Stochastic modelling of tracer transport in three dimensions

CYRIL FLEURANT & JAN VAN DER LEE

Ecole des Mines de Paris, Centre d'Informatique Géologique, 35 rue St-Honoré, F-77305 Fontainebleau Cedex, France

e-mail: fleurant@cig.ensmp.fr

Abstract Modelling of solute transport remains a key issue in the area of groundwater contamination. The fundamental processes of solute transport are advection and dispersion and an accurate description is needed for all modelling studies. The most common approach (advection–dispersion equation) considers an average advective flow rate and a Fickian-like dispersion. Consequently, advection is independent of dispersion. Here we propose a more accurate approach: advection is a function of the dispersive behaviour of the solute and of the characteristics of the medium. This method provides useful insight of the dispersion process in general. The aim of this article is to present the mathematical background of the random walk model and a simple numerical application.

INTRODUCTION

Solute transport model has been the subject of an intense research effort in recent years and remains a key research area in hydrogeology. The motivations are the problems of aquifer contamination and particularly migration of radionuclides from repository sites.

The movement of solute in porous media is commonly described by the advection–dispersion equation:

$$div\left(\overline{D}\,\overline{grad}C - C\overline{U}\right) = \frac{\partial C}{\partial t} \qquad (1)$$

where C is the concentration, t is the time, U is the average velocity, and D is the dispersion tensor. This classical approach considers the dispersive mass flux equal to Fick's first law. With this approach, dispersion is said to be diffusive or Gaussian. The most important drawbacks of use of the advection-dispersion equation (1) to simulate solute transport can be attributed to the non-Fickian behaviour of the dispersive transport as well as the apparent scale dependence of the dispersivity (Matheron & de Marsily, 1980; Neuman, 1990; Dagan, 1990; Gelhar, 1993).

The fit of the advection–dispersion equation (1) to experimental data sometimes fails because of non-Fickian behaviour leading to long tails in breakthrough curves and skewness in the spatial dissemination of the solute.

PRINCIPLES OF THE 3-D MODEL

Transport of matter in a porous medium is a function of the pore-velocity. Its random nature leads to an average *advective* velocity U but also to a random noise which represents the dispersion. Increasing the spatial scale will increase the number of movements, hence the noise. Consequently, dispersion is scale-dependent.

Notations are introduced according to an orthonormal coordination system (i,j,k) such that i points to X, the direction of the average flow velocity vector. As schematically shown in Fig. 1, vector $\mathbf{u}^j$ can be expressed relative to the basis (i,j,k) in terms of the angles θ and ϕ. Then, the change in position of a particle during one time step is written:

$$\frac{\mathrm{d}x^j}{\mathrm{d}t} = u^j \cos\theta \qquad \frac{\mathrm{d}y^j}{\mathrm{d}t} = u^j \sin\theta\cos\phi \qquad \frac{\mathrm{d}z^j}{\mathrm{d}t} = u^j \sin\theta\sin\phi$$

where u^j is the velocity of the particle j.

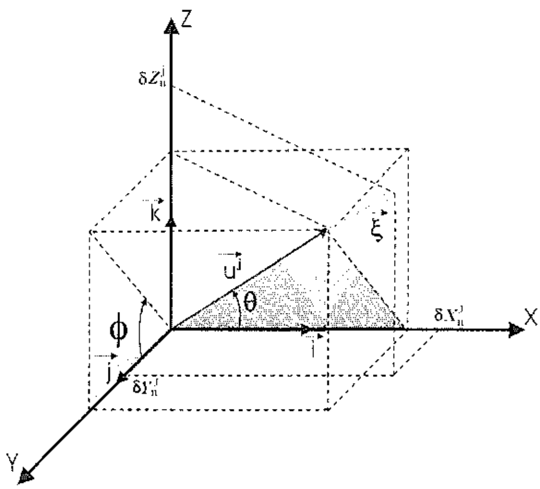

Fig. 1 Geometrical principles and general notation of the approach.

The stochastic behaviour of angles θ and ϕ represents the spatial variance of the vector $\mathbf{u}^j$. The azimuthal angle ϕ is distributed within $[0,\pi]$ in the plane perpendicular to the main flow direction according to a uniform probability density function.

The polar angle θ is distributed such that the probability of moving in the main flow direction (X, by definition) is large, while a pathway perpendicular to X is very weak. This probability is well described by a cosine function:

$$\mathrm{pdf}(\theta) = \frac{2}{\pi}\cos^2\theta \qquad -\frac{\pi}{2} \le \theta \le \frac{\pi}{2}$$

Even in a homogeneous porous medium, the porosity distribution is scattered leading to variation of particle velocities. A straightforward particle velocity distribution is the Gaussian pdf, but also lognormal (like) distributions are plausible as tracers may move in almost stagnant zones:

$$\mathrm{pdf}(u^j) = \frac{1}{\sigma\sqrt{2\pi}\left(u_{\max} - u^j\right)}\exp\left(-\frac{\ln^2\left(\dfrac{u_{\max} - u^j}{U}\right)}{2\sigma^2}\right)$$

where u_{max} is a parameter which denotes the faster velocity. Here, σ denotes the skewness of the distribution, defined within 0 (no skewness, Gaussian) and ~2 (left-skewed, lognormal).

The diffusion process is superimposed on the advective motion using the common Gaussian law, here denoted by:

$$\mathrm{pdf}(\xi) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{\xi^2}{2\sigma^2}\right) \qquad \sigma = \sqrt{2D_0 \mathrm{d}t}$$

where $\mathrm{d}t$ is the time step and D_0 denotes the molecular diffusion coefficient. The complete Markovian process including advection–diffusion–dispersion is then:

$$X_n^j = \sum_{i=1}^{n} \left(x^{\xi,i} + u^j \mathrm{d}t \cos\theta_i \right)$$

$$Y_n^j = \sum_{i=1}^{n} \left(y^{\xi,i} + u^j \mathrm{d}t \sin\theta_i \cos\phi_i \right)$$

$$Z_n^j = \sum_{i=1}^{n} \left(z^{\xi,i} + u^j \mathrm{d}t \sin\theta_i \sin\phi_i \right)$$

Dispersion is governed by parameter σ. Figure 2 shows the resulting breakthrough curves after transport through a simple column system.

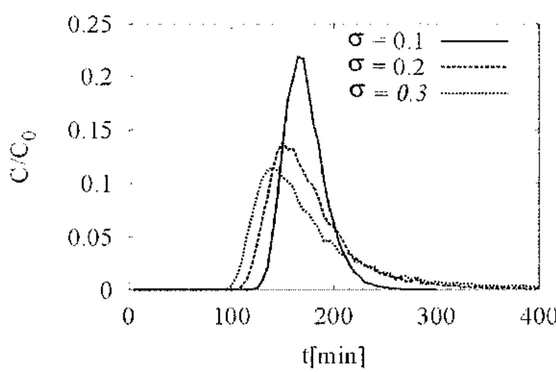

Fig. 2 Breakthrough curves for different values of the parameter σ.

NUMERICAL MODEL VALIDATION TEST

In order to validate the mathematical basis of the model, it is useful to compare the numerical calculations with an analytical solution. As we have no reliable solutions for non-Fickian dispersion, the tests have been limited to Fickian transport, i.e. the classical one-dimensional (1-D) advection–dispersion. The model is tested for a pulse injection with variations of molecular diffusion coefficient, of the average velocity and of the spatial scale. The transport model is forced to be 1-D, i.e. the column length is very long compared to the diameter. In a semi-infinite medium subjected to a uniform flow, the analytical solution of a variable time injection is (Bear, 1972; de Marsily, 1986):

$$C(x,t) = \frac{C_0}{2}\left[\operatorname{erfc}\left(\frac{x-Ut}{2\sqrt{D_x t}}\right) + \exp\left(\frac{Ux}{D_x}\right)\operatorname{erfc}\left(\frac{x+Ut}{2\sqrt{D_x t}}\right)\right] \tag{2}$$

where C_0 is the initial injected concentration, U is the average velocity, x is the observation point, D_x is the longitudinal dispersion coefficient and t is the time, and erfc denotes the complementary error function.

Variations of diffusion coefficient

Three simulations were carried out with three different values of the diffusion coefficient. For these three simulations, the average velocity is constant ($U = 10^{-5}$ m s^{-1}) and the dispersion parameters of the random walk model (σ) is equal to 0.05. The control location (x) is at 0.1 m from the injection point. The dispersivity of the analytical solution is fitted ($\alpha_x = 1.5 \times 10^{-4}$). Figure 3 confirms that the random walk transport model compares well with the advection–dispersion equation.

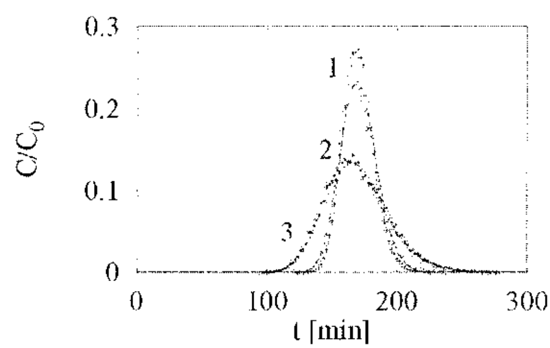

Fig. 3 Comparison between curves simulated by the random walk model and analytical solution (equation (1)) for different values of the molecular diffusion coefficient. Column length is 10 cm and average velocity is 10^{-5} m s^{-1}. The dispersivity of the analytical solution is fit to 1.510^{-4} m and the random walk model parameter is $\sigma = 0.05$. Diffusion coefficients are 9.310^{-10} m^2 s^{-1} (1), 1.8610^{-9} m^2 s^{-1} (2) and 9.310^{-9} m^2 s^{-1} (3).

Variations of the average velocity

Simulations were carried out with three values of the average velocity. The system parameters are the same as those described in the previous section. The diffusion coefficient is constant and equal to 9.310^{-10} m^2 s^{-1}. The simulation shown in Fig. 4 also confirms the mathematical basis of the random walk model. The fitting value of the dispersivity is the same that in the previous section ($\alpha_x = 1.510^{-4}$ m).

These two tests are a validation of use of the numerical model to simulate a Fickian dispersive transport as the classical advection–dispersion equation.

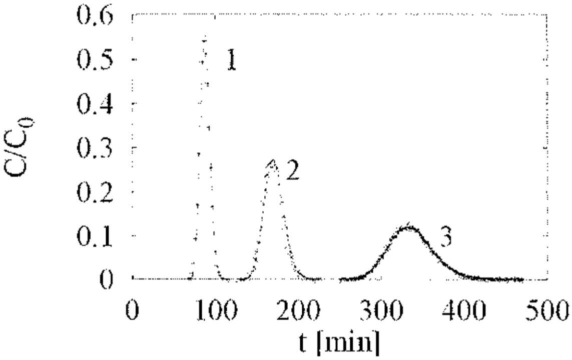

Fig. 4 Comparison between curves simulated by the random walk model and analytical solution (equation (1)) for different values of the average velocity. Column length is 10 cm and diffusion coefficient is 9.310^{-10} $m^2 s^{-1}$. The dispersivity of the analytical solution is fit to 1.510^{-4} m and the random walk model parameter is σ = 0.05. Average velocities are 210^{-5} $m s^{-1}$ (1), 10^{-5} $m s^{-1}$ (2) and 510^{-6} $m s^{-1}$ (3).

Scale variations

One simulation was carried out at constant velocity ($U = 10^{-5}$ m s^{-1}) and with a constant value of the dispersion parameter of the random walk model (σ = 0.05). Control planes were set at x = 0.05, 0.1, 0.15 and 0.2 m (Fig. 5).

This test is of significance to the random walk model behaviour: even though σ is constant, the values of the dispersivity have to be increased with the distance from the injection point to fit the model (see Table 1). The intrinsic dispersion of the random walk model allows for the non-scale-dependent nature of the parameter σ.

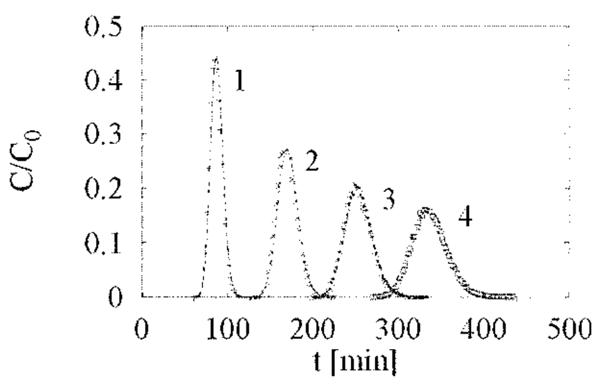

Fig. 5 Comparison between curves simulated by the random walk model and analytical solution (equation (1)) for different transport scale. Results are summarized in Table 1. Distance locations are 20 cm (1), 15 cm (2), 10 cm (3) and 5 cm (4).

Table 1 Comparison between values of analytical dispersivities and the dispersion parameter values of the model. Average velocity is 10^{-5} m s^{-1} and diffusion coefficient is 9.310^{-10} $m^2 s^{-1}$.

Control locations (m)	Dispersivity ($m^2 s^{-1}$)	σ
0.05	1.510^{-5}	0.05
0.1	4.510^{-5}	0.05
0.15	5.510^{-5}	0.05
0.2	6.510^{-5}	0.05

CONCLUSION

The random walk model presented is based on a mechanistic description of solute dispersion in a porous medium. Trajectories of solute particles are described in three dimensions by a random walk equation. The random pathways of a particle are determined by two random angles. The heterogeneity of the porous medium is described by a law of the velocities; the randomness of the particle's velocity is actually a representation of the distribution of the heterogeneity (porosity or permeability). These heterogeneities are described by a parameter (σ) which is the variance of the microscopic velocities around the average velocity.

Some simulations were then carried out in order to validate the random walk model with a 1-D analytical solution in the case of Fickian transport, and for a small dispersive medium. It is important to note that breakthrough curves are obtained without use of a numerical method which could introduce numerical dispersion. Indeed, particles are simply counted when they go through a virtual plane which corresponds to the distance location of the concentration control. The analytical solution and breakthrough curves of the random walk model were in good agreement for the three kinds of test made. The last test (scale test) is a significant demonstration of the random walk model behaviour and shows that when advection and dispersion are dependent, dispersion of a solute increases with the distance from its injection point. This allows the use of scale-constant dispersion parameters.

This model is an interesting tool for study of more complex systems such as transport of colloidal suspensions, including the volume and charge exclusion effects, and the porosity occlusion by particle filtration. In fact, colloidal transport lends itself to this kind of model because it is very easy to distinguish precisely, the dispersive behaviour of the colloids on one hand, and on the other, the dispersive behaviour of the solute.

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