# A Numerical Study on Solute Transport in Heterogeneous Porous Media

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ABSTRACT: The solute transport in a two-dimensional heterogeneous porous medium is numerically studied by using a random walk particle tracking (RWPT) method. Lognormally isotropic hydraulic conductivity fields are generated by using the turning band methods with mean zero and four different values of standard deviation. The numerical transport experiments are carried out to investigate the large time and spatial effects of the variable pore velocity field on solute plumes. The behavior of the solute plume through numerical simulations is presented in terms of longitudinal and transverse spatial moments: displacement of center-of-mass, plume spread variance and skewness coefficient. It was observed that the dispersive behavior of the solute plume is strongly affected by the degree of heterogeneity in the flow domain.

## 1 INTRODUCTION

Natural geological formations generally exhibit a large degree of spatial variability in terms of hydrogeologic properties such as hydraulic conductivity, porosity, etc. It is widely recognized that solute transport is strongly affected by this spatial variability (Dagan, 1989). The effect of a spatially variable hydraulic conductivity on solute transport has been studied analytically (Gelhar and Axness, 1983; Dagan, 1984, 1989) and numerically (Bellin et al., 1992). The aim of this study is to examine numerically the dispersive behavior of solute plumes in a 2-D heterogeneous porous medium with statistically isotropic hydraulic conductivity field. The solute transport is simulated by using the random walk particle tracking method and results obtained are expressed in terms of longitudinal and transverse spatial moments: displacement of center-of-mass, plume spread variance and skewness coefficient

## 2 HETEROGENEOUS VELOCITY FIELD

For solute transport simulations, a velocity field within a heterogeneous porous medium must be initially established. This can be performed by assigning spatially variable hydraulic conductivities to a flow domain. We assume a normally log conductivity $Y(\mathbf{x})$, defined as $Y(\mathbf{x}) = \ln\left[K(\mathbf{x})\right]$ with mean $\mu_Y$ and variance $\sigma_Y^2$, where $K$ is the hydraulic conductivity and $\mathbf{x}$ is the spatial coordinate vector. To represent a spatially correlated characteristics of $Y$, an exponential covariance function is assumed and given by (Dagan, 1989)

$$C_Y(\mathbf{h}) = \sigma_Y^2 \, exp\left(\frac{-\mathbf{h}}{\lambda_Y}\right) \tag{1}$$

where $\mathbf{h}$ is the distance vector between two points and $\lambda_Y$ is the spatial correlation scale of $Y$.

In the present study, the second order stationary is considered for stochastic process of $Y$. This is anisotropic if the covariance function depends on the direction of $C_Y(\mathbf{h})$, otherwise it is isotropic and the covariance function is determined by the length of $\mathbf{h}$. With the covariance function of Eq. (1), a spatially correlated hydraulic conductivity distribution is generated in our simulations through the use of a two-dimensional turning bands algorithm (Thompson et al, 1989; Langtuejoul, 1994).

The governing equation for steady-state groundwater flow in a saturated porous medium is

$$\nabla \cdot (K \nabla h) = 0 \tag{2}$$

where $h$ [L] is the hydraulic head and $K$ [$LT^{-1}$] is the hydraulic conductivity tensor.

The Galerkin finite element approach is used to compute the hydraulic head distribution from each realization of hydraulic conductivity field. The pore velocity can be determined from

$$\mathbf{v} = -\frac{K}{\omega} \nabla h \tag{3}$$

where $\omega$ is the porosity.

## 3 RANDOM WALK PARTICLE TRACKING METHOD

In a steady-state saturated porous medium, the transport of a non-reactive solute including a retardation factor due to adsorption can be described by the well known advection-dispersion equation (Bear, 1972)

$$R\frac{\partial C}{\partial t} + \nabla \cdot (C\mathbf{v}) - \nabla \cdot (\mathbf{D} \cdot \nabla C) = 0 \tag{4}$$

where $C$ [$ML^{-3}$] is the solute concentration, $R$ is the retardation factor, $\mathbf{v}$ [$LT^{-1}$] is the local velocity vector, $t$ [T] is time and $\mathbf{D}$ [$L^2T^{-1}$] is the local hydrodynamic dispersion tensor which is expressed by

$$\mathbf{D} = (\alpha_T V + D_m)\mathbf{I} + (\alpha_L - \alpha_T)\frac{\mathbf{vv}}{V} \tag{5}$$

where $D_m$ [$L^2T^{-1}$] is the molecular diffusion coefficient and is usually neglected in a field scale mass transport, $V$ [ $LT^{-1}$] is the magnitude of the velocity vector $(=|\mathbf{v}|)$, $\alpha_L$ and $\alpha_T$ [L] are the longitudinal and transverse dispersivities, respectively, and $\mathbf{I}$ is the identity matrix.

Conventional numerical techniques, such as finite difference and finite element methods, to solve the above advection-dispersion equation appears a numerical dispersion near a sharp front of solute concentration when there are its abrupt changes in space and time (Huyakorn and Pinder, 1983; Kinzelbach, 1990). In order to reduce this numerical dispersion, the spatial and/or temporal discretizations must be small enough to satisfy a grid Peclet number smaller than 2 or a Courant number smaller than 1. However, this criterion is not always possible due to significantly computational costs in a large scale of transport problems.

An alternative numerical technique to solve solute transport problems is a random-walk particle tracking (RWPT) method (Uffink, 1985; Kinzelbach, 1990; Tompson and Gelhar, 1990; Aboulaban and Nieber, 2000). This method is based on the assumption that a solute plume can be represented with a large number of particles moving in a flow field with spatially variable local velocities. A dispersion process is treated by adding the convective particle movement to a random movement that is proportional to the local dispersivity of the porous medium (Kinzelbach, 1990).

The mathematical treatment of RWPT method is based on the similarity between the advection-dispersion equation and the Fokker-Planck equation, and also a conservation equation for the probability distribution of particles moving independently in a flow field. The displacement of a particle can be described by the following equation (Thompson and Gelhar, 1990)

$$\mathbf{X}^{n} = \mathbf{X}^{n-1} + A\left(\mathbf{X}^{n-1}\right)\Delta t + B\left(\mathbf{X}^{n-1}\right)\cdot \mathbf{Z}\sqrt{\Delta t} \tag{6}$$

where $\mathbf{X}^{n}$ is the position of the particle at time level $n\Delta t$, $A\left(\mathbf{X}^{n-1}\right)$ is a known spatial and temporal function that is used to represent the deterministic forcing vector acting to change $\mathbf{X}^{n-1}$, $B\left(\mathbf{X}^{n-1}\right)$ is also a known spatial and temporal function that incorporates the random forces with $A\left(\mathbf{X}^{n-1}\right)$ and $\mathbf{Z}$ is a vector of normally distributed random numbers with mean zero and standard deviation 1. If a large number of particles displace simultaneously, their spatial and temporal probability distribution $f$ will obey the Ito-Fokker-Planck equation (Kinzelbach, 1990)

$$\frac{\partial f}{\partial t} + \nabla\cdot\left(Af\right) - \nabla^{2} : \left[\frac{1}{2}B\cdot B^{T} f\right] \tag{7}$$

For the case of conservative and linearly sorbing solutes, Eqs. (1) and (4) will be equivalent if $A$ and $B$ are defined by

$$A = \mathbf{v} + \nabla\cdot\mathbf{D}, \qquad B\cdot B^{T} = 2\mathbf{D} \tag{8}$$

It is well known that the RWPT method does not exhibit a numerical dispersion (Kinzelbach, 1990) and is superior in accuracy, efficiency and computational cost compared to conventional numerical schemes such as finite element and finite difference methods (Kinzelbach, 1990; Tompson and Gelhar, 1990).

However, a drawback of the RWPT method is the low computational efficiency in strongly heterogeneous porous medium. This is due to the use of a large number of particles and a small time step $\Delta t$ to obtain more accurate results. Thus when the conventional constant time (CT) scheme is used to solve solute transport problems in a strongly heterogeneous porous medium, it requires a very large computational effort. To avoid this computational problem, the constant displacement (CD) scheme developed by Wen and Kung (1995) is used in our simulation. In this scheme, the time step used for the displacement of each particle is adjusted automatically according to the pore velocity value at the present location of the particle. Unlike the CT scheme, the travel time and concentration associated with each particle can be calculated independently by using different time steps for its different displacement steps. More detailed information for CD scheme can be found in works of Wen and Kung (1995).

The concentration $C_{ij}$ in a cell $(i, j)$ at time $t$ can be determined from

$$C_{ij}\left(t\right) = \frac{NP_{ij}\left(t\right)CP\left(t\right)}{\omega\Delta x\Delta y} \tag{9}$$

where $NP_{ij}$ is the particle number in the cell $(i, j)$, $CP(t)$ is the solute mass of each particle, $\Delta x$ and $\Delta y$ are cell size and $\omega$ is the porosity.

## 4 NUMERICAL EXPERIMENTS

A rectangle (100m × 20m) is used as the areal domain with constant thickness of 1.0m (Fig. 1). This domain is discretized into 1m square elements and thus consists of 2000 elements and 2121 nodes. Particles are injected as an instantaneous pulse in the horizontal plane. In order to avoid very high initial concentrations, particles are uniformly distributed over a square area involving 4 elements located at the center of the transversal direction and 10m apart from the inflow boundary in the horizontal direction. This is to ensure that no particle would cross initially the upstream boundary in the simulation.

Two constant values of $h$ = 1.0 and 0.0 are prescribed at two opposite vertical boundaries of the domain, respectively, while no-flux conditions are imposed on the remaining boundaries (Fig. 1). Thus the hydraulic head gradient is 0.01 and the groundwater flows from the left to the right along $x$ direction.

Log hydraulic conductivity fields in the domain are generated for mean zero and four values of $\sigma_{\ln K}$ = 0.25, 0.50, 0.75 and 1.00 with isotropic spatial correlation length of 5.0m. In the present study, all transport simulations are carried out using 100g of solute and the number of particles is 100000 with constant particle mass of 1.0mg. The porosity of 0.35 and the retardation factor of 1.0 are assumed in each simulation.

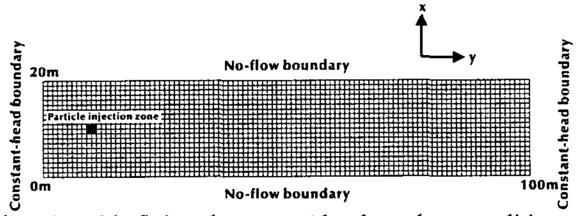
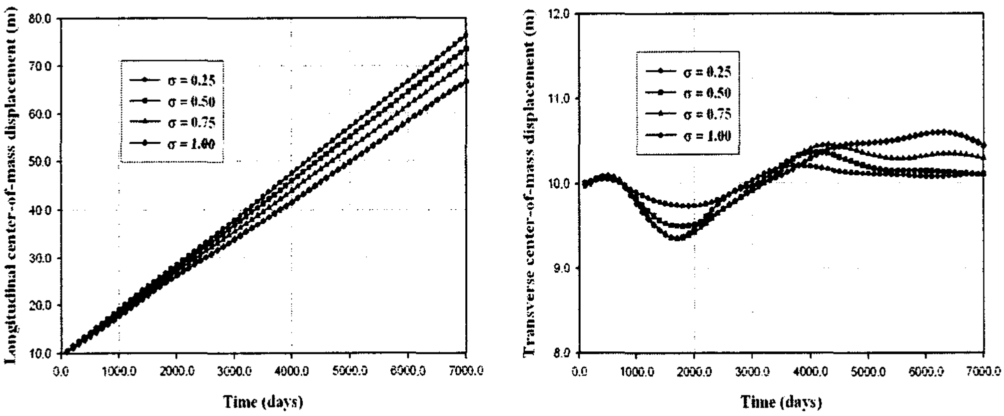



Fig. 1. Rectangular flow domain with finite elements. Also boundary condition and location of the particle injection zone are shown.

Results obtained from numerical experiments are presented in terms of longitudinal and transverse center-of-mass displacements, longitudinal and transverse spatial moments. Also they are expressed in terms of longitudinal and transverse plume skewness. Detailed mathematical definitions of these spatial moments can be found in the paper of Tompson and Gelhar (1990).

Our transport simulation is based on 10 independent log hydraulic conductivity field. Thus results we will present below correspond to mean values for these 10 realizations.

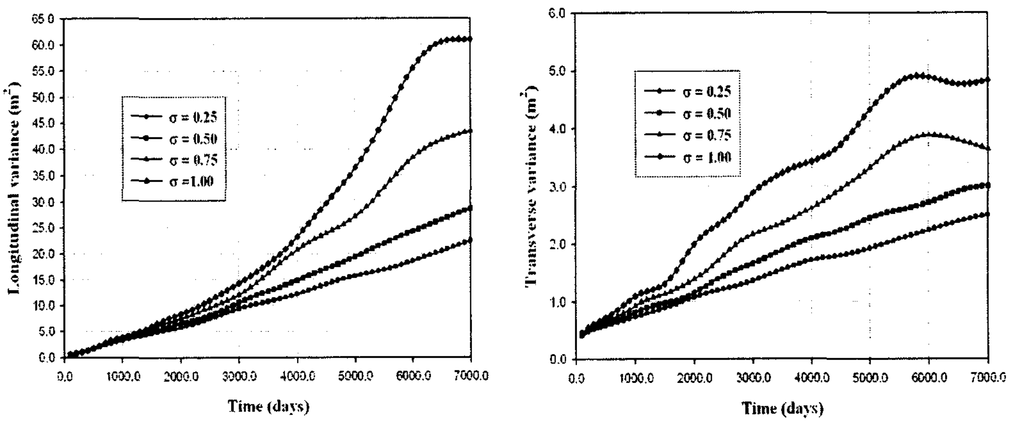



(a) (b)

Fig. 3. Longitudinal and transverse displacement of plume center-of-mass as a function of time (a) longitudinal case (b) transverse case.

The longitudinal and transverse displacements of the plume center-of-mass are depicted in Fig. 3 for those four standard deviations and for the correlation length of 5m. In the case of the longitudinal displacement, the general behavior of the curves shows that the displacement increases linearly according to the increasing time but the slope decreases as $\sigma_{\ln K}$ increases (Fig. 3a). In the case of the transverse displacement, the up and down deviation from the center of the transverse direction (10.0m) tends to increase as $\sigma_{\ln K}$ increases (Fig. 3b). If the porous medium is homogeneous, we can expect that these transverse displacement curves become straight lines along the flow direction.

The longitudinal and transverse spread variance of the plume for the four values of $\sigma_{\ln K}$ is shown in Fig. 4. The effect of the flow domain heterogeneity on the solute plume variance is significant. It is obvious that both longitudinal and transverse variances increase rapidly for larger values of $\sigma_{\ln K}$. Similar behavior was also observed by Berllin et al (1992). For the case of the transverse spread variance, it is observed that curves become undulant as $\sigma_{\ln K}$ increases. This behavior is due to the presence of a zone of high velocity contrast increasing as $\sigma_{\ln K}$ increases.




(a) (b)

Fig. 4. Longitudinal and transverse plume spread variance as a function of time (a) longitudinal case (b) transverse case.

Finally, Fig. 5 shows the longitudinal and transverse coefficient of skewness (i.e. third central moment) as a function of time. In the longitudinal case (Fig. 5a), we observe that the solute plume is generally skewed to the right (i.e. the flow direction) for four values of $\sigma_{\ln K}$, which is indicated by the positive value. We can also see that the longitudinal and transverse skewness coefficients tend to increase as $\sigma_{\ln K}$ increases. This is due to the fact that larger values of $\sigma_{\ln K}$ have a shaper plume front and longer tail relative to the size of the plume. However, the skewness coefficient for $\sigma_{\ln K}$ = 0.75 and 1.00 tends to zero after certain long time (i.e. after about 5300days). This behavior is due to the breakup of the initial solute plume in certain flow fields (Fig. 6b). The plume breakup is owing to the small size of the initial solute plume relative to the scale of flow domain heterogeneities. Thus in the cases of the larger heterogeneities the solute plumes are broken up at the beginning of the transport simulations (Fig. 5a). This causes the spatial moments to oscillate erratically around the values of the moments derived for the homogeneous flow domain (Fig.4). Moreover, the presence of this plume breakup causes the increase of the transverse skewness coefficient (Fig. 5b) instead of the increase of longitudinal skewness coefficient.

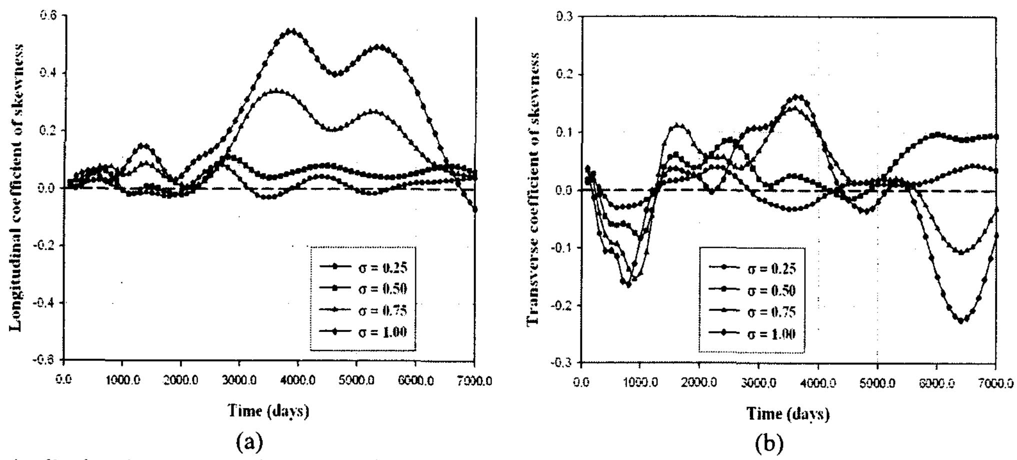



Fig. 5. Longitudinal and transverse plume spread variance as a function of time (a) longitudinal case (b) transverse case.

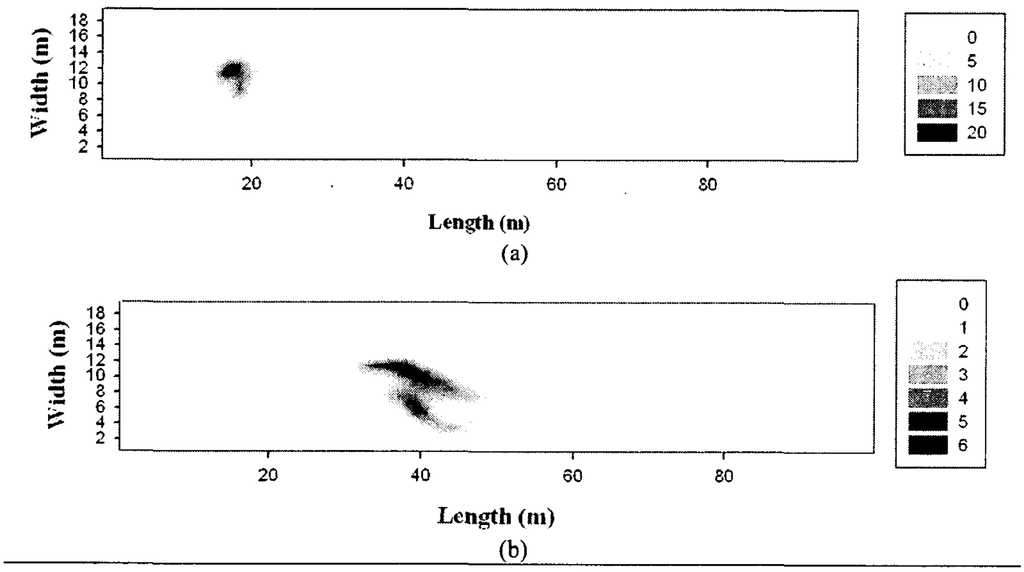



Fig. 6. A typical solute plume associated with $\sigma_{\ln K}$ of 1.00 and the correlation length of 5.00m at the time of (a) 1000 and (b) 5000days.

## 5 CONCLUSIONS

Numerical simulations were.peformed to examine the spatial behavior of nonreactive solute plume in a two-dimensional heterogeneous porous medium, using the random walk particle tracking method. The heterogeneity was generated by assuming a random variable with spatial correlation of hydraulic conductivity lognormally distributed in a flow domain and by using the turning bands method. Four the four log hydraulic conductivity standard deviations of 0.25, 0.50, 0.75 and 1.00 and one correlation length of 5m are considered. Results were presented in terms of spatial moments of the solute plume: center of mass, variance and skewness. From our numerical experiments, we observed that the dispersive behavior of the solute plumes is significantly affected by the flow domain heterogeneity. As the standard deviation of log hydraulic conductivity increases, both longitudinal and transverse plume spread variances increase, especially nonlinearly for a larger standard deviation. In the longitudinal and transverse spread skewness, the oscillatory behavior was especially prevalent for skewness since it is the moment most sensitive to any irregularity in the solute distribution.

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