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Application of Fourier series expansion to two-dimensional stochastic advection-dispersion equation for designing monitoring network and real-time prediction of concentration

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Abstract Various numerical methods are nowadays applied for the prediction of pollutant transport, assuming that the parameters necessary for the governing equations are given beforehand. However, the questions about the uncertainties in the parameters and boundary and initial conditions arise when predicting accuracy is of great importance. Even though an introduction of macro-scale dispersion coefficients is one of the smoothing methods for a large areal distribution of pollutant, a result from such approach may not always be satisfactory when pollutant transport through high permeable zones is critical. Besides, it is also important to consider of how pollutant varies temporally and locally. It is therefore desired that a real-time prediction of pollutant evolution is established as an alternative methodology based on the stochastic advection-dispersion pollutant transport equation. In this paper several advantages of the proposed method for handling the various types of boundary conditions and inclusion of information from the spatially distributed observation points are discussed through several simulation examples.

INTRODUCTION

Due to an increasing demand for protecting of groundwater and soil environment from waste disposal sites and farm land where human and agricultural activities result in excess load of toxic materials and fertilizers, numerical simulations of both groundwater flow and pollutant transport are commonly applied for practical problems. In most of the cases, however, a numerical prediction seldom meets a set of observed data for pollutant concentration due to a random nature of aquifer system and hydrological variations. Even though an idea such as the macroscopic dispersion is adapted, the numerical solutions may not be fully reliable because the deviation from observed values often includes important information on local concentration variation which should not be overlooked. In other words, the interpretation based on the macroscopic dispersion may result in the neglection of random fluctuation in model formulation and a calculation algorithm. Therefore real-time information which undergoes the change during a transport process should also be analyzed.

In the present paper, an idea of locally homogeneous advection-dispersion equation is presented instead in order to avoid heavy computational load and to efficiently utilize the filtering technique. The major advantages of the present methodology are the aptness of treating boundary conditions, of making use of observed time series of pollutant concentration at measuring wells, and of incorporating stochastic processes. Through a discussion of this methodology and several examples, the above mentioned advantages will be clarified.

STOCHASTIC POLLUTANT TRANSPORT EQUATION

The one-dimensional fundamental equation for pollutant transport considered herein is as follows

$$\frac{\partial C(x,t)}{\partial t} + \frac{\partial\{uC(x,t)\}}{\partial x} = \frac{\partial}{\partial x}\left\{D\frac{\partial C(x,t)}{\partial x}\right\} - \gamma C(x,t) + S(x,t) \quad (1)$$

where $C(x,t)$ is the pollutant concentration, $u(x,t)$ is the groundwater flow velocity (advection), $D(x,t)$ is the dispersion coefficient, $\gamma(x,t)$ is the degradation coefficient, and $S(x,t)$ is the external source/sink term. Even though actual hydrogeological situations in large scale may not allow the assumption of locally homogeneous conditions for groundwater flow velocity, dispersivity, and other physical parameters, we separate both the parameters and the pollutant concentration into (a) locally homogeneous and (b) remaining components. Consequently:

$$u(x,t)=u_0(t) + u'(x,t)\,,\ D(x,t)=D_0(t) + D'(x,t)\,,\ \gamma(x,t)=\gamma(t)_0 + \gamma'(x,t)$$
$$S(x,t)=S_0(t) + S'(x,t)\,,\ C(x,t)=c(x,t) + c'(x,t) \quad (2)$$

where $u_0(t)$, $D_0(t)$, $\gamma_0(t)$, $S_0(t)$, and $c(x,t)$ are, respectively, the locally homogeneous advection velocity, the dispersion coefficient, the degradation coefficient, the source/sink term, and the updated concentration to which the filtering technique is adapted. The remaining terms with " ' " are assumed to be random components. The randomness in the physical parameters will come from hydrogeological structures, reactable soil chemistries, and the external disturbances in the source/sink term due to hydrological variation, artificial groundwater recharge or uptake, agricultural activities, multi-chemical reactions among various species (Kinzelbach & Schäfer, 1989). The situations of the spatially randomness is illustrated in Figs 1a and 1b.

Substituting equation (2) into equation (1) and rearranging the terms, the following expression is obtained as

$$\begin{aligned}\frac{\partial c(x,t)}{\partial t} + u_0(t)\frac{\partial c(x,t)}{\partial x} = {} & D_0(t)\frac{\partial^2 c(x,t)}{\partial x^2} - \gamma_0(t)c(x,t) + S_0(t)\\ & + D_0(t)\frac{\partial^2 c'(x,t)}{\partial x^2} + \frac{\partial}{\partial x}\left\{D'\frac{\partial c(x,t)}{\partial x}\right\} + \frac{\partial}{\partial x}\left\{D'\frac{\partial c'(x,t)}{\partial x}\right\}\\ & + u_0(t)\frac{\partial c'(x,t)}{\partial x} - \frac{\partial}{\partial x}\left\{u'c(x,t)\right\} - \frac{\partial}{\partial x}\left\{u'c'(x,t)\right\}\\ & - \gamma'(x,t)c(x,t) - \gamma_0(t)c'(x,t) - \gamma'(x,t)c'(x,t) + S'(x,t)\end{aligned} \quad (3)$$

The terms with the notation " ' " in the right hand of equation (3) are conveniently replaced by the term $\varepsilon(x,t)$, so that

$$\frac{\partial c(x,t)}{\partial t} + u_0(t)\frac{\partial c(x,t)}{\partial x} = D_0(t)\frac{\partial^2 c(x,t)}{\partial x^2} - \gamma_0(t)c(x,t) + S_0(t) + \varepsilon(x,t) \quad (4)$$

Employing the similar assumption, the two-dimensional advection-dispersion pollutant transport equation is expressed as

$$\frac{\partial c(x,y,t)}{\partial t} + u_0(t)\frac{\partial c(x,y,t)}{\partial x} = D_{0x}(t)\frac{\partial^2 c(x,y,t)}{\partial x^2} + D_{0y}(t)\frac{\partial^2 c(x,y,t)}{\partial y^2} - \gamma_0(t)c(x,y,t) + S_0(t) + \varepsilon(x,y,t) \quad (5)$$

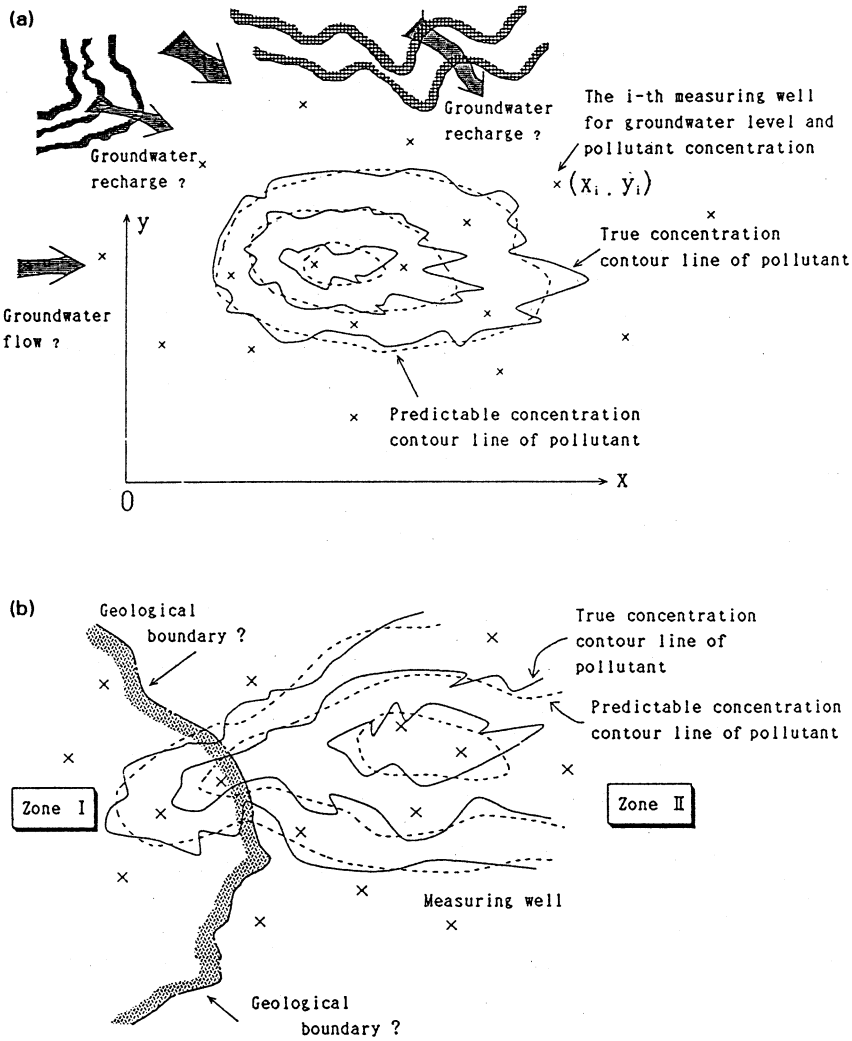

Fig. 1 Uncertain mass transport process: (a) schematic illustration of pollutant transport under uncertain conditions of groundwater recharge; (b) uncertainty for unspecified geological boundary.

if the coordinates of x and y axes are taken parallel and perpendicular to the major groundwater flow direction. An identification of two velocity components and four components of dispersion tensor in general case can also be easily done in the algorithm formulation that will be presented later. The random term $\varepsilon(x,y,t)$ needs to be clarified based on physical interpretations. If an assumption of the locally homogeneous parameters are valid, then it will be possible to assume that the random term is white both for space and time. On the other hand, if neither information on such hydrogeological structure nor external pollutant infiltration is sufficient for the confirmation of the whiteness, then the random term needs to be treated as colored. This clarification can be made only when either detail information on hydrogeological structure and sufficient concentration time series from measuring wells are obtained.

APPLICATION OF THE EXTENDED KALMAN FILTER FOR THE FOURIER SERIES COEFFICENT AND PARAMETER IDENTIFICATION

Fourier series expansion

The finite element approach would be possible for the discretization of the advection-dispersion pollutant transport equation where the parameters are not necessarily homogeneous. However, this approach does not only require heavy computational load but also becomes unreliable due to the numerical error at the advection term and the boundary conditions. An adjustment of nodal points of the finite elements to measuring wells should be done in order to incorporate the measured pollutant concentration. Moreover, readjustment of the nodal points needs to be done when some measuring wells are additionally installed. Considering these disadvantages of the finite element approach, the Fourier series expansion is used instead in the present paper assuming the locally homogeneous parameters in the governing equation. If this assumption is valid, then several advantages can be found as:

(a) numerical error at the advection term does not occur;
(b) measuring wells can be arbitrarily treated since the observation equation in the present approach is directly related with the location of a measuring well;
(c) boundary conditions are also incorporated into the observation equation, and
(d) the random term can be mathematically discussed without extinguishing true mean of "randomness".

The two-dimensional Fourier series expansion for the pollutant concentration is as follows

$$c(x,y,t) = \frac{A_{0,0}(t)}{2} + \sum_{m=1}^{M}\sum_{n=0}^{N} [\, A_{m,n}(t) \cos L_1(x,y,m,n) + B_{m,n}(t) \sin L_1(x,y,m,n) \,] + \sum_{m=0}^{M}\sum_{n=1}^{N} [\, C_{m,n}(t) \cos L_2(x,y,m,n) + D_{m,n}(t) \sin L_2(x,y,m,n) \,] \tag{6}$$

The coordinates x and y are illustrated in Fig. 1a, in which several measuring wells are arbitrarily distributed. Similarly, the Fourier series expansion for the random term in equation (5) is

$$\varepsilon(x,y,t) = \frac{R_{0,0}(t)}{2} + \sum_{m=1}^{M}\sum_{n=0}^{N} [\, E_{m,n}(t) \cos L_1(x,y,m,n) + F_{m,n}(t) \sin L_1(x,y,m,n) \,] + \sum_{m=0}^{M}\sum_{n=1}^{N} [\, G_{m,n}(t) \cos L_2(x,y,m,n) + H_{m,n}(t) \sin L_2(x,y,m,n) \,] \tag{7}$$

The functions appeared in the above equations are as follows

$$L_1(x,y,m,n) = 2\pi mx / \lambda_x + 2\pi ny / \lambda_y , \qquad L_2(x,y,m,n) = 2\pi mx / \lambda_x - 2\pi ny / \lambda_y \tag{8}$$

Suppose that the solid lines in Fig. 1 are the true concentration contours which should occur in a natural aquifer. The dotted lines indicate the possible predictions of the concentration distribution which can be filtered out by applying the filtering technique explained later. The symbols λ_x and λ_y denote the basic wave lengths which need to be taken so that the area to be studied is covered. Substituting the Fourier series expansions of equations (6) and (7) into equation (5) and separating the coefficients which have the same wave numbers, a set of ordinary differential equations are obtained as follows

$$dA_{0,0}(t)/dt = -\gamma_0(t)A_{0,0}(t) + 2\,S_0(t) + R_{0,0}(t)$$

$$\begin{pmatrix} dA_{m,n}(t)/dt \\ dB_{m,n}(t)/dt \\ dC_{m,n}(t)/dt \\ dD_{m,n}(t)/dt \end{pmatrix} = \begin{pmatrix} -P_{m,n} & Q_m & 0 & 0 \\ Q_m & -P_{m,n} & 0 & 0 \\ 0 & 0 & -P_{m,n} & Q_m \\ 0 & 0 & Q_m & -P_{m,n} \end{pmatrix} \begin{pmatrix} A_{m,n}(t) \\ B_{m,n}(t) \\ C_{m,n}(t) \\ D_{m,n}(t) \end{pmatrix} + \begin{pmatrix} E_{m,n}(t) \\ F_{m,n}(t) \\ G_{m,n}(t) \\ H_{m,n}(t) \end{pmatrix} \tag{9}$$

where the functions $P_{m,n}$ and Q_m are

$$P_{m,n} = D_{0x}(t)\;(2\pi m/\lambda_x)^2 + D_{0y}(t)\;(2\pi n/\lambda_y)^2 + \gamma_0(t)$$
$$Q_m = u_0(t)\;(2\pi m/\lambda_x) \tag{10}$$

If the spatially averaged value of the random term $R_{0,0}(t)/2$, or the source/sink term $S_0(t)$, is not zero and is unknown, then the evolution of these quantities need to be modelled.

State equation

As explained below, the Fourier coefficients will be predicted and hence the concentration distribution will be calculated once the parameters in equation (10) are identified. A set of equation (9) consists a so-called state equation of the filtering technique. Let us briefly recall the fundamental procedures of the filtering technique (Athans *et al.*, 1968; Jinno *et al.*, 1989; Kawamura *et al.*, 1991, 1992; Jinno *et al.*, 1993).

Let us denote the state variable by $X(t)$ as

$$\mathbf{X}(t) = [u_0\, D_{0x}\, D_{0y}\, \gamma_0\, A_{0,0}(t) \cdots A_{m,n}(t)\;B_{m,n}(t)\;C_{m,n}(t)\;D_{m,n}(t) \cdots]^T \tag{11}$$

The quantities after the first 4 variables in equation (11) obey the time evolution equation (9). On the other hands, the parameters are assumed to satisfy the following state equations if they are time invariant as

$$du_0(t)/dt = 0\,,\quad dD_{0x}(t)/dt = 0\,,\quad dD_{0y}(t)/dt = 0\,,\quad d\gamma_0(t)/dt = 0 \tag{12}$$

However, this does not mean that the parameters do not change in time during the filtering processes, because they are updated through the filter equation. In the case of the colored random noise, an evolution equation of the Fourier coefficients for the noise term $\varepsilon(x,y,t)$ need to be modelled.

A set of equations (9) and (12) is simply denoted by the vector differential equation as follows

$$d\mathbf{X}(t)/dt = f(\mathbf{X}(t)) + \mathbf{v}(t) \tag{13}$$

where the term v(t) represents the random noise which is related to the Fourier coefficients of $\varepsilon(x,y,t)$ as seen in the right hand of equation (9).

Interpretations of the observed values and various boundary conditions as a set of observation equations

1) Utilization of observed values Unlike an ordinary boundary value problem where boundary conditions are completely prescribed, our concerns with groundwater flow and pollutant transport are usually uncertain for boundary geometries of a study region and boundary conditions. An utilization of the Fourier series expansion automatically assumes a periodic boundary condition which is dependent on the wave lengths λ_x and λ_y. The effect of the basic wave lengths on the parameter estimations have been confirmed to be less through the preliminary tests done by the authors. The observed values are utilized by substituting the locations of measuring wells denoted by (x_i, y_i) as follows

$$c(x_i, y_i, t) = \frac{A_{0,0}(t)}{2} + \sum_{m=1}^{M}\sum_{n=0}^{N} [A_{m,n}(t)\cos L_1(x_i, y_i, m, n) + B_{m,n}(t)\sin L_1(x_i, y_i, m, n)]$$
$$+ \sum_{m=0}^{M}\sum_{n=1}^{N} [C_{m,n}(t)\cos L_2(x_i, y_i, m, n) + D_{m,n}(t)\sin L_2(x_i, y_i, m, n)] + w(x_i, y_i, t) \quad (14)$$
$$(i = 1, 2, \cdots, M_o)$$

The last term in equation (14) considers the possible noise inherent in the measurement.

This expression can be transformed into the matrix, so that a so-called set of observation equations is formulated in the algorithm of the filtering technique.

2) Cauchy type boundary condition If an area to be studied has the boundary where deterministic boundary conditions like constant pollutant concentration and pollutant flux are prescribed, then the Fourier coefficients need to be determined to satisfy them. Here, the Cauchy type boundary condition is discussed first. Suppose as shown in Fig. 2, that a certain point is located in the immediate vicinity of a lake where the pollutant concentration is zero, for example, then the Cauchy type boundary condition can be interpreted

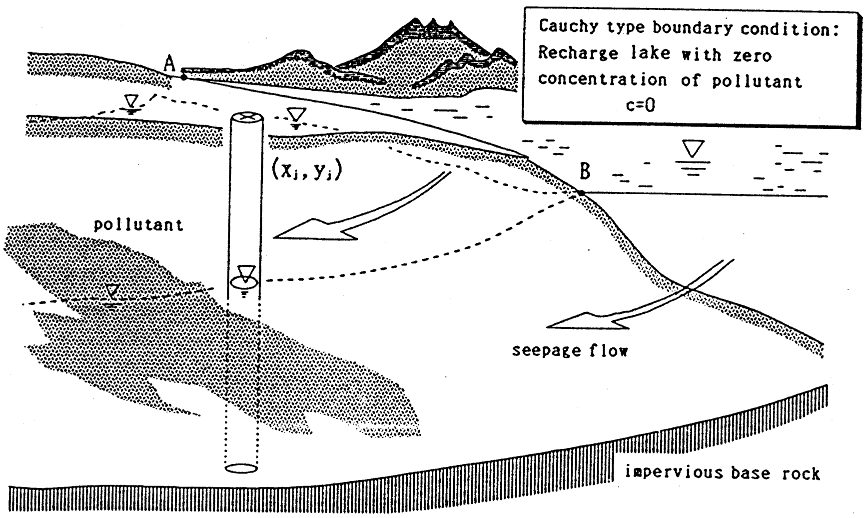

Fig. 2 Cauchy type boundary condition.

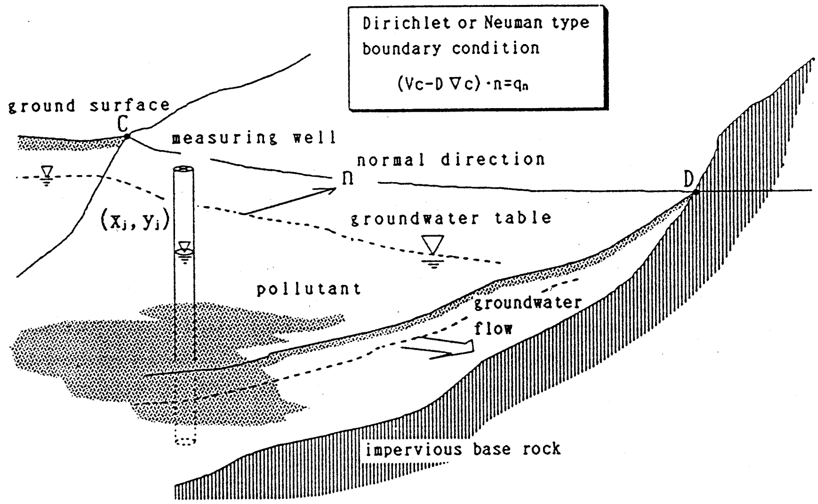

Fig. 3 Dirichlet or Neuman type boundary condition.

from equation (6) as follows

$$c(x_j, y_j, t) = 0 = \frac{A_{0,0}(t)}{2} + \sum_{m=1}^{M}\sum_{n=0}^{N} [A_{m,n}(t)\cos L_1(x_j, y_j, m, n) + B_{m,n}(t)\sin L_1(x_j, y_j, m, n)]$$
$$+\sum_{m=0}^{M}\sum_{n=1}^{N} [C_{m,n}(t)\cos L_2(x_j, y_j, m, n) + D_{m,n}(t)\sin L_2(x_j, y_j, m, n)] \tag{15}$$
$$+w(x_j, y_j, t) \qquad (j = 1, 2, \cdots, M_C)$$

An arbitrary number of boundary points can be allocated along the boundary from the points A through B so that the sufficient boundary geometry is described.

3) Dirichlet or Neuman type boundary condition Similarly, the Dirichlet or Neuman type boundary condition in Fig. 3 can also be easily incorporated as a regime of the observation equations. The partial derivatives of *c(x,y,t)* with respect to *x* and *y* are

$$\frac{\partial c(x,y,t)}{\partial x} = \sum_{m=1}^{M}\sum_{n=0}^{N}\left[-\left(\frac{2\pi m}{\lambda_x}\right)A_{m,n}(t)\sin L_1(x,y,m,n) + \left(\frac{2\pi m}{\lambda_x}\right)B_{m,n}(t)\cos L_1(x,y,m,n)\right]$$
$$+\sum_{m=0}^{M}\sum_{n=1}^{N}\left[-\left(\frac{2\pi m}{\lambda_x}\right)C_{m,n}(t)\sin L_2(x,y,m,n) + \left(\frac{2\pi m}{\lambda_x}\right)D_{m,n}(t)\cos L_2(x,y,m,n)\right] \tag{16}$$

and

$$\frac{\partial c(x,y,t)}{\partial y} = \sum_{m=1}^{M}\sum_{n=0}^{N}\left[-\left(\frac{2\pi n}{\lambda_y}\right)A_{m,n}(t)\sin L_1(x,y,m,n) + \left(\frac{2\pi n}{\lambda_y}\right)B_{m,n}(t)\cos L_1(x,y,m,n)\right]$$
$$= \sum_{m=0}^{M}\sum_{n=1}^{N}\left[+\left(\frac{2\pi n}{\lambda_y}\right)C_{m,n}(t)\sin L_2(x,y,m,n) + \left(\frac{2\pi n}{\lambda_y}\right)D_{m,n}(t)\cos L_2(x,y,m,n)\right] \tag{17}$$

Therefore, the boundary condition shown in Fig. 3 can be written using the relations of equations (16) and (17) as follows

$$q_n = [\, V \cdot c(x,y,t) - D\, \nabla \cdot (x,y,t)\,]\, n$$
$$= V_n \cdot [\, eq.(6)\,] - n_x \cdot D_{0x} \cdot [\, eq.(16)\,] - n_y \cdot D_{0y} \cdot [\, eq.(17)\,] \qquad (18)$$
$$+\, w(x_j, y_j, t) \qquad (j = 1, 2, \cdots, M_D)$$

where n_x and n_y are the components of the normal vector $\boldsymbol{n}$. Again, this constraint can be imposed on the arbitrary points along the boundary from the points from C through D. Both equations (15) and (18) need to be rearranged so that the Fourier coefficients $A_{m,n}(t)$, $B_{m,n}(t)$, $C_{m,n}(t)$, and $D_{m,n}(t)$ constitute the part of the unknown state variables and that the remaining parts like $-(2\pi m/\lambda_x)\ sinL_1(x_j, y_j, m,n)$ can be matrix components of the observation equations. It is therefore summarized that equations (15) and (18) describing various types of boundary conditions can also be treated as a regime of the observation equation like equation (14).

Algorithm of the extended Kalman filter

The set of necessary equations in the algorithm of the extended Kalman filter is as follows (Athans *et al.*, 1968):

(a) State equation: see equation (13)

(b) Observation equation:see equation (14)

(c) Covariance matrix evolution $\Gamma(t)$:

$$\frac{d\,\Gamma(t)}{dt} = \Phi\, \Gamma(t) + \Gamma(t)\, \Phi^T + U(t) \qquad (19)$$

(d) Updating equations(Filter equations):

$$\hat{\mathrm{X}}(t+1|t+1) = \hat{\mathrm{X}}(t+1|t) + \mathrm{K}(t+1) \times \{Prediction\ Innovation\} \qquad (20)$$

$$\Sigma(t+1|t+1) = \Gamma(t+1) - \Gamma(t+1)\,\Psi^T[\,\Psi\, \Gamma(t+1)\,\Psi^T + R(t+1)\,]^{-1}\,\Psi\, \Gamma(t+1) \qquad (21)$$

(e) Gain matrix $K(t)$:

$$\Sigma(t+1|t+1) = \Gamma(t+1) - \Gamma(t+1)\,\Psi^T[\,\Psi\, \Gamma(t+1)\,\Psi^T + R(t+1)\,]^{-1}\,\Psi\, \Gamma(t+1) \qquad (22)$$

The notations used above are the Jacobian matrix Φ for the vector function $f(X)$, the updated state variable $\hat{X}(t+1|t+1)$, the updated covariance matrix Σ, the observation matrix Ψ, $U(t)$ and $R(t)$ for the system and observation noise covariance matrices. It should be noticed that the system noise covariance matrix $U(t)$ includes partly the spectral components of the covariance of the random noise $\varepsilon(x,y,t)$ and hence the level of each component needs to be changed with respect to the wave numbers if the random noise is not white.

EXAMPLES FOR THE SYNTHETICALLY GENERATED CONCENTRATION DISTRIBUTION

Several cases for both the one-dimensional and two-dimensional advection-dispersion equations with locally homogeneous parameters have been examined (Jinno *et al.*, 1989; Kawamura & Jinno, 1991). Figs 4, 5, and 6 are the illustrations of how the filtering technique worked. Figure 4 is the comparisons of the predictions of the pollutant distribution and the synthetically generated contours under the random disturbances. The predicted contours do not only present a general movement but also the distorted phases that can hardly be obtained by a deterministic equation. Figure 5 is the change in the concentration at the points no.1 and no.2 depicted in Fig. 4. An agreement of them seems reasonable. The 50 step ahead prediction at the point no.2 is improved after around 150 time step whereas 60 time step at the point no.1. This is due to the difference in the locations of the two points:the point no.2 is located downstream of no.1 and hence major change in the concentration appeared later. The changes in various parameters and the Fourier coefficients are of great interesting. Figure 6 illustrates the changes of them. The parameters $u_0(t)$ and $D_{ox}(t)$ and the constant term $A_{0,0}(t)$ seem to slowly converge to the true values. This fact means that long term observations would be necessary in order to obtain converged values. If the physical parameters can be obtained preliminarily by solving flow equation, then remarked improvement is expectable as demonstrated previously by the authors (Jinno *et al.*, 1989). The updating process for the Fourier coefficient $A_{5,0}(t)$ seems more sensitive than those of the parameters. The change in $B_{1,8}(t)$ seems to be flat around zero compared to the true fluctuation. This means that the Fourier coefficient $B_{1,8}(t)$ does not significantly contribute to the prediction. Whether or not the inclusion such high wave number component will not be

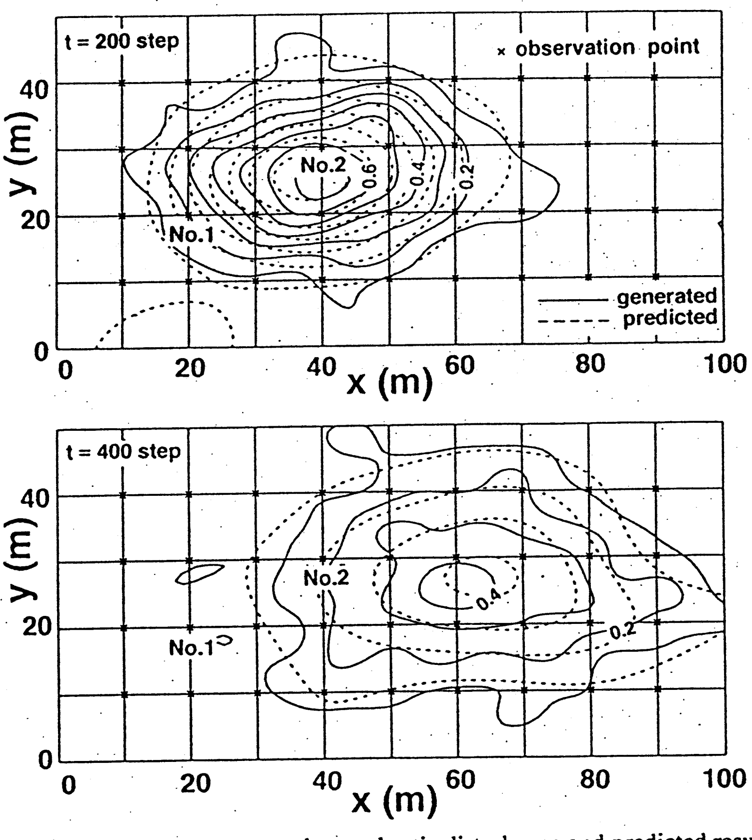

Fig. 4 Pollutant transport under stochastic disturbance and predicted results.

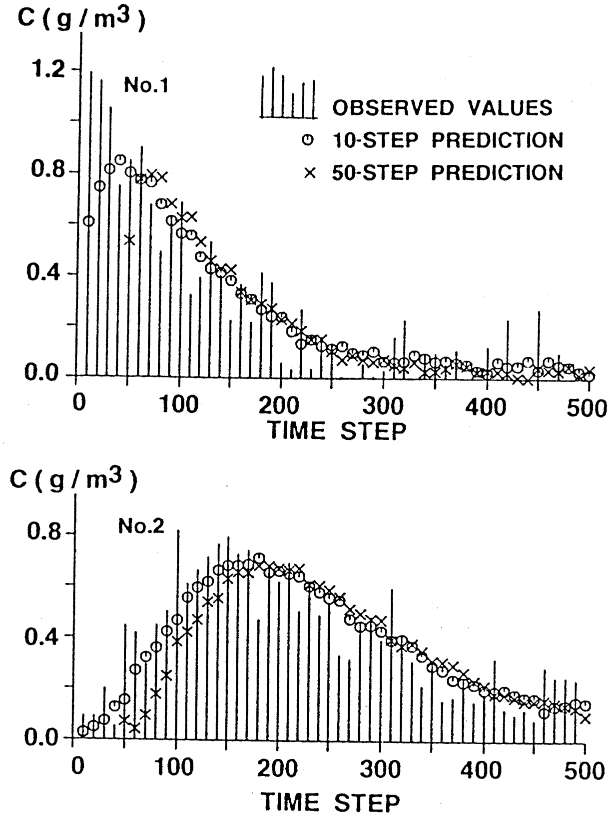

Fig. 5 Predictability of pollutant concentration at the points no. 1 and no. 2.

easily decided prior to a calculation, hence several attempts have to be done if computational load is expected heavy. In the present example, 10 wave numbers for both M and N are equally chosen and therefore a total of 445 state variables including the parameters have been calculated. Even though the number of the state variables may sound large, several advantages of the present method can be promised as mentioned before.

FUTURE WORK

Up to now the authors have confirmed the availability of the present method through one-dimensional and two-dimensional cases where the synthetically generated time series of the pollutant concentration in an infinite study region are tested. Besides, as an example of real applications, although the problem studied is not the groundwater pollution, the present method has been applied to the change in the rainfall intensity using an identical advection-dispersion equation and is found sufficiently available (Kawamura *et al.*, 1992; Jinno *et al.*, 1993). In the practical cases, however, the nature of the hydrogeological randomness needs to be carefully considered. Detailed examinations of the workability of the present method should be done further in future work.

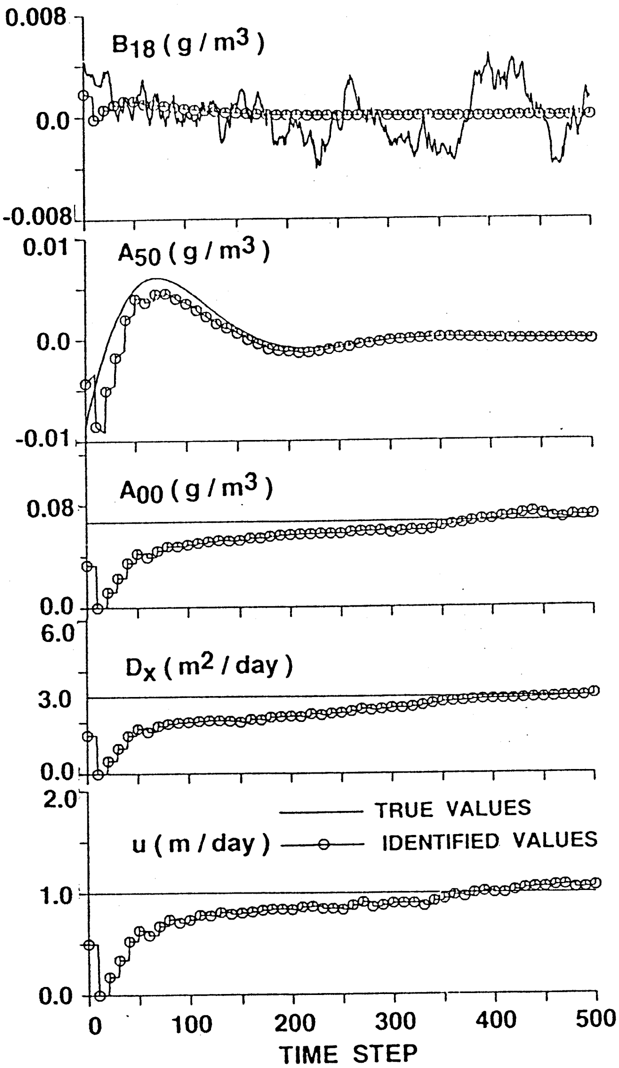

Fig. 6 Identifications of the parameters and the Fourier coefficients.

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