Backward simulation of the probability of a trace particle reaching a given region

Jiannong Fang *, Laurent Tacher, Aurèle Parriaux,

GEOLEP-ICARE-ENAC, Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Abstract

This paper describes the solution of the backward-type Kolmogorov equation (backward method) as an alternative to the forward method to determine the probability (P) of a trace particle reaching a given region within a time τ, which is of interest in groundwater contamination investigation, such as pollution monitoring and controlling. The backward-type Kolmogorov equation describing P was theoretically derived under the assumption that the divergence of the velocity field is zero. We here verify that this assumption is unnecessary and therefore the equation can be used in general cases when various recharge/discharge sources in the flow equation are considered. The backward method is validated by comparing its results with that from the forward method. We find that boundary conditions must be properly imposed in the backward method in order to obtain the same results as from the forward method. The backward method is much more efficient than the forward method.

Key words: Probability, Stochastic process, Ground water, Pollution, Protection zones, Mathematical models, Numerical Modelling

1 Introduction

In this paper we focus on the problem of calculating the probability (P) of a trace particle (pollutant) reaching a target region (such as the proximity of a drinking well) within a time τ, which is of interest in groundwater contamination investigation, such as pollution monitoring and controlling. Traditionally, a problem like this is solved by the forward random walk particle tracking [1,2]. According to the forward method, particles are dropped somewhere in the domain, the path of each particle is calculated by superimposing to the fluid velocity field a random path, one then counts how many among them reach the target region after a time τ. The result is obviously an approximation of the probability P. Repeating this procedure in many places in the domain, the protection zone is defined by grouping the areas where the probabilities for the particles to reach the target region are over a threshold value.

It is intuitively known that the probability for a particle to reach a region within a certain time is described by the Kolmogorov backward equation (KBE) with proper boundary conditions [3,4]. Indeed, this was theoretically proved by Cai et al. [5] under the assumption that the divergence of the velocity field is zero ($\frac{\partial v_i}{\partial x_i} = 0$). In this paper, we first theoretically shown that the assumption is unnecessary and therefore the backward-type Kolmogorov equation (KBE) derived by them can be used in general cases where various recharge/discharge sources are considered, e.g. when rain recharge is modelled through the source term in the two dimensional flow equation. We propose a backward method, i.e. solving the KBE directly by finite element methods. The backward method is then validated by comparing its results with that

* Corresponding author. Email: jiannong.fang@epfl.ch; Fax: 0041-21-6936330.

from the forward method for both $\frac{\partial v_i}{\partial x_i} = 0$ and $\frac{\partial v_i}{\partial x_i} \neq 0$ cases. Boundary conditions are carefully examined in order to get consistent results between the two methods. The backward method is more efficient than the forward method because it can obtain P for the whole domain in a single calculation.

2 Theory

The particle (pollutant) concentration $C(\mathbf{x}, t)$, defined as mass of solute per unit volume of fluid at location $\mathbf{x}$ at time t, satisfies the following advection-dispersion equation (ADE):

$$\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x_i}(v_i C) + \frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right) \tag{1}$$

In equation (1), a repeated subscript in a product denotes a summation, x_i are components of coordinate vector $\mathbf{x}$, v_i are components of fluid velocity vector $\mathbf{v}$, and D_{ij} are elements of dispersion matrix $\mathbf{D}$, which may be expressed as follows:

$$D_{ij} = (D_d + \alpha_{_T} v)\delta_{ij} + (\alpha_{_L} - \alpha_{_T})\frac{v_i v_j}{v}, \tag{2}$$

where $\alpha_{_L}$ and $\alpha_{_T}$ are known as the longitudinal and transverse dispersivities, respectively, D_d is the molecular diffusion coefficient, δ_{ij} is the Kronecker delta and v is the magnitude of the velocity.

Consider a random walk particle with a drift vector $\mathbf{a}$ and a noise tensor $\mathbf{B}$. Let $p(\mathbf{x}, t \mid \tilde{\mathbf{x}}, t_0)$ be the conditional probability density, i.e. $p(\mathbf{x})d\mathbf{x}$ is the probability to find the particle in the interval $(\mathbf{x}, \mathbf{x} + d\mathbf{x})$ at t, given it was in position $\tilde{\mathbf{x}}$ at time t_0 $(t > t_0)$. It can be shown that p satisfies the forward

Kolmogorov equation (3)

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial x_i}(a_i p) + \frac{\partial^2}{\partial x_i \partial x_j}(B_{ij} p). \tag{3}$$

Kolmogorov [6] stated the analogy between this equation and the advection-dispersion equation (1), based on the derivation of the dispersion coefficient from a random process [7]. The practical consequence is to allow to read concentrations calculated according to (1) in terms of probability densities or vice versa [8]. In fact, the analogy between randomly moving particles and the spreading of contaminants in reality is one of the appealing features of the forward random walk method. It can be readily shown that a complete similarity between the two equations is obtained under the following transforms:

$$B_{ij} = D_{ij}; \tag{4}$$

$$a_i = v_i + \frac{\partial D_{ij}}{\partial x_j}. \tag{5}$$

The transition probability density p is also governed by the backward Kolmogorov equation,

$$\frac{\partial p}{\partial t_0} = -a_i \frac{\partial p}{\partial \tilde{x}_i} - B_{ij} \frac{\partial^2 p}{\partial \tilde{x}_i \partial \tilde{x}_j}, \tag{6}$$

which is the adjoint of the forward equation. In Eq. (6) $\tilde{\mathbf{x}}$ and t_0 are independent variables, and a_i and B_{ij} are functions of $\tilde{\mathbf{x}}$ and t_0. This equation gives the probability density to find the particle in position $\tilde{\mathbf{x}}$ at a past time t_0 ($t_0 < t$), given its position $\mathbf{x}$ at time t.

Delineation of groundwater protection zones while accounting for dispersion asks for calculating the probability P for particles injected at a certain position $\mathbf{x}$ to reach a target region (e.g., the proximity of a drinking well, which may be defined as a circle with a given radius centered on the well) within a certain time τ. This can be done by using the forward method. However the forward

method is time-consuming since the calculation has to be performed for each starting position, and hence it has to be repeated many times in order to obtain the protection zone. Practically, the probability P is known intuitively to be also described by the backward Kolmogorov equation with compatible boundary conditions [3,4]. Under the assumption that the divergence of the velocity field is zero ($\frac{\partial v_i}{\partial x_i} = 0$), Cai et al. [5] derived the equation for P. Indeed, the equation happens to be a backward-type Kolmogorov equation

$$\frac{\partial P}{\partial \tau} = (v_i + \frac{\partial D_{ij}}{\partial x_j})\frac{\partial P}{\partial x_i} + D_{ij}\frac{\partial^2 P}{\partial x_i \partial x_j} \tag{7}$$

subject to the initial condition

$$P(\mathbf{x}, 0) = 0,\ \mathbf{x} \in \Omega \tag{8}$$

and the boundary condition

$$P(\mathbf{x}, \tau) = 1,\ \mathbf{x} \in S_1, \tag{9}$$

where S_1 denotes the boundary of the target region, which is treated as absorbing boundary in the forward method. The boundary condition expressed by Eq. (9) is simply due to the definition of P.

In the following we will derive the equation for P without invoking the assumption $\frac{\partial v_i}{\partial x_i} = 0$. Under the transform (4) and (5), the equation (3) describing the transient probability density p now reads

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial x_i}(v_i p) + \frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial p}{\partial x_j}\right). \tag{10}$$

Following the derivation procedure of Cai et al. [5], equation (10) is cast in the form of the Fokker-Planck equation as follows:

$$\frac{\partial}{\partial t}p(\mathbf{x}, t \mid \tilde{\mathbf{x}}, t_0) + \frac{\partial}{\partial x_i}G_i(\mathbf{x}, t \mid \tilde{\mathbf{x}}, t_0) = 0, \tag{11}$$

where each G_i is a component of the probability flux vector $\mathbf{G}$. Comparing equations (10) and (11), we obtain

$$G_i(\mathbf{x}, t \mid \tilde{\mathbf{x}}, t_0) = \left[v_i(\mathbf{x}, t) + \frac{\partial D_{ij}(\mathbf{x}, t)}{\partial x_j} \right] p - \frac{\partial}{\partial x_j}[D_{ij}(\mathbf{x}, t)p]. \tag{12}$$

Let $\bar{p}(\mathbf{x}, \tilde{\mathbf{x}}, \tau)dS(\mathbf{x})$ be the probability that one tracer particle initially located at $\tilde{\mathbf{x}}$ at time t_0, has reached $dS(\mathbf{x})$ on boundary S_1 before time $t = t_0 + \tau$. From the physical meaning of the probability flow $\mathbf{G}$, we obtain

$$\begin{aligned} \bar{p}(\mathbf{x}, \tilde{\mathbf{x}}, \tau)dS(\mathbf{x}) &= \int_0^\tau \mathbf{G}(\mathbf{x}, u + t_0 \mid \tilde{\mathbf{x}}, t_0) \cdot d\mathbf{S}(\mathbf{x})du \\ &= \int_0^\tau G_k(\mathbf{x}, u + t_0 \mid \tilde{\mathbf{x}}, t_0)dS_k(\mathbf{x})du, \end{aligned} \tag{13}$$

where $dS(\mathbf{x})$ is the magnitude of vector $d\mathbf{S}(\mathbf{x})$, and $dS_k(\mathbf{x})$ are components of $d\mathbf{S}(\mathbf{x})$. We now consider a special case, in which the flow velocity and the dispersion matrix are independent of time. Using equations (13) and (12), we obtain

$$\frac{\partial \bar{p}}{\partial \tilde{x}_i} dS(\mathbf{x}) = \int_0^\tau \left[v_k(\mathbf{x}) + \frac{\partial D_{kl}(\mathbf{x})}{\partial x_l} \right] \frac{\partial p}{\partial \tilde{x}_i} - \frac{\partial}{\partial x_l} \left[D_{kl}(\mathbf{x}) \frac{\partial p}{\partial \tilde{x}_i} \right] dS_k(\mathbf{x})du \tag{14}$$

and

$$\frac{\partial^2 \bar{p}}{\partial \tilde{x}_i \partial \tilde{x}_j} dS(\mathbf{x}) = \int_0^\tau \left[v_k(\mathbf{x}) + \frac{\partial D_{kl}(\mathbf{x})}{\partial x_l} \right] \frac{\partial^2 p}{\partial \tilde{x}_i \partial \tilde{x}_j} - \frac{\partial}{\partial x_l} \left[D_{kl}(\mathbf{x}) \frac{\partial^2 p}{\partial \tilde{x}_i \partial \tilde{x}_j} \right] dS_k(\mathbf{x})du. \tag{15}$$

Introducing the operator $F(\bar{p})$ as

$$F(\bar{p}) = \left[v_i(\tilde{\mathbf{x}}) + \frac{\partial D_{ij}(\tilde{\mathbf{x}})}{\partial \tilde{x}_j} \right] \frac{\partial \bar{p}}{\partial \tilde{x}_i} + D_{ij}(\tilde{\mathbf{x}}) \frac{\partial^2 \bar{p}}{\partial \tilde{x}_i \partial \tilde{x}_j}, \tag{16}$$

we then obtain from equations (14) and (15)

$$\begin{aligned} F(\bar{p})dS(\mathbf{x}) = \int_0^\tau & \left\{ \left[v_k(\mathbf{x}) + \frac{\partial D_{kl}(\mathbf{x})}{\partial x_l} \right] - \frac{\partial}{\partial x_l} D_{kl}(\mathbf{x}) \right\} \\ & \times \left\{ \left[v_i(\tilde{\mathbf{x}}) + \frac{\partial D_{ij}(\tilde{\mathbf{x}})}{\partial x_j} \right] \frac{\partial p}{\partial \tilde{x}_i} + D_{ij}(\tilde{\mathbf{x}}) \frac{\partial^2 p}{\partial \tilde{x}_i \partial \tilde{x}_j} \right\} dS_k(\mathbf{x})du. \end{aligned} \tag{17}$$

By using the fact that $p(\mathbf{x}, t_0+u \mid \tilde{\mathbf{x}}, t_0)$ satisfies the following alternative form of the Kolmogorov backward equation:

$$\frac{\partial p}{\partial u} = \left[v_i(\tilde{\mathbf{x}}) + \frac{\partial D_{ij}(\tilde{\mathbf{x}})}{\partial x_j} \right] \frac{\partial p}{\partial \tilde{x}_i} + D_{ij}(\tilde{\mathbf{x}}) \frac{\partial^2 p}{\partial \tilde{x}_i \partial \tilde{x}_j}, \tag{18}$$

equation (17) then yields

$$F(\bar{p}) dS(\mathbf{x}) = \int_0^\tau \left\{ \left[v_k(\mathbf{x}) + \frac{\partial D_{kl}(\mathbf{x})}{\partial x_l} \right] \frac{\partial p}{\partial u} - \frac{\partial}{\partial x_l} D_{kl}(\mathbf{x}) \frac{\partial p}{\partial u} \right\} dS_k(\mathbf{x}) du. \tag{19}$$

Since $\mathbf{v}$ and $\mathbf{D}$ are independent of time, equation (19) can be equivalently written as

$$F(\bar{p}) dS(\mathbf{x}) = \int_0^\tau \frac{\partial}{\partial u} [G_k(\mathbf{x}, u + t_0 \mid \tilde{\mathbf{x}}, t_0) dS_k(\mathbf{x})] du \tag{20}$$

by using the definition of G_k in equation (12). After using the following equivalences: (a) $\mathbf{G}(\mathbf{x}, t_0 \mid \tilde{\mathbf{x}}, t_0) = 0$; (b) $G_k(\mathbf{x}, t_0 + \tau \mid \tilde{\mathbf{x}}, t_0) dS_k(\mathbf{x}) = \frac{\partial \bar{p}}{\partial \tau} dS(\mathbf{x})$ obtained from equation (13), the equivalence in equation (20) can be further expressed as

$$F(\bar{p}) dS(\mathbf{x}) = G_k(\mathbf{x}, t_0 + \tau \mid \tilde{\mathbf{x}}, t_0) dS_k(\mathbf{x}) = \frac{\partial \bar{p}}{\partial \tau} dS(\mathbf{x}) \tag{21}$$

The above equivalence shows that $\bar{p}(\mathbf{x}, \tilde{\mathbf{x}}, \tau)$ also satisfies the Kolmogorov backward equation, namely

$$\frac{\partial \bar{p}}{\partial \tau} = \left[v_i + \frac{\partial D_{ij}}{\partial \tilde{x}_j} \right] \frac{\partial \bar{p}}{\partial \tilde{x}_i} + D_{ij} \frac{\partial^2 \bar{p}}{\partial \tilde{x}_i \partial \tilde{x}_j}. \tag{22}$$

The probability for tracer particle reaching anywhere on boundary S_1 by time τ is given by

$$P(\tilde{\mathbf{x}}, \tau) = \int_{S_1} \bar{p}(\mathbf{x}, \tilde{\mathbf{x}}, \tau) dS(\mathbf{x}). \tag{23}$$

From equations (22) and (23), it can be readily shown that $P(\tilde{\mathbf{x}}, \tau)$ also satisfies the Kolmogorov backward-type equation (7) with $\tilde{\mathbf{x}}$ replaced by $\mathbf{x}$ there. Eq. (7) was derived by Cai et al. [5] under the assumption $\frac{\partial v_i}{\partial x_i} = 0$. As far as we

know, the assumption was adopted by the authors only because they started from the convective form of the advection-dispersion equation (see equation (1) of [5]) which is a special form of Eq. (1) in this paper under the assumption of incompressible flow, and hence the transform (5) for complete similarity between their Eq. (1) and the forward Kolmogorov equation (Eq.(3)) could only be valid by invoking the assumption again. Since such an assumption is not needed to obtain the complete similarity between our Eq. (1) (more general) and the forward Kolmogorov equation (Eq.(3)) and it is not used in the proof from Eq.(3) to Eq.(7) given above, we therefore verify that this assumption is unnecessary and therefore the backward-type equation (7) can be used for the case $\frac{\partial v_i}{\partial x_i} \neq 0$. We note that Eq. (7) is only valid when the flow velocity and the dispersion matrix are independent of time, which is required in the intermediate derivation step from Eq. (19) to Eq. (20). Otherwise, additional integral terms would occur.

We propose to solve directly the backward-type Kolmogorov equation (7) by finite element methods. In practice, the equation is rewritten as

$$\frac{\partial P}{\partial \tau} = v_i \frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_i}\left(D_{ij} \frac{\partial P}{\partial x_j} \right). \tag{24}$$

The velocity field is first calculated from the flow equation, and then inserted in (24). For steady horizontal (2D) flows in confined aquifers considered in the next section, the flow equation is given by

$$\begin{aligned} \frac{\partial \overline{q}_i}{\partial x_i} &= Q \\ \overline{q}_i &= -BK_{ij} \frac{\partial h}{\partial x_j} \\ v_i &= \frac{\overline{q}_i}{B\theta} \end{aligned} \tag{25}$$

where $\overline{q}_i$ is the integrated Darcy velocity, Q is the recharge/discharge source, h

is the hydraulic head, B is the thickness of the aquifer, θ is the porosity and K_{ij} are the elements of the hydraulic conductivity tensor $\mathbf{K}$. Here the flow equation (25) is solved by the Galerkin finite element method and the equation (24) is solved by the streamline-upwind-Petrov-Galerkin (SUPG) method. The whole procedure will be denoted as the backward method.

3 Numerical example

In this section the proposed backward method is validated numerically by comparing its results with that from the standard forward method. Although the hydraulic velocity field must be steady, the probability field may be calculated in both steady and transient state.

Steady state On the boundary of the target region under consideration, a probability $P = 1$ (first-type) is imposed for the backward method since particles are yet in the region, while $p = 0$ is imposed there in the forward method. On the absorbing boundaries, $P = p = 0$ (first-type) is imposed for both forward and backward methods. On the boundaries where the hydraulic flux exits in the forward model (enters in the backward model), if the dispersive probability flux (second-type)

$$-D_{ij}\frac{\partial p}{\partial x_j}n_i = 0$$

is imposed for the forward method, then, the total probability flux (third-type)

$$-[Pv_i + D_{ij}\frac{\partial P}{\partial x_j}]n_i = 0$$

must be imposed in the backward method. On the boundaries where the hydraulic flux enters in the forward model (exits in the backward model),

the boundary conditions are opposite to the previous case. The above two matching rules between the forward and backward boundary conditions is intuitive and inspired by the same matching rules obtained by the adjoint method [9]. On the impervious boundaries, the second-type boundary condition

$$-D_{ij}\frac{\partial P}{\partial x_j}n_i = 0$$

is imposed. The calculated P field is the probability for a particle to reach the target region eventually.

Transient state Initials conditions are set to $P = 0$ everywhere. Imposing the same boundary conditions as in steady state, the calculated P field of time τ describes the probability for particles to reach the target region before τ.

Multiple target regions Imposing $P = 1$ at more than one target region, the calculated P field describes the probability for particles to reach one of these regions, without discerning which one among them. This P field is equal to the sum of the fields calculated for each target region separately. This has sense in steady or transient state.

To validate the backward method numerically, we here consider the two-dimensional, rectangular, 800 m $\times$ 200 m confined aquifer shown in Figure 1. Flow is steady, and the flow boundaries are specified head on the east and west boundaries and no flow in the north and south boundaries, with flow from west to east. A pumping well is located at $(x, y) = (500\text{m}, 100\text{m})$ and pumps at a rate of $Q_w = 10\text{m}^3/\text{d}$. The target region associated with the well is defined as a square of 20 m centered on the well. The aquifer thickness is $B = 1$ m, and the transmissivity is $T = 10^{-4}\text{m}^2/\text{s}$. The molecular diffusion coefficient is $D_d = 10^{-9}\text{m}^2/\text{s}$. The longitudinal and transverse dispersivity are

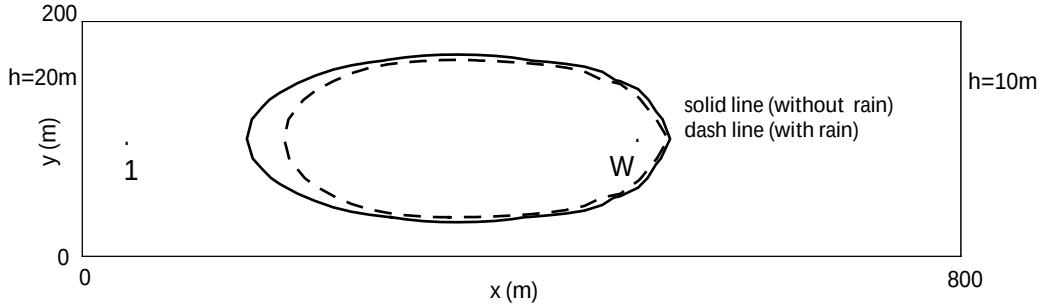

Fig. 1. Aquifer geometry, boundary conditions, and protection zones calculated. The point with symbol "W" denotes the pumping well location and the point with number 1 denotes the observation point. The solid line and the dash line envelop the protection zones corresponding to $\tau = 365$d obtained by the backward method for $Q = 0$ and $Q = 2 \times 10^{-4}$m/d, respectively.

$\alpha_{_L} = 10$m and $\alpha_{_T} = 2$m respectively. The aquifer porosity is $\theta = 0.2$.

We choose one point from the domain to compare the results from the forward and backward methods. The point is located at $(x, y) = (50\text{m}, 100\text{m})$ with the number 1 as shown in Figure 1. The results obtained by the two methods are compared in Figure 2 for $Q = 0$ and $Q = 2 \times 10^{-4}$m/d, respectively. We find that, in both cases, the results from the backward method are in excellent agreement with that from the forward method. This supports that the two methods are equivalent for whatever $\frac{\partial v_i}{\partial x_i}$. Not shown are the results of the backward method with the boundary conditions disobeying the rules mentioned before, which are inconsistent with those from the forward method. This suggests that the two methods are equivalent only with matching boundary conditions. Needless to say, the backward method is much more efficient than the forward method in the sense that it can obtain the entire time-dependent protection zone with one simulation. As an example, the protection zone for $\tau = 365$ d obtained by the backward method is shown in Figure 1 for $Q = 0$ and $Q = 2 \times 10^{-4}$m/d, respectively, where the protection zone is defined by

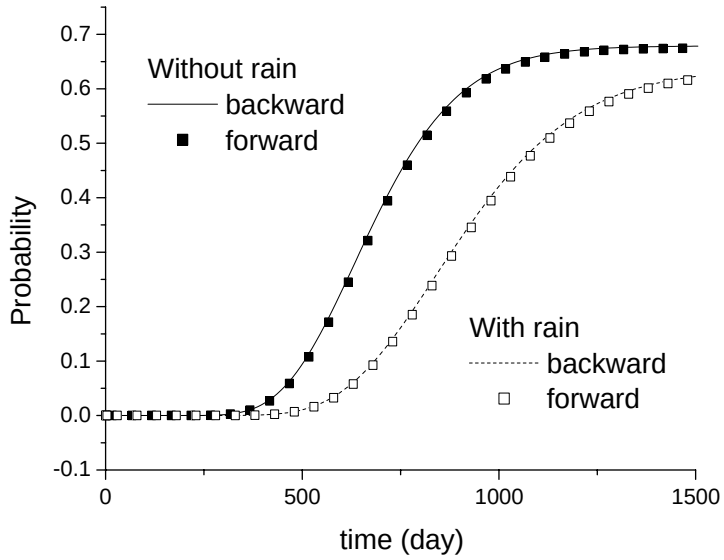

Fig. 2. The probability P for the observation point calculated by the forward and backward methods for $Q = 0$ and $Q = 2 \times 10^{-4}$m/d, respectively.

choosing a threshold value, $P = 0.1$. The protection zone for $Q = 2 \times 10^{-4}$m/d is smaller than that for $Q = 0$ due to the spatially uniform recharge, which was also reported by others [10].

4 Conclusions

The backward method is presented to calculate the probability of a trace particle reaching a target region within a given time and to delineate probabilistic protection zones associated with the target region. The method and the boundary conditions are validated by comparing the results with those from the standard forward method. It has been shown theoretically and numerically that the method works for more general problems where the assumption (the divergence of the velocity field is zero) does not hold. The removing of the assumption expands the application of the backward equation and therefore is practically very important especially in the field of groundwater protection

where various recharge/discharge sources (such as rain recharge) are often encountered. The method is simple and more efficient than the forward method. It may be easily included in Monte-Carlo processes to address the probability for a particle of contaminant to reach a target region also with respect for the uncertainty on the physical parameters.

References

[1] Kinzelbach W. The random walk method in pollutant transport simulation. In: Custodio E, Gurgui A, Lobo Ferreira JP. Goundwater flow and quality modelling. NATO ASI Series, Serie C: Math. and Phys. Sci. 224. Reidel Publishing Company, 1988. p. 227-246.

[2] EPA. Literature review of methods for delineating wellhead protection areas. Report EPA, United States Environmental Protection Agency, Office of Water, Office of Ground Water and Drinking Water, No. 816-R-98-021.

[3] Kunstmann H, Kinzelbach W. Computation of stochastic wellhead protection zones by combining the first-order second-moment method and Kolmogorov backward equation analysis. Journal of Hydrology 2000;237:127–146.

[4] Uffink G. Application of Kolmogorov's backward equations in random walk simulations of groundwater contaminant transport. In: Kobus D, Kinzelbach W. Contaminant transport in groundwater. Brookfield (VT): A.A. Balkema, 1989. p. 283–289.

[5] Cai GQ, Qiu X, Su TC, Lin YK. Markov process modeling of groundwater contamination problems. Probabilistic Engineering Mechanics 1996;11:243–250.

[6] Kolmogorov A. Uber die analytischen Methoden in der Wahrscheinlichkeitsrechnung. Math Ann 1931;104:415–458.

[7] Harr ME. Mechanics of particulate media. New York: McGraw Hill, 1977.

[8] de Marsily G. Quantitative Hydrogeology. New York: Academic Press, 1986.

[9] Neupauer RM, Wilson JL. Adjoint method for obtaining backward-in-time location and travel time probabilities of a conservative groundwater contaminant. Water Resources Research 1999;35:3389–3398.

[10] Cole BE, Silliman SE. Utility of simple models for capture zone delineation in heterogeneous unconfined aquifers. Ground Water 2000;38:665–672.