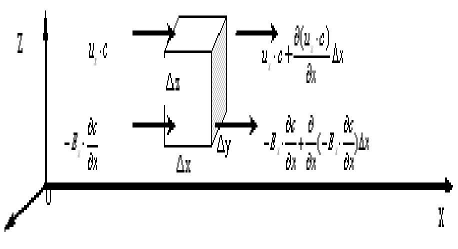

Figure 1. Mass balance in a volume element

As shown in Fig.1, pollutant inputting of each volume element in X direction at unit time is $[u_x \cdot c + (-D_{xx} \cdot \frac{\partial(c)}{\partial x})]\Delta y \Delta z$

Pollutant outputting of each volume element in X direction at unit time is

$$u_x \cdot c + \frac{\partial u_x \cdot c}{\partial x}\Delta x + (-D_{xx}\frac{\partial c}{\partial x}) + \frac{\partial}{\partial x}(-D_{xx} \cdot \frac{\partial c}{\partial x})\Delta x]\Delta y \Delta z$$

So the pollutant change quantity in X direction at unit time is

$$[u_x \cdot c + (-D_{xx} \cdot \frac{\partial c}{\partial x})]\Delta y \Delta z - u_x \cdot c + \frac{\partial u_x \cdot c}{\partial x}\Delta x + (-D_{xx}\frac{\partial c}{\partial x}) + \frac{\partial}{\partial x}(-D_{xx} \cdot \frac{\partial c}{\partial x})\Delta x]\Delta y \Delta z$$
$$= -[\frac{\partial(u_x \cdot c)}{\partial x} + \frac{\partial}{\partial x}(-D_{xx} \cdot \frac{\partial(c)}{\partial x})]\Delta x \Delta y \Delta z$$

Similarly, the pollutant change quantities in Y,Z direction at unit time respectively are

$$-[\frac{\partial(u_y\cdot c)}{\partial y}+\frac{\partial}{\partial y}(-D_{yy}\cdot\frac{\partial(c)}{\partial y})]\Delta x\Delta y\Delta z-[\frac{\partial(u_z\cdot c)}{\partial z}+\frac{\partial}{\partial z}(-E_z\cdot\frac{\partial(c)}{\partial z})]\Delta x\Delta y\Delta z$$

If pollutant takes place attenuation reactions and contains sources and sinks in the volume element, corresponding pollutant change quantity will be $(\otimes s-\otimes k\cdot\otimes c)\Delta x\Delta y\Delta z$. Thereupon, in the unit time pollutant change quantity of the volume element is

$$\frac{\partial(c)}{\partial t}\Delta x\Delta y\Delta z=-[\frac{\partial(u_x\cdot c)}{\partial x}+\frac{\partial}{\partial x}(-E_x\cdot\frac{\partial c}{\partial x})]\Delta x\Delta y\Delta z$$
$$-[\frac{\partial(u_y\cdot c)}{\partial y}+\frac{\partial}{\partial y}(-E_y\cdot\frac{\partial(c)}{\partial y})]\Delta x\Delta y\Delta z-[\frac{\partial(u_z\cdot c)}{\partial z}+\frac{\partial}{\partial z}(-E_z\cdot\frac{\partial c}{\partial z})]\Delta x\Delta y\Delta z$$
$$-(s-k\cdot c)\Delta x\Delta y\Delta z$$

In a homogeneous flow field, u_x and E_y are the non-dynamic volumes, which can be taken as constants. Order the volume element $\Delta x\Delta y\Delta z=1$, then the following equation can be obtained

$$\frac{\partial c}{\partial t}=E_x\cdot\frac{\partial^2 c}{\partial x^2}+E_y\cdot\frac{\partial^2 c}{\partial y^2}+E_z\cdot\frac{\partial^2 c}{\partial z^2}-u_x\cdot\frac{\partial c}{\partial x}-u_y\cdot\frac{\partial c}{\partial y}-u_z\cdot\frac{\partial c}{\partial z}+s-k\cdot c \quad (11)$$

Where， c ——the concentrations of pollutants， mg/m^3；

E_y ——the grey diffusion coefficients in the landscape orientation， m^2/s；

u_x ——the grey wind speed in the predominant direction (vertical)， m/s；

s ——the sources and sinks of air pollutants， $mg/m^3\cdot s$；

k ——the attenuation coefficient of air pollutants， s^{-1}；

t ——the migration time of air pollutants， s；

$$\frac{\partial(\otimes C)}{\partial t}=(D_{xx})\frac{\partial^2(\otimes C)}{\partial x^2}+(\otimes D_{yy})\frac{\partial^2(\otimes C)}{\partial y^2}-(\otimes u)\frac{\partial(\otimes C)}{\partial x}-(\otimes k)(\otimes C) \quad (12)$$

According to the above analysis, the governing gray equation of groundwater pollution is:

$$\frac{\partial(\otimes C)}{\partial t}=(D_{xx})\frac{\partial^2(\otimes C)}{\partial x^2}+(\otimes D_{yy})\frac{\partial^2(\otimes C)}{\partial y^2}-(\otimes u)\frac{\partial(\otimes C)}{\partial x}-(\otimes k)(\otimes C) \quad (13)$$

The initial and boundary condition:

$$\begin{aligned}&\otimes c(x,0)=0 && x>0\\ &\otimes c(0,t)=c_0 && t\ge 0\\ &\otimes c(\infty,0)=0 && t=0\end{aligned} \quad (14)$$

Using finite difference equation to replace differential equation as followings:

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

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 [7], [9], [10]. If terms of third and higher orders are neglected, then:

$$(\otimes c)_{i,j}^{n+1}\approx(\otimes c)_{i,j}^n+\Delta t\frac{\partial(\otimes c)}{\partial t}+\frac{\Delta t^2}{2}\frac{\partial^2(\otimes c)}{\partial t^2} \quad (15)$$

$$(\otimes c)_{i\pm1,j}^n\approx(\otimes c)_{i,j}^n\pm\Delta x\frac{\partial(\otimes c)}{\partial x}+\frac{\Delta x^2}{2}\frac{\partial^2(\otimes c)}{\partial x^2}+0(\Delta x^3) \quad (16)$$

$$(\otimes c)_{i,j\pm1}^n\approx(\otimes c)_{i,j}^n\pm\Delta y\frac{\partial(\otimes c)}{\partial y}+\frac{\Delta y^2}{2}\frac{\partial^2(\otimes c)}{\partial y^2}+0(\Delta y^3) \quad (17)$$

The second-order temporal derivative of c is written in terms of spatial derivatives using the differentiated form of [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:

$$\frac{\partial^2(\otimes C)}{\partial t^2}=[(\otimes u)^2-2(\otimes k)(\otimes D_{xx})]\frac{\partial^2(\otimes C)}{\partial x^2}-2(\otimes k)(\otimes D_{yy})\frac{\partial^2(\otimes C)}{\partial y^2}+2(\otimes u)(\otimes k)\frac{\partial(\otimes C)}{\partial x}+(\otimes k)^2(\otimes C) \quad (18)$$

Equation (8) may then be written as:

$$\frac{\partial(\otimes C)}{\partial t}=\left\{(\otimes D_{xx})-\frac{\Delta t}{2}[(\otimes u)^2-2(\otimes k)(\otimes D_{xx})]\right\}\frac{\partial^2(\otimes C)}{\partial x^2}+[(\otimes D_{yy})+\Delta t(\otimes k)(\otimes D_{yy})]\frac{\partial^2(\otimes C)}{\partial y^2}-[(\otimes u)+\Delta t(\otimes u)(\otimes k)]\frac{\partial(\otimes C)}{\partial x}-[(\otimes k)+\frac{\Delta t}{2}(\otimes k)^2](\otimes C)+s(x,y,t) \quad (19)$$

namely:

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

Equation (9) can be simplified as

$$\frac{\partial(\otimes C)}{\partial t}=(\otimes D_{xx})^*\frac{\partial^2(\otimes C)}{\partial x^2}+(\otimes D_{yy})^*\frac{\partial^2(\otimes C)}{\partial y^2}-(\otimes u)^*\frac{\partial(\otimes C)}{\partial x}-(\otimes k)^*(\otimes C)+s(x,y,t) \quad (20)$$

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

$$
\begin{aligned}
&(D_{xx})^* \frac{(\otimes C)_{i-1,j}^{n+1} - 2(\otimes C)_{i,j}^{n+1} + (\otimes C)_{i+1,j}^{n+1}}{(\Delta x)^2} + \\
&(D_{yy})^* \frac{(\otimes C)_{i,j-1}^{n+1} - 2(\otimes C)_{i,j}^{n+1} + (\otimes C)_{i,j+1}^{n+1}}{(\Delta y)^2} \\
&-(\otimes u)^* \frac{(\otimes C)_{i+1,j}^{n+1} - (\otimes C)_{i-1,j}^{n+1}}{2\Delta x} - \\
&(\otimes k)^* (\otimes C)_{i,j}^{n+1} = \frac{(\otimes C)_{i,j}^{n+1} - (\otimes C)_{i,j}^{n}}{\Delta t}
\end{aligned} \tag{21}
$$

Where

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

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

$$
\begin{aligned}
&[2(\otimes A) + 2(\otimes B) + (\otimes k)\cdot \Delta t + 1](\otimes C)_{i,j}^{n+1} \\
&-[(\otimes A) + (\otimes M)](\otimes C)_{i-1,j}^{n+1} \\
&-[(\otimes A) - (\otimes M)](\otimes C)_{i+1,j}^{n+1} \\
&-(\otimes B)(\otimes C)_{i,j-1}^{n+1} - (\otimes B)(\otimes C)_{i,j+1}^{n+1} = (\otimes C)_{i,j}^{n}
\end{aligned} \tag{22}
$$

Adopting the same picking-number with the gray number, the two following equations can be obtained [3].

$$
\begin{aligned}
&(2[A_b] + 2[B_b] + [k_b]\cdot \Delta t + 1)[C_b]_{i,j}^{n+1} - ([A_a] + [M_a])[C_a]_{i-1,j}^{n+1} \\
&-([A_a] - [M_b])[C_a]_{i+1,j}^{n+1} - [B_a][C_a]_{i,j-1}^{n+1} - [B_a][C_a]_{i,j+1}^{n+1} = [C_a]_{i,j}^{n}
\end{aligned} \tag{23}
$$

$$
\begin{aligned}
&(2[A_a] + 2[B_a] + [k_a]\cdot \Delta t + 1)[C_a]_{i,j}^{n+1} - ([A_b] + [M_b])[C_b]_{i-1,j}^{n+1} \\
&-([A_b] - [M_a])[C_b]_{i+1,j}^{n+1} - [B_b][C_b]_{i,j-1}^{n+1} - [B_b][C_b]_{i,j+1}^{n+1} = [C_b]_{i,j}^{n}
\end{aligned} \tag{24}
$$

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

$$
\begin{bmatrix}
a_{11}C_{1b} & a_{12}C_{2a} & a_{13}C_{3a} & \cdots & a_{1l}C_{la} \\
a_{21}C_{1a} & a_{22}C_{2b} & a_{23}C_{3a} & \cdots & a_{2l}C_{la} \\
a_{31}C_{1a} & a_{32}C_{2a} & a_{33}C_{3b} & \cdots & a_{3l}C_{la} \\
 & \cdots & & \cdots & \\
a_{l1}C_{1a} & a_{l2}C_{2a} & a_{l3}C_{3a} & \cdots & a_{ll}C_{lb}
\end{bmatrix}
=
\begin{bmatrix} f_{1a} \\ f_{2a} \\ f_{3a} \\ \cdots \\ f_{la} \end{bmatrix} \tag{25-1}
$$

$$
\begin{bmatrix}
b_{11}C_{1a} & b_{12}C_{2b} & b_{13}C_{3b} & \cdots & b_{1l}C_{lb} \\
b_{21}C_{1b} & b_{22}C_{2a} & b_{23}C_{3b} & \cdots & b_{2l}C_{lb} \\
b_{31}C_{1b} & b_{32}C_{2b} & b_{33}C_{3a} & \cdots & b_{3l}C_{lb} \\
 & \cdots & & \cdots & \\
b_{l1}C_{1b} & b_{l2}C_{2b} & b_{l3}C_{3b} & \cdots & b_{ll}C_{la}
\end{bmatrix}
=
\begin{bmatrix} f_{1b} \\ f_{2b} \\ f_{3b} \\ \cdots \\ f_{lb} \end{bmatrix} \tag{25-2}
$$

Where $l = m \times n$

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

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

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

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

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

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

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

The two equations can be solved by turns as followings, the gray concentration of groundwater quality $[c_{ai} \quad c_{bi}]$ can be got.

$$
\begin{aligned}
&c_{ai}^0 \xrightarrow{(15\text{-}2)} c_{bi}^1 \xrightarrow{(15\text{-}1)} c_{ai}^2 \xrightarrow{(15\text{-}2)} c_{bi}^3 \cdots\cdots \\
&c_{bi}^0 \xrightarrow{(15\text{-}1)} c_{ai}^1 \xrightarrow{(15\text{-}2)} c_{bi}^2 \xrightarrow{(15\text{-}1)} c_{ai}^3 \cdots\cdots
\end{aligned} \tag{26}
$$

A. Grey numerical model for one-dimensional water quality

The mathematic model of solute transport equation can be got as followings

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

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

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

$$\otimes c(x,0) = 0 \qquad x > 0$$

$$\otimes c(0,t) = c_0 \qquad t \geq 0$$

$$\otimes c(L,t) = 0 \qquad t = 0$$

Using finite difference equation to replace differential equation as followings

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

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

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

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:

$$\frac{(\otimes c)_i^{n+1} - (\otimes c)_i^n}{\Delta t} = (\otimes E)\frac{(\otimes c)^{n+1}{}_{i+1} - 2(\otimes c)^{n+1}{}_i + (\otimes c)^{n+1}{}_{i-1}}{(\Delta x)^2} - (\otimes u)\frac{(\otimes c)^{n+1}{}_{i+1} - (\otimes c)^{n+1}{}_i}{\Delta x} - (\otimes k)(\otimes c)^{n+1}{}_i$$

$$\frac{(\otimes E)\cdot \Delta t}{(\Delta x)^2} = \otimes A \quad \frac{(\otimes u)\cdot \Delta t}{\Delta x} = \otimes B$$

$$[(\otimes B) - (\otimes A)](\otimes c)_{i+1}^{n+1} + [1 + 2(\otimes A) + (\otimes k)\Delta t](\otimes c)_i^{n+1} - (\otimes A)(\otimes c)_{i-1}^{n+1} = (\otimes c)_i^n$$

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

$$([B_a]-[A_b])[c_a]_{i+1}^{n+1}+(1+2[A_a]+[k_a]\Delta t)[c_a]_i^{n+1}-[A_b][c_b]_{i-1}^{n+1}=[c_b]_i^n$$

$$([B_b]-[A_a])[c_b]_{i+1}^{n+1}+(1+2[A_b]+[k_b]\Delta t)[c_b]_i^{n+1}-[A_a][c_a]_{i-1}^{n+1}=[c_a]_i^n$$

The equation has an special structure as followings:

$$\begin{bmatrix} a_{11}c_{1a}^{n+1} & a_{12}c_{2a}^{n+1} & & & & \\ a_{12}c_{1b}^{n+1} & a_{22}c_{2a}^{n+1} & b_{23}c_{3a}^{n+1} & & & \\ & a_{32}c_{2b}^{n+1} & a_{33}c_{3a}^{n+1} & a_{34}c_{4a}^{n+1} & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & \ddots & \ddots \\ & & & \ddots & \ddots & a_{m-1m}c_{ma}^{n+1} \\ & & & & a_{m-1m-1}c_{m-1b}^{n+1} & a_{mm}c_{ma}^{n+1} \end{bmatrix} = \begin{bmatrix} c_{1a}^n \\ c_{2a}^n \\ c_{3a}^n \\ c_{4a}^n \\ \vdots \\ \vdots \\ c_{ma}^n \end{bmatrix}$$

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$$\begin{bmatrix} b_{11}c_{1b}^{n+1} & b_{12}c_{2b}^{n+1} & & & & \\ b_{21}c_{1a}^{n+1} & b_{22}c_{2b}^{n+1} & b_{23}c_{3b}^{n+1} & & & \\ & b_{32}c_{2a}^{n+1} & b_{33}c_{3b}^{n+1} & b_{34}c_{4b}^{n+1} & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & \ddots & \ddots \\ & & & \ddots & \ddots & b_{m-1m}c_{nb}^{n+1} \\ & & & & b_{m-1m-1}c_{m-1a}^{n+1} & b_{mm}c_{nb}^{n+1} \end{bmatrix} = \begin{bmatrix} c_{1b}^n \\ c_{2b}^n \\ c_{3b}^n \\ c_{4b}^n \\ \vdots \\ \vdots \\ c_{mb}^n \end{bmatrix} \quad ($$

(27)

From the equation (27), c_{ai}^{n+1} can be obtained as followings:

$$c_{ia}^{n+1}=(c_{i+1b}^n-b_{i+1(i+1)}c_{i+1b}^{n+1}-b_{i+1(i+2)}c_{i+2b}^{n+1})/b_{i+1(i)}$$

So the equation (27) can be changed as the followings:

$$\begin{bmatrix} 0 & d_{12} & d_{13} & d_{14} & & & & \\ d_{21} & 0 & d_{23} & d_{24} & d_{25} & & & \\ & d_{32} & 0 & d_{34} & d_{35} & d_{36} & & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & & \ddots & \ddots & \ddots & \ddots & \ddots \\ & & & & \ddots & \ddots & \ddots & \ddots \\ & & & & & \ddots & \ddots & \ddots \\ & & & & & d_{m-1(m-2)} & 0 & d_{m-1(m)} \\ & & & & & & d_{m(m-1)} & d_{mm} \end{bmatrix} \begin{bmatrix} c_{1b}^{n+1} \\ c_{2b}^{n+1} \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ c_{nb}^{n+1} \end{bmatrix} = \begin{bmatrix} f_{1b} \\ f_{2b} \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ f_{nb} \end{bmatrix} \quad (28)$$

The equation (17) is a five-diagonal matrix , Solving the equation, C_{bi}^{n+1} (i=1,2…..m) can be easily got, then put it into the below equation , C_{ai}^{n+1} can be also obtained.

B. Application

To one-dimensional river water pollution problem, the governed equation and constraint condition can be described as equation1 and equation2. in order to verificate 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 $[c_a,c_b]$, velocity u and $[u_a,u_b]$ with pollutant concentration c and $[c_a,c_b]$ is needed to be considered. In order to analysis the sensitivity, when analyzing one parameter's influence on pollutant concentration, other parameters remains unchanged, grey parameter can float its lower and upper value 10%. The parameters are as followings

$$k=0.2 \;\; k_a=0.18 \;\; k_b=0.22\text{；}\;\; u=4m/s$$
$$u_a=3.6m/s \;\; u_b=4.4m/s\text{；}\;\; E=400$$
$$E_a=360 \;\; E_b=440$$

The calculate result can be seen in figure 1 to 3

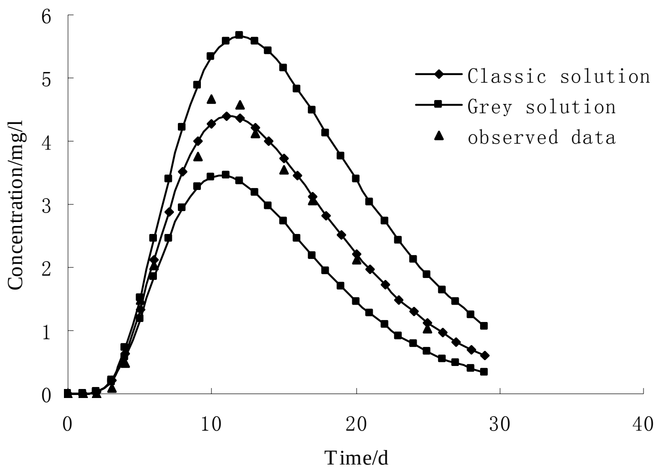

Figure 2. Influence of grey dispersion coefficient on pollutant migration

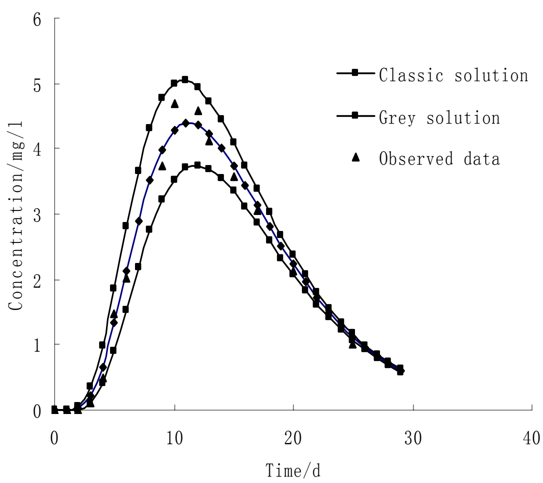

Figure 3. Influence of grey velocity on pollutant migration

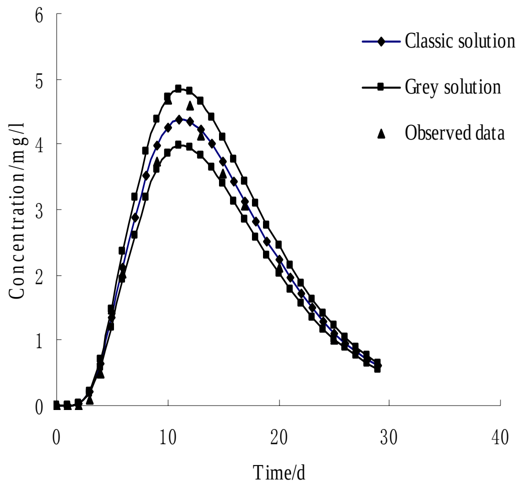

Figure 4. Influence of grey attenuation coefficient on pollutant migration

Seen From Fig1 to fig.3 ,we can see that the curve of contaminant transport by grey numerical model is one "gray strip". That is to say the value of gray 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, the data of hydraulic and water quality in river water system is absent, so the grey mathematic can be applied to the fields. Influence scope of Decay coefficient is lager than other parameters.

IV. GRAY MATHEMATIC MODEL AND NUMERICAL SOLUTION ON TWO-DIMENSIONAL RIVER MODEL

According to the above analysis, the governing gray equation of groundwater pollution is:

$$\frac{\partial(\otimes C)}{\partial t} = (D_{xx})\frac{\partial^2(\otimes C)}{\partial x^2} + (\otimes D_{yy})\frac{\partial^2(\otimes C)}{\partial y^2} - (\otimes u)\frac{\partial(\otimes C)}{\partial x} - (\otimes k)(\otimes C) \quad (11)$$

The initial and boundary condition:

$$\otimes c(x,0) = 0 \qquad x > 0$$
$$\otimes c(0,t) = c_0 \qquad t \geq 0 \quad (12)$$
$$\otimes c(\infty,0) = 0 \qquad t = 0$$

Using finite difference equation to replace differential equation as followings:

As a discussion in theory, the contaminant transport in straight river is discussed as an example. Supposing instant point source is in river center. The parameters are as followings:

M , 100kg, velocity 1.0m/s ; k , 0; E_x , 100m^2/s E_y ,1.0 m^2/s. $E_{xa} = 95m^2/s$, $E_{xb} = 105m^2/s$; $E_{ya} = 0.95m^2/s$, $E_{yb} = 1.05m^2/s$ $u_a = 0.95m/s$, $u_b = 1.05m/s$.

The influence of reflection of bank can be ignored for simple. The known data is put into Eq.11 and Eq.12, the distribution of contaminant in river can be simulated. The location below instant point source 1000km is considered as governed section. The coordinate is （1000，0），（1000，20），（1000，40）.When t=3600s, the contaminant density in this three point can be seen in table1

TABLE I. THE POLLUTANT CONCENTRATION VALUES IN THE SECTION X_0 AT TIME T

coordinates	Contaminant value	Upper value of grey model	Lower value of grey model
（1000，0）	0.00604	0.00674	0.00521
（1000，20）	0.00587	0.00651	0.00509
（1000，40）	0.00541	0.00606	0.00474

Seen from table1, the calculated value according to the certainty model is among the grey belt which is proved that the grey model is feasible. Under the goal of water quality, water quality of the governed point can be analyzed and evaluation.

V. SO THE CONTAMINANT GRAY DENSITY $[c_{ai}^{n+1} \quad c_{bi}^{n+1}]$ CAN BE SOLVED.

VI. APPLICATION

As a discussion in theory, the contaminant transport in straight river is discussed as an example. Supposing instant point source is in river center. The parameters are as followings:

M , 100kg, velocity 1.0m/s ; k , 0; E_x , 100m^2/s E_y ,1.0 m^2/s. $E_{xa} = 95m^2/s$, $E_{xb} = 105m^2/s$; $E_{ya} = 0.95m^2/s$, $E_{yb} = 1.05m^2/s$ $u_a = 0.95m/s$, $u_b = 1.05m/s$.

The influence of reflection of bank can be ignored for simple. The known data is put into Eq.11 and Eq.12, the distribution of contaminant in river can be simulated. The location below instant point source 1000km is considered as governed section. The coordinate is （1000，0），（1000，20），（1000，40）.When t=3600s, the contaminant density in this three point can be seen in table1

TABLE II. THE POLLUTANT CONCENTRATION VALUES IN THE SECTION X_0 AT TIME T

coordinates	Contaminant value	Upper value of grey model	Lower value of grey model
（1000，0）	0.00604	0.00674	0.00521
（1000，20）	0.00587	0.00651	0.00509
（1000，40）	0.00541	0.00606	0.00474

Seen from table1, the calculated value according to the certainty model is among the grey belt which is proved that the grey model is feasible. Under the goal of water quality, water quality of the governed point can be analyzed and evaluation.

VII. CONCLUSIONS

- A differential model of two-dimensional river water quality is proposed according to grey theory and water quality model. The distribution of contaminant below the gage of pollutant can be got.
- The model in this paper is clear in concept and feasible, which reflects the influence of grey parameters on contaminant distribution.
- Comparison with classic numerical model, the results of grey model is a "grey belt" ,not a precison value.
- As a discussion of theory, only the contaminant transport in straight river is studied. To the complex river, it should be further studied.

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