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ABSTRACT

A simple particle tracking technique based on an Eulerian-Lagrangian finite element approach was used to solve the solute transport equation. The method introduces only one moving particle to track each concentration front continuously forward in one-dimensional transport problems. At each time step, all element nodes are taken as moving particles along the characteristic path. The single-step reverse particle tracking technique was adopted to obtain the 'convective components' of concentrations for nodes away from the concentration front, whereas the convective components for nodes within the front area were obtained by the single-step forward particle tracking technique. Results from a large number of simulations showed that the numerical solution improved when the Lagrangian derivative was multiplied with a correction factor larger than one.

INTRODUCTION

Numerical simulators of the convection-dispersion equation (CDE) are widely used for predicting solute transport in soil and aquifer systems. Application of conventional finite element and finite difference numerical methods to the solution of convection-dominated transport problems often results in oscillatory behavior and/or numerical dispersion, unless very fine temporal and spatial steps are adopted. The mixed Eulerian-Lagrangian method has proven to be quite effective in eliminating or reducing oscillations and numerical dispersion. This type of method has been used extensively in the past to solve a variety of surface and subsurface transport problems (Konikow and Bredehoeft [6], Neuman and Sorek [8], Neuman [9], Molz et al. [7], Huang [5], Yeh [ll], Dimou and Adams [l]). The method uses a Lagrangian approach to treat the convection term along characteristic paths, while all other terms are solved on a fiied Eulerian grid. The Lagrangian approach usually involves either continuous forward particle tracking (CFPT) (Carder et al. [4], Konikow and Bredehoeft [6], Dimou and Adams [l], among others), or a single-step reverse particle tracking (SRPT) method (Molz et al. [7], Yeh [Il], Galeati et al. [3]).

As shown by Neuman and Sorek [8], the SRPT method can still result in significant numerical dispersion. The CFPT method, on the other hand, is virtually free of numerical dispersion but suffers from instability when the time step size exceeds a certain limit (Neuman.[9]). Complex boundary conditions and nonlinearities are also not easily incorporated. In addition, the numerical implementation of a large number of particles can become quite time-consuming and laborious. In Neuman's hybrid method [9], the convective contribution to the concentration near a steep concentration front is tracked forward-using moving particles clustered around the front. Away from a front, however, the convection problem is being handled with the SRPT method. This approach has proven to be very effective in eliminating most of the numerical difficulties.

Unfortunately, one drawback of Neuman's hybrid method is that a sophisticated procedure must be used at each time step to map concentrations from particles to nodes of the fixed grid, and to re-establish the concentration of particles from those at the nodes. The objective of this paper is to describe a much simpler and more efficient particle tracking technique for solving the one-dimensional CDE.

THEORY

The governing equation for one-dimensional solute transport in a porous medium is taken as

$$R\frac{\partial c}{\partial t} = \frac{1}{\theta}\frac{\partial}{\partial x}(\theta D\frac{\partial c}{\partial x}) - v\frac{\partial c}{\partial x} - \mu c + \gamma \qquad (1)$$

where c is the solution concentration, t is time, x is distance, $R = 1 + \rho k/\theta$ is the retardation factor, ρ is the porous medium bulk density, k is an empirical distribution constant, θ is the volumetric moisture content, v is the pore-water velocity, and μ and y are rate constants for first-order decay and zero-order production, respectively. Equation (1) will be solved subject to the initial and boundary conditions

$$c(x, 0) = C_i(x) \qquad (2a)$$

$$(-\beta D\frac{\partial c}{\partial x} + vc)\Big|_{x=0} = vC_0 \qquad (2b)$$

$$\frac{\partial c}{\partial x}(L, t) = 0 \qquad (2c)$$

where $C_i(x)$ and C,,(t) are prescribed functions of x and t, respectively; β controls the type of boundary condition imposed at the inlet position (β =0 for prescribed concentration conditions and β = 1 for prescribed flux conditions); and *L* is the-length of the medium being considered. Using the Lagrangian derivative

$$\frac{Dc}{Dt} = \frac{\partial c}{\partial t} + v^* \cdot \frac{\partial c}{\partial x} \tag{3}$$

where $v^* = v/R$, Equation (1) can be rewritten in Lagrangian form as

$$R\frac{Dc}{Dt} = \frac{1}{\theta}\frac{\partial}{\partial x}(\theta D \frac{\partial c}{\partial x}) - \mu c + \gamma \tag{4}$$

in which c no longer represents the concentration at a point in space and time, but rather the concentration of a fluid particle moving along a characteristic path described by the equation

$$\frac{dx}{dt} = v^* \tag{5}$$

PROPOSED PARTICLE-TRACKING METHOD

Assume that the concentration c_k at time t_k is known. Equation (4) subject to auxiliary conditions (2a, b, c) will be used to solve for c_{k+1} at time step $t_{k+1} = t_k + At$, where *At* is the time increment, using the following four consecutive steps:

1. Tracking the Concentration Front

Since numerical difficulties are expected to occur primarily near sharp concentration fronts, the first and foremost step is to find as accurately as possible the positions of the concentration fronts. This is done by introducing a moving particle at the input boundary and at the center of each source or sink location, and subsequently tracking these particles continuously forward at each time step along their characteristic paths. Let particle P represent the center of a concentration front. If this particle at time t_k is located at x_k^P, its position at time t_{k+1} will be

$$x_{k+1}^P = x_k^P + \int_{t}^{t_{k+1}} v^* dt \tag{6}$$

We note that a new moving particle must be introduced at the inflow boundary each time the concentration there changes. Similarly, a new particle is needed each time the concentration of a source or sink changes.

2. Single-Step Forward Tracking

Next., the nodes around each concentration front are considered to be moving particles and tracked forward for the duration of one time step. As a moving particle, the position of node n at time t_{k+1} will be

$$x_{k+1}^{n} = x_n + \int_{t_k}^{t_{k+1}} v^* dt \qquad (n=1,2,...,N_P) \tag{7}$$

where x_n is the fiied position of node n, and N_P is the number of nodes considered to be moving particles. The convective component for nodes covered by moving particles was estimated from particle concentrations, c_j^k, using the inverse distance interpolation formula (Fujinawa [2])

$$\overline{c}_n = \begin{cases} \sum_{j=1}^{2} c_j^k / r_j \Big/ \sum_{j=1}^{2} 1/r_j & \min r_j > \epsilon \\ c_j & \min r_j \le \epsilon \end{cases} \tag{8}$$

where ϵ is some limiting value of the distance $r_j = | x_n - x_j^{k+1} |$ between node n and moving particle j.

3. Sinele-Sted Reverse Tracking

In areas where the concentration gradients are weak, the convective component was obtained using the efficient single-step reverse particle tracking technique (Neuman [9]). Each node, n, in these areas is considered to be a fictitious particle and sent backward during a particular time step along its characteristic path to the point

$$x_n' = x_n - \int_{t_k}^{t_{k+1}} v^* dt \tag{9}$$

This means that a particle leaving at t_k will reach the grid point location x_n exactly at t_{k+1}. For a steady-state flow field, x_n' is the same for all nodes, and hence needs to be calculated only once. The convective component, $\overline{c}_n$, for node n can be computed by the finite element method. In our analysis, the convective component takes the concentration of the down-stream node of the element where x_n' was located.

4. Finite Element Approximation

Define the finite element approximation of c as

$$c^N(x,t) = \sum_{i=1}^{N} c_i(t)\, \varphi_i(x) \tag{10}$$

where N is the number of nodes placed in the solution domain, and $\varphi_i(x)$ are the linear basis functions. Application of the Galerkin procedure to Equation (4) leads to

$$\int_L [R\frac{Dc}{Dt} - \frac{1}{\theta}\frac{\partial}{\partial x}(\theta D\frac{\partial c}{\partial x}) + \mu c - \gamma]\varphi_i dx \qquad (i=1,2,...,N) \qquad (11)$$

where L is the solution domain. By applying mass-lumping to the time-derivative term,. integrating by -parts, and using Equation (10) for c, Equation (11) can be rewritten in matrix form as

$$([E] + [F])\{c\} - [G] + [H]\left\{\frac{Dc}{Dt}\right\} = 0 \qquad (12)$$

where

$$E_{ij} = \int_L \theta D\frac{\partial(\varphi_i/\theta)}{\partial x}\frac{\partial \varphi_j}{\partial x} dx \approx \int_L D\frac{\partial \varphi_i}{\partial x}\frac{\partial \varphi_j}{\partial x} dx \qquad (13a)$$

$$F_{ij} = \int_L \mu \varphi_i \varphi_j dx \qquad H_{ij} = \int_L R \varphi_i \varphi_j dx \qquad (13b)$$

$$G_{ij} = \int_1 \gamma \varphi_i \varphi_j dx + \varphi_i D\frac{\partial c}{\partial x}\Big|_0^L \qquad (13c)$$

in which the Lagrangian derivative was approximated by

$$\frac{Dc_i}{Dt} \approx \frac{c_i^{k+1} - \overline{c_i}}{\Delta t} \qquad (14)$$

Solving Equation (12) leads to the solution, c_n^{k+1}. As will be shown later, we found that the numerical results could be further improved by multiplying the Lagrangian derivative with an empirical correction factor larger than one.

EXAMPLES

The proposed particle tracking method was used to simulate convective-dispersive solute transport in a homogeneous medium during steady-state water flow (θ and v are constant), and without considering adsorption (R = 1) and zero- or first-order reactions ($\gamma = \mu = 0$) in Equation (1). i.e.,

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - v\frac{\partial c}{\partial x} \tag{15}$$

subject to the initial and boundary conditions

$$c(x,0) = 0 \qquad c(0,t) = \begin{cases} 1 & 0 < t \le t_0 \\ 0 & t > t_0 \end{cases} \qquad \frac{\partial c}{\partial x}(L,t) = 0 \tag{16}$$

Using any arbitrary buf con&tent set of units, the physical and finite element grid parameters are v = 0.5, L =2.5, Ax = 0.05, and D = 10^{-2}, lo", 10^{-4}, and 10^{-5}, resulting in mesh Peclet numbers, $Pe = v\Delta x/D$, of 2.5,25,250, and 2500. The selected time steps At are 1.25 and 2.5, giving local Courant numbers, Cu $= v\Delta t/\Delta x$, of 1.25 and 2.5, respectively. Results obtained with our method will be compared with those computed using Neuman's hybrid method (Neuman [9]) assuming 20 moving particles, and the analytical solution of Equations (15) and (16) as given by van Genuchten and Alves [10].

Figure 1 shows very good agreement between our solution (solid circles), Neuman's method (dashed lines) and the analytical solution (solid lines). Numerical oscillations were completely eliminated by both methods. Actually, our results appear slightly better than those obtained with Neuman's approach.

Figure 2 presents simulation results for a transport problem with a step input concentration pulse (t_0 = 1) at the inlet boundary. The numerical solution closely approximates the analytical results at the lower Peclet number. However, some numerical dispersion is apparent in our as well as Neuman's method when the Peclet number becomes very large.

Figure 3 shows comparisons of the maximum error (ME) and the sum of squared error (SE) between the analytical and numerical results. SE reflects primarily the amount of numerical dispersion. These and other results indicate that the errors generated with our relatively simple particle tracking method are generally smaller than those obtained with Neuman's approach at relatively low to intermediate values of the Peclet number, *Pe*. Table 1 further demonstrates that for relatively large Peclet numbers the amount of numerical dispersion introduced with our scheme (as reflected by the value of SE) is the same or only slightly higher than SE obtained with Neuman's approach. On the other hand, the maximum error, ME, produced with our method was always smaller than the maximum error generated with Neuman's scheme.

By multiplying the Lagrangian derivative with a factor, ω, larger than one, the accuracy of the simulated results by our as well as Neuman's method can be further improved. For-Peclet numbers larger than about 10^2, the computed result becomes better as ω increases. More dramatic

improvements in accuracy were observed within a given range of ω values. As shown in Figure 3, an optimal value of ω exists for Peclet numbers of order 10^1. For Peclet number of order 10^0, a value of slightly more than one appears optimal. One likely explanation for these numerical effects is that a larger ω value makes the capacity matrix, H, in Equation (12) more diagonally dominant, a feature which is known to increase numerical stability.

The simulated solutions were found to be sensitive to the size of the concentration front area to which the single-step forward particle tracking technique was applied. The errors increased significantly when the method was applied to areas over where the concentration fronts were poorly defined. Our results suggest that for relatively large Peclet numbers it is sufficient to use only two or three nodes ahead and behind the concentration front as the forward tracking particles. More nodes should be considered when the Peclet number becomes less than about 100.

The results given here show that the proposed particle-tracking method virtually eliminates numerical oscillations and artificial dispersion for convection-dispersion problems involving a wide range of mesh Peclet numbers, and for local Courant numbers well above 1. Compared with other particle tracking techniques for solving solute transport problems, our method is also much simpler and easier to implement, especially for transient velocity fields.

Table 1. Maximum errors (ME) and sum of squared errors (SE) obtained with the method proposed in this study and Neuman's approach ($\omega = 1$).

	Pe = 250				Pe = 2500			
	This study		Neuman		This study		Neuman	
	ME	SE	ME	SE	ME	SE	ME	SE
t=2	0.216	0.080	0.231	0.059	0.219	0.082	0.228	0.056
t=3	0.205	0.085	0.266	0.088	0.214	0.093	0.276	0.070
t=4	0.242	0.114	0.279	0.110	0.269	0.132	0.305	0.120

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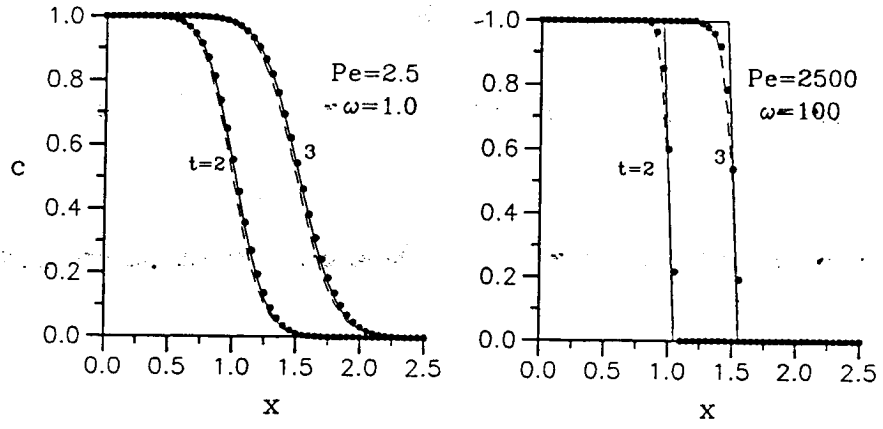

Fig. 1 Comparison of simulated results using the method described in this study (solid circles), Neuman's approach (dashed lines), and the analytical solution (solid lines).

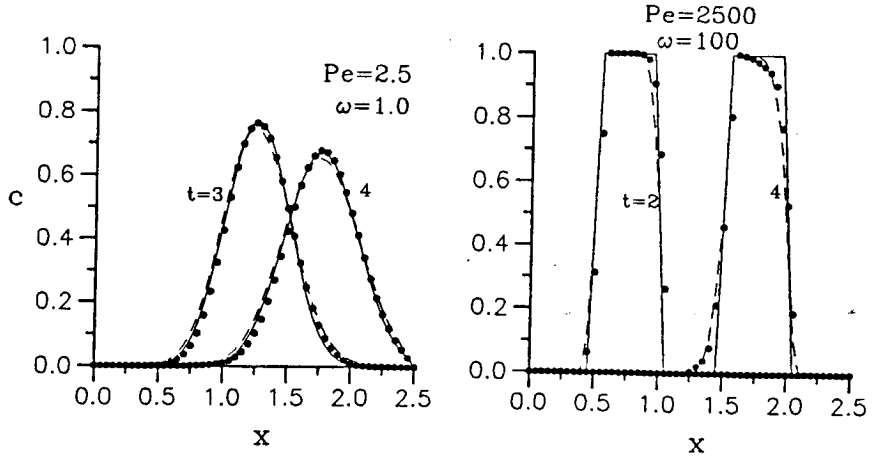

Fig. 2 Comparison of concentration distributions obtained with our method (solid circles) and the analytical solution (solid lines).

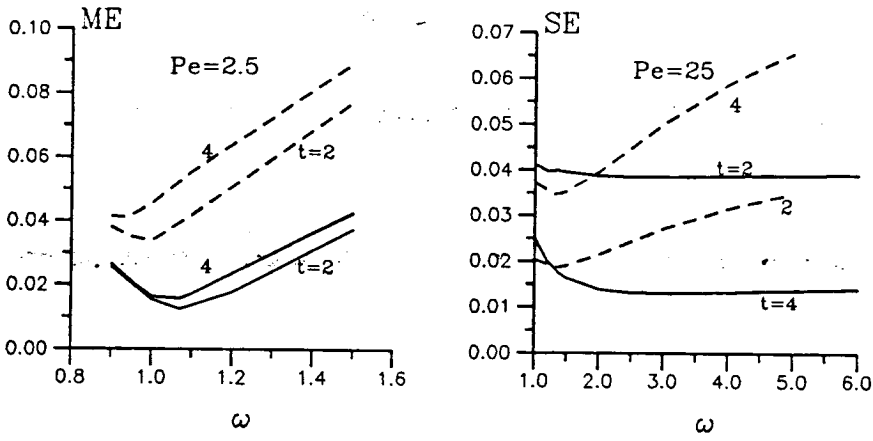

Fig. 3 Mean error (ME) and sum of squared error (SE) as a function of the correction factor, ω, obtained with the method proposed in this study (solid lines) and Neuman's approach (dashed lines).