Monte Carlo simulations of non-ergodic reactive solute transport in random porous media

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Abstract Monte Carlo simulations of transport of reactive solute plumes of finite sizes by steady-state groundwater flow were performed in a two-dimensional heterogeneous aquifer. The results were compared with the first-order theoretical results. Physical and chemical heterogeneity are described with random transmissivity and retardation factor fields, respectively. The transmissivity and retardation factor are assumed to be lognormally distributed and correlated. Three correlation models are considered: the perfectly positive correlation, the perfectly negative correlation, and no correlation. Ensemble averages of the second spatial moments of a plume about its centre of mass and the plume centroid covariance were simulated for the variances of log transmissivity: 0.1, 0.5 and 1.0 and line sources normal to the mean velocity of three dimensionless lengths: 1, 5, and 10. The results show that the first-order theory may significantly overestimate the longitudinal second spatial moments but underestimates transverse moments of reactive solute plumes, especially after long time periods.

INTRODUCTION

Transport of reactive solutes in physically and chemically heterogeneous aquifers has been investigated increasingly in recent years. Most studies were carried out under the assumption of ergodicity. This condition is often unsatisfied in the field. Therefore, it is important to study the effect of the plume size on the spreading of a solute plume. Recently, Zhang & Lin (1998) conducted Monte Carlo simulations of non-ergodic plumes of a conservative solute in two-dimensional heterogeneous aquifers and compared their simulated results with the first-order analytical solutions (Zhang & Zhang, 1997). The purpose of this study is to extend the work of Zhang & Lin (1998) to reactive solutes, i.e. to conduct Monte Carlo simulations of transport of non-ergodic plumes of reactive solutes. The simulated results are then compared with the first-order theoretical results derived recently by Zhang (1998).

SIMULATION DESIGN AND PROCEDURE

The simulation domain is a two-dimensional rectangle where constant hydraulic heads are assigned at the left and right boundary and the no-flow condition on top and bottom to create a uniform mean velocity \( \mu \). The domain is divided into 256 \( \times \) 128 square cells of one unit length. The integral scale, \( L \), of log transmissivity, \( Y = \log T \), is taken to be 5 units. Three values of the variance of log transmissivity, \( \sigma_Y^2 \)
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= 0.1, 0.5, and 1.0, were simulated. An inner region where the velocity field is stationary was found to be 15 cells or 3 integral scales to the outside boundaries. A line source of three dimensionless lengths, ѳ = l/L = 1, 5, and 10 normal to µ were simulated, where l is the length of the line source. Physical and chemical heterogeneities are described with random transmissivity and retardation factor fields, respectively. The transmissivity and retardation factor are assumed to be lognormally distributed and correlated. Three correlation models are considered: the perfectly positive correlation (model A), the perfectly negative correlation (model B), and no correlation (model C). The simulation starts by generating a random transmissivity field with the mean $E(Y)$, the variance $\sigma_Y^2$, and the isotropic exponential covariance function $\rho_Y = \sigma_Y^2 \exp(-r/L)$, where $r$ is the separation distance. The retardation factor field is then obtained with its correlation to $Y$. The hydraulic heads at nodal points are solved from the steady-state groundwater flow equation with the boundary conditions described above by using the mesh-centred finite difference method and the point successive over-relation scheme. The velocity at the interfaces between two cells are calculated with a linear interpolation. A line source normal to $\mu$ is represented by a number of particles (four particles per cell) which are placed 15 cells or 3L away from the left constant head boundary to avoid the boundary effect. These particles are tracked with a Euler algorithm. The retarded particle velocity, $v^r = v / R_d$, is calculated using the linear interpolation, where $R_d$ is the mean retardation factor. The tracking stops during each Monte Carlo (MC) run when any of the particles is moved closer than 3L to the boundaries. At the end of the $m$th MC run, the position of the centroid of the retarded plume, $R^m$, and their second spatial moments, $S^m_{ij}$ ($i, j = 1, 2$) are computed. The above procedures are repeated for $M (= 800)$ realizations of the $Y$ and $R$ field. The average positions, $\langle R(t) \rangle$, the average of the second spatial moments, $\langle S_y(t) \rangle$, and the plume centroid covariance, $R_y(t)$, are then calculated. Once $\langle S_y \rangle$ and $R_y$ are available, the second spatial covariance of an ergodic plume, $X_y$, can be obtained based on the fundamental relationship (Dagan, 1990):

$$X_y(t) = \langle S_y(t) \rangle - S_y(0) + R_y(t)$$

where $S_y(0)$ is the initial value of $S_y(t)$ and is assumed to be constant in this study.

RESULTS AND DISCUSSION

While the second spatial moments $\langle S_y(t) \rangle - S_y(0)$ and the plume centroid covariance, $R_y(t)$, were simulated, we present only the second spatial moments of an ergodic plume, $X_y(t)$, due to the limited space ($i = 1, 2$). The values of $X_y(t)$ are obtained by adding the simulated $\langle S_y(t) \rangle - S_y(0)$ to $R_y(t)$, based on the relationship (3). The ergodic moments, $X_y$, should be invariant with the initial size of a plume for a fixed value of $\sigma_Y^2$. This is indeed the case as shown in Fig. 1 where the simulation results are presented with the symbols and the first-order solutions are given by the solid lines. For any of the three values of $\sigma_Y^2$, say 1.0, all six symbols (triangle, diamond,
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Fig. 1 Comparison of the simulated second spatial moments (symbols) with the first-order analytical solutions (solid lines), (a) $X_{11}$ for model A, (b) $X_{22}$ for model A, (c) $X_{11}$ for model B, (d) $X_{22}$ for model B, (e) $X_{11}$ for model C, (f) $X_{22}$ for model C. In each graph, the top symbol and solid curves are for $\sigma_y^2 = 1.0$, the middle symbol and solid curves are for $\sigma_y^2 = 0.5$, and the bottom symbol and solid curves are for $\sigma_y^2 = 0.1$. The value of $i_j$ is the length of a line source normal ($i_j = 1$) or parallel ($i_j = 1$) to $\mu$.

star, plus, cross, and asterisk curves), representing $X_{11}$ (Fig. 1(a), (c), (e)) and $X_{22}$ (Fig. 1(b), (d), (f)) for the line sources of three different lengths either normal or parallel to the mean flow and for model A (Fig. 1(a), (b)), model B (Fig. 1(c), (d)), and model C (Fig. 1(e), (f)), fall on each other to form a single curve for the simulated $X_{11}$ and $X_{22}$. The more or less same values of $X_{11}$ obtained for each value of $\sigma_y^2$ may be viewed as validation of the simulation results. By comparing the simulated results with the analytical solutions (the solid curves) derived by Zhang (1998), one may conclude that the first-order theory overestimates the longitudinal moment, $X_{11}$, but it significantly underestimates the transverse moments, $X_{22}$, especially in late time. The results obtained here for a reactive plume are different from those for a conservative plume found by Zhang and Lin (1998) in that the first-order theory provides a fairly accurate approximation to $X_{11}$ but in both studies the first-order theory consistently underestimates $X_{22}$.

REFERENCES


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