A numerical assessment of the random walk particle tracking method for heterogeneous aquifers

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Abstract The random walk particle tracking method has become an important tool for the uncertainty assessment of solute transport models due to its computational efficiency and the non-existence of numerical dispersion. Yet, in highly heterogeneous aquifers the smoothness assumption of the velocity field, requisite for a correct solution of the random walk equations, may not hold anymore. Three different numerical methods to overcome this problem are numerically evaluated. The results demonstrate that in an aquifer with an isotropic spatial correlation, and following a multi-Gaussian random function with a small connectivity of extreme values, all techniques are able to model solute transport correctly, even for a hydraulic conductivity variance of $\sigma^2_{lnK} = 4$.

Keywords heterogeneity; local mass conservation; numerical implementation; random walk particle tracking; solute transport

INTRODUCTION

Eulerian transport models are often plagued by numerical dispersion or artificial oscillations, especially for advection-dominated problems. To reduce these problems, a higher grid resolution and smaller time steps may be applied, resulting in large computational times.

One alternative to solve transport in heterogeneous porous media is the Lagrangian approach. In particular, the random walk particle tracking (RWPT) method, treats the transport of a solute by partitioning the solute mass into a large number of particles. It moves each particle through the porous medium using the velocity field obtained from the solution of the flow equation to simulate advection, and adds a Brownian random displacement to simulate dispersion. This approach avoids solving the transport equation directly and therefore is virtually free of numerical dispersion and artificial oscillations. Furthermore, computational times, even for models with a high grid resolution and characterized by strong heterogeneities, are significantly smaller than using the traditional Eulerian, mixed Eulerian-Lagrangian, or total variation diminishing (TVD) schemes (e.g. Tompson & Gelhar, 1990; Zheng & Bennett, 2002). These advantages have made the RWPT method a popular choice for complex, high-resolution transport problems, inverse modelling, and uncertainty assessment of contaminant transport.

BASIC PRINCIPLES

Random walk particle tracking is a method from statistical physics which has been used in the analysis of dispersion and diffusion processes in porous media. It is based on a similarity between the Fokker-Planck equation and the advection–dispersion equation. Using the similarity between these equations, solute concentrations are represented by the density function of particles that are moving following the Itô-Taylor integration scheme (Gardiner, 1990):

$$\mathbf{X}_{p}(t + \Delta t) = \mathbf{X}_{p}(t) + \mathbf{A}(\mathbf{X}_{p}, t) \Delta t + \mathbf{B}(\mathbf{X}_{p}, t) \cdot \Delta w \sqrt{\Delta t}$$
with $\mathbf{A} = \mathbf{u} + \nabla \cdot \mathbf{D}$ and $2\mathbf{D} = \mathbf{B} \cdot \mathbf{B}^{\mathrm{T}}$
(1)

where $\mathbf{X}_p(t)$ is the position of a particle at time *t*; **A** is a "drift" vector; **B** is a tensor defining the strength of dispersion which is related to the dispersion tensor **D** as shown above; **u** is the groundwater velocity; and Δw , an uncorrelated stochastic force, is a vector of independent normally distributed random variables with zero mean and unit variance.

However, using Stratonovich's interpretation of a stochastic integral leads to the following equation, by which the density function of particles also fulfils the advection–dispersion equation:

$$\mathbf{X}_{p}(t + \Delta t) = \mathbf{X}_{p}(t) + \mathbf{A}\left(\mathbf{X}_{p}, t + \frac{\Delta t}{2}\right) \Delta t + \mathbf{B}\left(\mathbf{X}_{p}, t + \frac{\Delta t}{2}\right) \cdot \Delta w \sqrt{\Delta t}$$
(2)
with: $\mathbf{A} = \mathbf{u} + \frac{1}{2} \mathbf{B} \cdot \nabla \cdot \left(\mathbf{B}^{T}\right)$ and $2\mathbf{D} = \mathbf{B} \cdot \mathbf{B}^{T}$

It can be seen that the drift vector and the dispersion tensor are evaluated at a moment halfway along the time step to the next particle position. Equation (2) is rarely used for the RWPT method, as this procedure requires an additional iterative scheme within each time step. Nevertheless, the modified velocity contains a derivative term reduced by a factor of 1/2.

THE PROBLEM OF LOCAL SOLUTE MASS CONSERVATION

Numerical implementation of the random walk equations is relatively simple, with one exception. When solving the flow equation using numerical methods the resulting hydraulic heads and the associated velocity field are usually computed at discrete points. Yet, simulation of solute transport by the random walk methodology requires continuous information about the velocity field. Therefore, a map of velocities from this discrete information has to be generated. This velocity map should fulfil the local fluid mass balance at any location and the local solute mass conservation at any grid-cell interface. In general, there is not a simple solution to this problem, but several approaches have been proposed in the literature.

The interpolation method

The interpolation method is certainly the approach most commonly used to address this problem. It uses linear interpolation to obtain the groundwater velocity at any point and bilinear interpolation to calculate the gradient of the dispersion term and the dispersion tensor. By means of this so-called "hybrid" scheme, the interpolation method fulfils both the fluid mass balance and the local solute mass balance. Nevertheless, using bilinear interpolation introduces a greater smoothing, which can lead to errors especially for highly heterogeneous aquifers. LaBolle *et al.* (1996) presented a detailed analysis of this method.

The reflection principle

The reflection principle was first presented by Uffink (1985) and is based on the idea of diffusion across a boundary with different diffusion coefficients. He suggested that part of a set of particles crossing from one domain into another with different diffusion coefficients must be reflected in order to obtain the correct concentration distribution across the boundary between the domains. This is done in RWPT by assigning a certain probability for a particle of crossing the domain interface, which depends on the diffusion coefficients on either side. The local flow mass balance is satisfied by using linear interpolation to calculate groundwater velocity. Various authors (Ackerer, 1987; Cordes & Rouvé, 1991; Semra *et al.*, 1993; Hoteit *et al.*, 2002) have used this approach and suggested slight modifications.

Generalized stochastic differential equations

Strictly speaking, stochastic theory only applies when transport properties are smooth functions in space. LaBolle *et al.* (2000) presented generalized stochastic differential equations (GSDE) for the case of discontinuous transport properties and their numerical integration for RWPT. In practical terms this means that, for the case of isotropic dispersion and homogeneous porosity, a two-step procedure is used in order to account for the local solute mass balance. First, the velocity at the particles position, shifted only by the dispersive part, is evaluated. Then, this velocity is used to calculate the final particle step. The local fluid mass balance is fulfilled by using linear interpolation as in the other two approaches.

NUMERICAL ANALYSIS

The approaches were numerically implemented into the random walk transport model RW3D (Fernàndez-Garcia *et al.*, 2005). Solute transport in the following synthetic cases is conservative, two-dimensional and pore-scale dispersion is assumed to be isotropic ($\alpha = 0.01$ m). A constant displacement scheme is used as it is computationally more efficient than the constant time step scheme (Wen & Gómez-Hernández, 1996). MODFLOW (McDonald & Harbaugh, 1988) was used to solve the flow equation and to compute the cell-interface velocities.

Two heterogeneous hydraulic conductivity fields with a discretization of $\Delta x = \Delta y = 0.3$ m and a total domain size of x = 60 m and y = 21 m were generated using stochastic

simulation techniques as shown in Fig. 1. Whereas for model A a Gaussian random function is used, model B was created using indicator simulation. Spatial correlation is isotropic for model A ($\lambda_x = \lambda_y = 1.2 \text{ m}$) and strongly anisotropic for model B ($\lambda_x = 20 \text{ m}$, $\lambda_y = 1.2 \text{ m}$). The spatial correlation for both fields is modelled using an exponential semivariogram and the indicator simulation was performed using a mosaic model with nine thresholds. The variance is increased from $\sigma_{lnK}^2 = 0.5$ to 4 in order to simulate increasing heterogeneity and the mean hydraulic conductivity is kept constant at $\ln K = -6.908 \text{ m s}^{-1}$. In this article, the interpolation method, using the Itô or the Stratonovich interpretation of a stochastic integral, and the GSDE method in highly heterogeneous aquifers are evaluated.

The third order TVD (ULTIMATE) scheme, included in the MT3DMS model (Zheng & Wang, 1999), was used for comparison with these methods. This scheme offers an attractive alternative to the traditional mixed Eulerian-Lagrangian schemes (e.g. method of characteristics, MOC) due to its mass conservation property and the ability of reducing numerical dispersion (Zheng & Wang, 1999; Zheng & Bennett, 2002). Nevertheless, as the present problem is strongly advection-dominated, the domain was refined to a discretization of $\Delta x = \Delta y = 0.1$ m to minimize any possible numerical dispersion. One model run for model B with $\sigma^2_{lnK} = 2$ was repeated with a discretization of $\Delta x = \Delta y = 0.075$ m and the two results obtained with the TVD scheme were compared. Neither artificial oscillations nor numerical dispersion were observed.

The differences between the different numerical schemes are investigated by comparing the time-dependence of corresponding solute plume spatial moments. The spatial moments are calculated following Tompson & Gelhar (1990).



Fig. 1 Models generated using sequential Gaussian simulation (Model A) and indicator simulation (Model B) with different spatial correlation. Model dimensions are given in metres; hydraulic conductivity is as $\ln K$.

RESULTS

All methods performed well for model A, even when presenting an extreme heterogeneity of $\sigma_{lnK}^2 = 4$ (Fig. 2). For model B, all the techniques illustrate good results up to a hydraulic conductivity variance of $\sigma_{lnK}^2 = 2$. Increasing the heterogeneity for this model, only the interpolation method in combination with the Itô- or Stratonovich-Fokker-Planck equation is able to reproduce the average velocity and the macrodispersivity correctly (Fig. 3). The GSDE method underestimates the average velocity and overestimates the macrodispersivity as depicted in Fig. 3.

With respect to the numerical implementation, the interpolation method in combination with the Itô-Fokker-Planck equation is the easiest method. All other









approaches require either an additional iterative scheme (Stratonovich interpretation), or are complex to implement for three-dimensional, heterogeneous systems (reflection principle, GSDE).

Finally, it should be noted that computation times, especially for the strongly heterogeneous cases, are significantly lower for the RWPT method than for the TVD scheme. Whereas the TVD scheme required from approximately 30 minutes (for model A with $\sigma^2_{lnK} = 0.5$) to several hours (for model B with $\sigma^2_{lnK} = 4$) to solve the transport equation, RWPT, using 2000 particles, required approximately 15 minutes, clearly demonstrating the computational efficiency.

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