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An Efficient Eulerian-Lagrangian Method for Solving Solute Transport Problems in Steady and Transient Flow Fields

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A computationally efficient, yet relatively simple Eulerian-Lagrangian method is proposed for solving the one-dimensional convection-dispersion solute transport equation assuming a steady or transient velocity field. The method uses a modified single-step reverse particle tracking (MSRPT) technique to handle steep concentration fronts. The scheme utilizes two weighting factors to control the movement of particles during a backward tracking step. One weighting factor greater than unity is used in the upstream region of the convection front, while another weighting factor less than unity is taken in the downstream region. The two factors were related empirically to the grid Peclet and Courant numbers. The MSRPT technique is carried out only within the concentration plume at each time step. For transient flow fields, the weighting factors were determined using an automatically adjustable procedure based on mass balance errors. The MSRPT method maintains the advantages of the traditional single-step reverse particle tracking (SRPT) procedure, i.e., producing efficient and oscillation-free calculations, but circumvents numerical dispersion introduced by SRPT. A large number of tests against analytical solutions for one-dimensional transport in uniform flow fields indicate that the proposed method can handle the entire range of Peclet numbers from zero to infinity. Numerical tests also show that the MSRPT method is a relatively accurate, efficient and mass-conservative algorithm for solute transport in transient flow fields. The Courant number at present cannot exceed 1. The MSRPT approach was found especially useful for convection-dominated problems; in fact, an exact numerical solution may be obtained with MSRPT for pure convection.

INTRODUCTION

Convection-dispersion type equations are being widely used to model solute transport in soil and groundwater. Owing to the particular combination of hyperbolic and parabolic terms, serious difficulties are often encountered in obtaining accurate numerical solutions of these equations. A variety of numerical schemes have been developed to deal with these difficulties, including an extensive number of Eulerian methods using fixed grid systems, and Lagrangian approaches involving moving coordinates. There is now a growing trend to combine the Eulerian and Lagrangian methods *[Garder et al.,* 1964; *Leith, 1965; Heinrich et al., 1977; Konikow and Bredehoeft, 1978; Varoglu and Finn, 1978; Cheng et al., 1984; Khaleel and Reddell, 1985; Fujinawa, 1986; Dimou and Adams, 1991; Leonard, 1991; Galeati et al., 1992; Huang et al., 1992,* among others]. Eulerian-Lagrangian methods treat the convection part of the transport problem using a Lagrangian formulation in a fixed Eulerian grid, while the dispersion term is treated by either an Eulerian or a Lagrangian formulation. As a typical example, *Neuman and Sorek [1982]* decomposed the concentration field into two parts, one controlled by pure convection, the other by dispersion. The convection part was handled with the help of moving particles, while the dispersion problem was solved using finite elements on a fixed grid. Neuman [1984] subsequently presented an adaptive Eulerian-Lagrangian finite element method for solving the convection-dispersion equation. The method is capable of dealing with the entire range of Peclet numbers from zero to infinity. However, the scheme is quite troublesome to implement and time consuming to execute because of the need to continuously track the front using numerous particles at each time step. In a related approach, *Yeh* [1990] used the Eulerian-Lagrangian method with a zoomable (or adjustable) hidden fine-mesh approach to resolve numerical difficulties. While this scheme reduces or virtually eliminates numerical dispersion and oscillations, the process of zooming and refining the elements at each time step is not straightforward in terms of its practical implementation. Also, the large number of elements needed for this approach requires excessive amounts of computer memory and execution time.

In the adaptive Eulerian-Lagrangian finite element method used by *Neuman [1984],* the convective components of steep concentration fronts were tracked forward with moving particles around each front. Away from the fronts, however, the convective problem was solved with a single-step reverse particle tracking (SRPT) method. The SRPT technique requires much less computer time and storage than continuous forward particle tracking. Unfortunately, one drawback of the SRPT method is that it introduces some numerical dispersion near sharp concentration fronts.

The objective of this paper is to present a simple and efficient particle tracking technique to solve the convection-dispersion equation. A modified single-step reverse particle tracking (MSRPT) method is used to deal with convection-dominated transport problems. We shall show that MSRPT maintains the advantages of the traditional single-step reverse particle tracking procedure, but eliminates numerical dispersion introduced by SRPT. Simulation results based on the scheme will be compared with analytical solutions as well as numerical results obtained with other methods.

GENERAL FORMULATION

Transport of miscible components in a one-dimensional transient flow field is described with the convection-dispersion solute transport equation

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$$\theta R \frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(\theta D \frac{\partial c}{\partial x}\right) - \theta v \frac{\partial c}{\partial x} \quad (1)$$

where c is the solution concentration, t is time, x is distance, D is the dispersion coefficient, $v = q/\theta$ is the pore water velocity, q is the Darcian fluid flux, θ is the volumetric water content, and R is a retardation factor accounting for linear equilibrium sorption; i.e.,

$$R = 1 + \rho k/\theta \quad (2)$$

in which ρ is the porous medium bulk density and k is an empirical distribution constant. The equation will be solved here subject to the initial and boundary conditions

$$c(x, 0) = C_0 \quad (3)$$

$$-\beta D \frac{\partial c}{\partial x} + v(c - C_1) = 0 \qquad \text{inflow boundary} \quad (4)$$

$$\frac{\partial c}{\partial x} = 0 \qquad \text{outflow boundary} \quad (5)$$

where C_0 and C_1 are prescribed constant concentrations, while β controls the type of boundary condition imposed at the inlet position ($\beta = 0$ for a prescribed concentration condition and $\beta = 1$ for a prescribed flux condition).

By using the Lagrangian derivative

$$\frac{dc}{dt} = \frac{\partial c}{\partial t} + v^* \frac{\partial c}{\partial x} \quad (6)$$

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

$$\theta R \frac{dc}{dt} = \frac{\partial}{\partial x}\left(\theta D \frac{\partial c}{\partial x}\right) \quad (7)$$

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

$$dx/dt = v^* \quad (8)$$

The Lagrangian formulation of the governing equation eliminates the convection term so that the equation takes on a purely parabolic appearance which can be solved efficiently with a finite element method.

Let us define the finite element approximation of the solute concentration at location x and time t as

$$\bar{c}(x, t) = \sum_{i=1}^{N} c_i(t)\varphi_i(x) \quad (9)$$

where N is the number of nodes in the solution domain, $\varphi_i(x)$ represents the linear shape function, and c_i is the concentration at node i ($i = 1, \cdots, N$). Applying the Galerkin procedure to (7) and incorporating (9) leads to

$$\int_L \left[\theta R \frac{d\bar{c}}{dt} - \frac{\partial}{\partial x}\left(\theta D \frac{\partial \bar{c}}{\partial x}\right)\right]\varphi_i \, dx = 0 \quad (10)$$

$$i = 1, 2, \cdots, N$$

where L is the solution domain. ***Neuman and Narasimhan*** [1977], among others, showed that parabolic problems such as (10) are more effectively solved by implementing a mass lumping scheme in which the first term of (10) is approximated by

$$\int_{I_L} \theta R \frac{d\bar{c}}{dt} \varphi_i \, dx \approx \frac{dc_i}{dt} \int_{I_L} \theta R \varphi_i \, dx \quad (11)$$

The Lagrangian derivative may be approximated by [*Neuman*, 1984]

$$\frac{dc_I}{dt} \approx \frac{c_i^{k+1} - \bar{c}_i}{\Delta t} \quad (12)$$

where $\bar{c}_i$ is the "convective concentration" of node i to be discussed in detail in the following section, and c_i^{k+1} is the concentration of node i at t_{k+1}. Following the procedure of ***Neuman*** [1984], ***we*** substitute (11) and (12) into (10) and use the linear basis functions to eventually obtain a system of linear equations for the concentration at time step $t_{k+1} = t_k + \Delta t$ as follows:

$$\left([E] + [H]^T + \frac{[W]}{\Delta t}\right)\{c^{k+1}\} = [G] + \frac{[W]}{\Delta t}\{\bar{c}\} \quad (13)$$

where

$$E_{ij} = \int_{I_L} \theta D \frac{d\varphi_i}{dx}\frac{d\varphi_j}{dx} \, dx \quad (14)$$

$$H_i = -q_i \qquad \text{inflow boundary}$$
$$H_i = 0 \qquad \text{outflow boundary} \quad (15)$$

$$w_{ij} = \delta_{ij} \int_{J_L} \theta R \varphi_i \, dx \quad (16)$$

$$G_i = -q_i C_1 \qquad \text{inflow boundary}$$
$$G_i = 0 \qquad \text{outflow boundary} \quad (17)$$

The global matrices H_i and G_i in these equations were derived assuming $\beta = 1$ (i.e., for prescribed flux conditions). When $\beta = 0$, c is known at the inflow boundary.

The relative accuracy of the different schemes will be evaluated, in part, by using the mass balance error ***(ME)*** as follows:

$$ME = 100(C_m - C_s)/C_m(\%) \quad (18)$$

with

$$C_m = C_{ini} + C_{in} - C_{out} \quad (19)$$

where C,, C_{ini}, C_{in}, and C_{out} are the amounts of solute stored in the profile, initially present in the profile, cumulative input, and cumulative output, respectively.

MODIFIED SINGLE-STEP REVERSE PARTICLE TRACKING

The convective concentration, $\bar{c}$ in (12), may be computed using a single-step reverse particle tracking (SRPT) tech-

nique. That is, a fictitious particle from each node i is sent backward to the point

$$x_i' = x_i - \int_{t_k}^{t_{k+1}} v^* \, dt \qquad (20)$$

during each time step. This means that a particle leaving x_i' at t_k will reach grid point location x_i exactly at t_{k+1}. The convective concentration is subsequently computed by the finite element approximation; i.e.,

$$\bar{c}(x_i, t_k) = c(x_i', t_k) \approx \sum_{j=1}^{N} c(x_j, t_k)\varphi_j(x_i') \qquad (21)$$

This technique works well in regions where the concentration gradients are small; however, the method introduces artificial dispersion near sharp concentration fronts.

To eliminate the numerical problem, a modified single-step reverse particle tracking (MSRPT) technique is formulated to compute the convective concentration. First, the single-step particle tracking method is carried out within a certain region determined by

$$x_t = x_0 + x_c + x_d \qquad (22)$$

where x_0 is the initial center location (at $t = 0$) of a sharp front, and x_c and x_d are the travel distances related to convection and dispersion, respectively; i.e.,

$$x_c = \int_0^t v^* \, dt \qquad (23)$$

$$x_d = 4\left(\int_0^t D \, dt\right)^{1/2} \qquad (24)$$

The term $x_0 + x_c$ in (22) indicates the center location of the sharp front at time t, while (24) is an empirical expression based on numerical experiments. For elements within x_t, the location at t_k of a particle which reaches x_i at t_{k+1} is computed by

$$x_i' = x_i - \int_{t_k}^{t_{k+1}} w_1 v^* \, dt$$

$$x < x_0 + x_c \qquad \text{upstream region} \qquad (25a)$$

$$x_i' = x_i - \int_{t_k}^{t_{k+1}} w_2 v^* \, dt$$

$$x_0 + x_c \le x \le x_t \qquad \text{downstream region} \qquad (25b)$$

where w_1 and w_2 are weighting factors for the upstream and downstream regions, respectively. Next the convective concentration is computed by (21) using the calculated x_i'.

The weighting factors w_1 and w_2 were found to change with different flow velocities, dispersion coefficients, and space and time discretizations. They were related empirically to the grid Peclet number (Pe) and Courant number (Cu) as follows:

$$w_1 = 1 + (1/Cu - 1) \exp\left[-41.02(1/PeCu)^{1.123}\right]$$

$$1/PeCu \text{ IO.05} \qquad (26a)$$

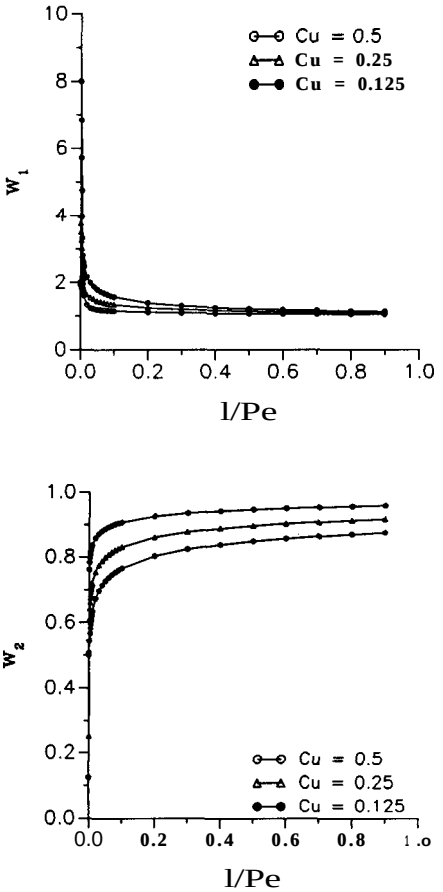

Fig. 1. Relationships between (top) w_1 and $1/Pe$ and (bottom) w_2 and $1/Pe$ for varying values of Cu.

$$w_1 = 1 + (1/Cu - 1) \exp\left[-2.63(1/PeCu)^{0.206}\right]$$

$$1/PeCu > 0.05 \qquad (26b)$$

$$w_2 = 1 - (1 - Cu) \exp\left[-2.9(Cu/Pe)^{0.18}\right] \qquad (27)$$

where

$$Pe = v^*\Delta x/D \qquad \text{Cu} = v^*\Delta t/\Delta x \qquad (28)$$

Equations (26) and (27) were obtained by carrying out a large number of simulations for a steady flow field using different values for Pe and Cu. For each pair of Pe and Cu values, w_1 and w_2 were adjusted by minimizing the mass balance error, and by minimizing deviations between the numerical and the available analytical solutions. Results of (26) and (27) are currently limited to $\text{Cu} \le 1$. Since the weighting factors depend only on the grid Peclet and Courant numbers and are computed for each grid, the MSRPT method can be used for problems with both uniform and varying element sizes.

Figure 1 shows families of curves of w_1 and w_2 versus 1/Pe for different values of Cu. The weighting factor w_1 is greater than unity, and increases as Pe increases and/or Cu decreases. On the other hand, the weighting factor w_2 is less than unity, and increases as Pe decreases and/or Cu increases. Figure 2 presents similar relationships between w_1 and w_2 and 1/Pe for Cu = 0.25. Notice that when $Pe \to \infty$, w_1 = 1/Cu, and $x_d = 0$. This means that in the region x ≤

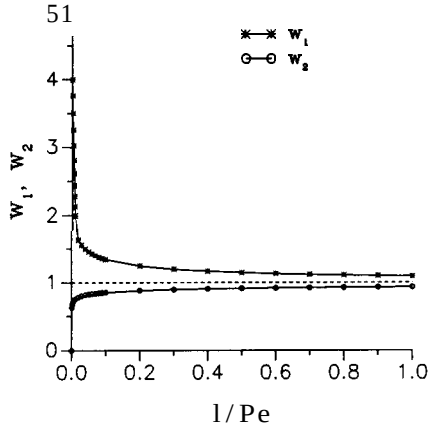

Fig. 2. Dependency of w_1 and w_2 on $1/Pe$ for $Cu = 0.25$.

x'_t, i.e., within $x_0 + x_c$, the location x'_i of a moving particle beginning from node i is given exactly by

$$x'_i = x_i - \mathrm{Ax} = x_{i-1} \tag{29}$$

In other words, the moving particles coincide perfectly with the nodes of the fixed grid system, and hence

$$\bar{c}(x_i, t_k) = c(x'_i, t_k) = c(x_{i-1}, t_k) \tag{30}$$

Since there is now no interpolation error for $\bar{c}$, exact results can be obtained for the pure convection problem. For dispersion-dominated problems, both w_1 and w_2 approach unity (Figure 2), and subsequently the MSRPT method reduces to the traditional SRPT technique which provides sufficiently accurate solutions for such problems [Neuman, 1984]. We note that the SRPT method was only used to compute the convective concentration of node i outside the region of x_t.

For transient problems the flow velocity and dispersion coefficient change with time and space, in which case the Peclet and Courant numbers become functions of time and spatially dependent. We introduced a correction factor a, with the weighting factors w_1 and w_2 in (25) to account for the transient effects; i.e.,

$$w'_1(t) = a_t w_1 \qquad w'_2(t) = a_t w_2 \tag{31}$$

where w_1 and w_2 are computed with (26) and (27) as before. The correcting factor a, in the numerical scheme is determined using an adaptive procedure which depends on the value of the mass balance error. The procedure consists of two steps. First, the initial value a_0 of a, at $t = 0$ is set equal to unity. Next, at each time step, the mass balance error (ME) is computed. If ME is within a preset tolerance (e.g., $|ME| < 0.1\%$), the value of a, is kept unchanged; i.e., a_{t+1} = a,. Otherwise, a_{t+1} is set equal to 0.95 a, if $ME < 0$, and to 1.05 a, if $ME > 0$.

In addition to the global mass balance error, the relative accuracy of the different schemes are also compared in terms of the sum-squared error E defined as

$$E(t) = \sum_{i=1}^{N} [C_i(t) - C_i^*(t)]^2 \tag{32}$$

where N is the number of nodes, C_i^* is the simulated concentration, and C_i is the presumed correct solution of the concentration at node i. For steady state flow, C_i will be evaluated using analytical solutions. No useful analytical solutions exist for problems of solute transport in transient flow fields. For these problems we used as our correct solution simulated results obtained with a finite element scheme which assumed very fine grid and time discretizations.

EXAMPLES

Problem 1 deals with the solution of an advancing concentration front. The analytical solution of the transport equation in a uniform flow field, i.e., for

$$R \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} \tag{33}$$

subject to

$$c(x, 0) = 0 \qquad 0 \le x < \infty \tag{34}$$

$$c(0, t) = 1 \qquad t > 0 \tag{35}$$

$$\frac{\partial c}{\partial x}(\infty, t) = 0 \qquad t > 0 \tag{36}$$

is given by [van *Genuchten and Alves, 1982]*

$$c(x,t) = \frac{1}{2}\left\{\mathrm{erfc}\left[\frac{x - vt}{2(DRt)^{1/2}}\right] + \exp\left(\frac{vx}{D}\right)\mathrm{erfc}\left[\frac{x + vt}{2(DRt)^{1/2}}\right]\right\} \tag{37}$$

which, for the limiting case when $D \to 0$, reduces to

$$c(x,t) = 1 \qquad x < vt$$
$$c(x,t) = 0 \qquad \text{otherwise} \tag{38}$$

Three simulations were carried out with the MSRPT scheme. For case 1, the following parameters were used: Ax = 200, At = 100, $t = 9600$, $v = 0.5$, $R = 1$, and $D = 0$ ($Pe = \infty$), and assuming a domain of $0 \le x \le 12800$ (any consistent set of units may be used for these parameters). Cases 2 and 3 were the same as for case 1 except for D which was set at 2 ($Pe = 50$) and 50 ($Pe = 2$), respectively. Figure 3 displays the calculated concentration profiles for the three cases. Results obtained with the SRPT and MSRPT methods are compared with the analytical solution. The calculations show that over the whole range of $0 \le Pe < \infty$, the MSRPT eliminates both numerical oscillation and artificial dispersion. The SRPT method on the other hand produces significant numerical dispersion, except for relatively small Pe values. Figure 4 further compares results obtained with MSRPT, the finite element method (FEM), and the upstream weighted method (UWM) [*Heinrich et al.,* 1977] against the analytical solution. The upstream weighted method uses nonlinear weighting functions so that greater weight is placed on variables associated with the upstream node of an element. The parameters used for this example were the same as those of case 1 except for $D = 1$ ($Pe = 100$). Notice the excellent results obtained with the MSRPT method. By

comparison, the FEM exhibits numerical oscillation, while the computations using UWM show extensive numerical dispersion.

Another class of problems amenable to indirect solution by the MSRPT is the initial value problem with a "step function" type initial condition. Problem 2 again concerns one-dimensional transport in a steady flow field, but now with the initial and boundary conditions given by

$$c(x, 0) = 1 \qquad 0 \le x < x_1$$
$$c(x, 0) = 0 \qquad x \ge x_1 \tag{39}$$

$$c(0, t) = 0 \qquad t > 0 \tag{40}$$

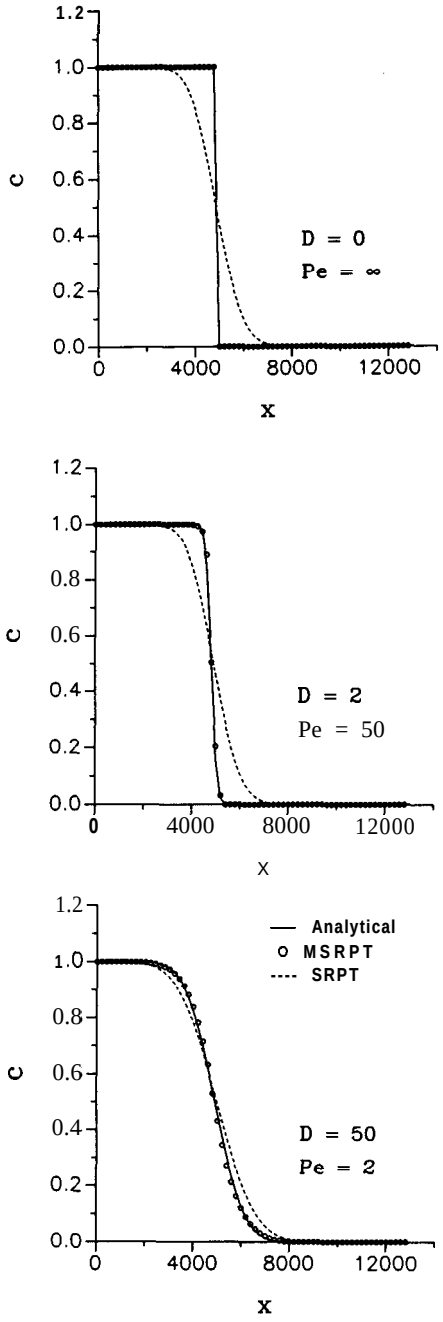

Fig. 3. Concentration profiles computed with the modified single-step reverse particle tracking method, the single-step reverse particle tracking method, and the analytical solution for $v = 0.5$, $R = 1$, and (top) $D = 0$ ($Pe = \infty$), (middle) $D = 2$ (Pe = 50), and (bottom) $D = 50$ ($Pe = 2$).

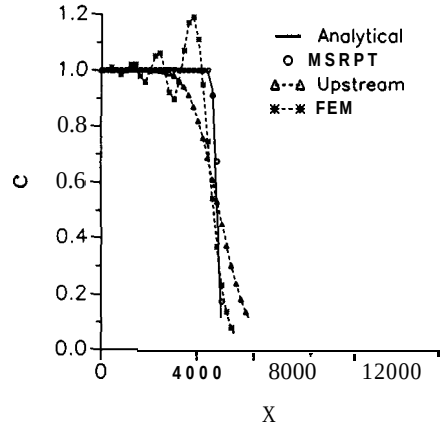

Fig. 4. Comparison of concentration profiles computed with the modified single-step reverse particle tracking method, the finite element method, the upstream weighted method, and the analytical solution for $v = 0.5$ and $D = 1$ ($Pe = 100$).

The exact solution for a semi-infinite profile is given by [van *Genuchten and* Alves, 1982]

$$c(x,t) = \frac{1}{2}\left\{\operatorname{erfc}\left[\frac{(x - x_1) - vt}{2(DRt)^{1/2}}\right] + \exp\,(vx/D)\operatorname{erfc}\left[\frac{(x + x_1) + vt}{2(DRt)^{1/2}}\right]\right\} \tag{41}$$

The initial condition (39) represents a unit step function near the inlet boundary. The center of the plume at time t is located at $x_c = 0.5x_1 + vt$. MSRPT was used to only compute $\bar{c}$ for nodes in the half region of the plume from the center to the extended area, i.e., between $0.5x_1 + vt$ and $x_1 + vt + 4(Dt)^{1/2}$. The convective concentrations of the nodes were subsequently mirrored to the other half region, i.e., between $vt - 4(Dt)^{1/2}$ and $0.5x_1 + vt$. Based on the mirrored concentration values, the convective concentration of the nodes in this region was calculated by linear interpolation. Using Ax = 200, At = 100, $t = 9600$, v = 0.5, $D = 0.2$, $R = 1$, and $x_1 = 1200$, we simulated solute movement in the same domain as problem 1, utilizing both SRPT and MSRPT. The results are compared in Figure 5 with the analytical solution. Again, MSRPT matches the analytical solution almost exactly, whereas SRPT leads to serious numerical dispersion.

Problem 3 involves the infiltration of water and a dissolved solute in an initially solute-free soil profile. The problem was designed to show the performance of MSRPT when simulating solute transport during transient unsaturated water flow. For this example we used MSRPT to solve (1) subject to the same initial and boundary conditions as Problem 1. Because of the transient flow conditions, θ and v, and hence also D and R in (1) are functions of time and space. At each time step, θ and v were obtained by numerically solving the Richards equation; i.e.,

$$C\frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left(K\frac{\partial h}{\partial x} - K\right) \tag{42}$$

where C is the soil water capacity, K is the hydraulic conductivity, and h is the pressure head. Equation (42) was

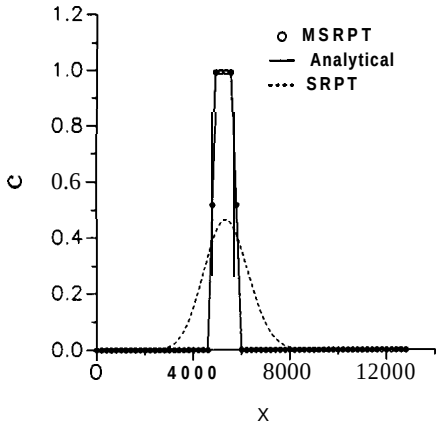

Fig. 5. Concentration distributions computed with the modified single-step reverse particle tracking method, the single-step reverse particle tracking method, and the analytical solution for $v = 0.5$ and $D = 0.2$ (Pe = 500).

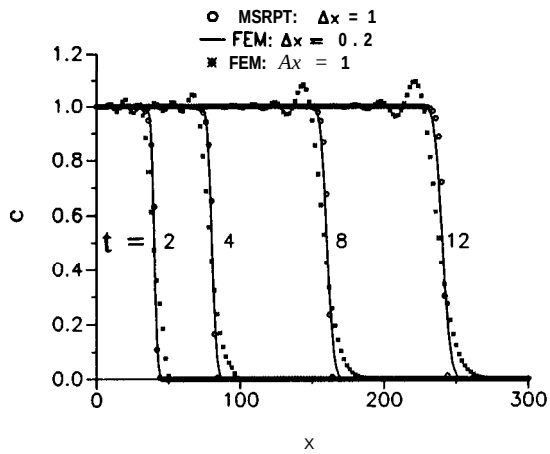

Fig. 6. Solute transport simulations at times $t = 2$, 4, 8, and 12 days for a transient flow field using the modified single-step reverse particle tracking method (Ax = 1), the finite element method with Ax = 1, and the FEM method assuming a more refined grid (Ax = 0.2).

solved using a mass-lumped linear finite element scheme as discussed by *Kool and van* Genuchten [1991]. The soil hydraulic properties in this equation were given by *[van Genuchten, 1980]*

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} = [1 + (\alpha|h|)^n]^{-m} \qquad (43)$$

$$K = K_s S_e^{1/2}[1-(1-S_e^{1/m})^m]^2 \qquad (44)$$

where θ_r and θ_s are the residual and saturated water contents, respectively, K_s is the saturated hydraulic conductivity, α and n are model parameters determined by experimental data, and $m = 1 - 1/n$. The dispersion coefficient in (1) was computed as [Bear, 1972]

$$D = \lambda|v| + D_0\tau \qquad (45)$$

where λ is the dispersivity of the medium, D_0 is the ionic or molecular diffusion coefficient in free water, and τ is a tortuosity factor. The tortuosity factor was evaluated as a function of the water content *[Millington and Quirk, 1961]* as follows:

$$\tau = \theta^{10/3}/\theta_s^2 \qquad (46)$$

Calculations were obtained for a 300-cm-deep soil profile, an infiltration rate of 8 cm day^{-1}, and the following hydraulic parameters: $n = 1.8$, $\alpha = 0.1$ cm-t, $\theta_r = 0.05$, $\theta_s = 0.4$, $D_0 = 0$, and $K_s = 10$ cm day-'. The concentration of the input solution was set at unity. We selected an element size Ax of 1 cm and a relatively small value of 0.04 cm for the dispersivity A, such that $Pe \approx \Delta x/\lambda = 25$. Numerical results obtained with the MSRPT and FEM methods are shown in Figure 6 at times $t = 2, 4, 8$, and 12 days. To eliminate or minimize oscillations and numerical dispersion in the FEM results, we had to further refine the element size. Figure 6 also displays the FEM concentration profiles using the refined grid (Ax = 0.2 cm, $Pe = 5$). The profiles obtained with FEM using the smaller elements (Ax = 0.2 cm) and MSRPT (Ax = 1 cm) are quite comparable; however, the FEM method took 25 times more computer time than MSRPT (approximately 5 hours versus 12 min on a 486 PC).

The MSRPT results in Figure 6 were obtained with an element size Ax of 1 cm. However, a much larger element size is possible with this scheme; this feature may further increase the computational efficiency of MSRPT relative to FEM. Figure 7 shows that some numerical dispersion occurred when the element size was increased. This numerical dispersion may have been caused by the process of choosing the weighting factors according to the mass balance error. The mass stored in the profile was calculated by summation of the element contributions. For smaller elements, the mass balance should be more accurate at each time step, which would result in more appropriate values for the weighting factors. Additionally, changing the element size likely affected the accuracy of the water flow simulation, which in turn should have impacted the accuracy of the solute transport simulation.

Transport simulations for a variably saturated flow field were also carried out using a solute flux boundary condition at the soil surface. The solute dispersivity was now taken as 0.01 cm. We used the simulated FEM results with the refined elements of Ax = 0.05 cm ($Pe = 5$) as a standard for

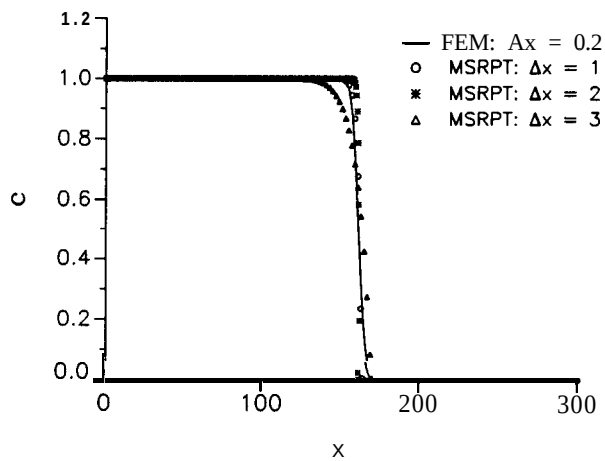

Fig. 7. Effect of element size on numerical results for a transient flow field obtained with the modified single-step reverse particle tracking method.

TABLE 1. Mass Balance Errors (ME) of the Modified Single-Step Reverse Particle Tracking (MSRPT) Method and Sum-Squared Errors (E) of the MSRPT and Finite Element Methods (FEM)

Day	Mass Error, *ME, %* (MSRPT)	Sum-Squared Error, *E* (MSRPT)	Sum-Squared Error, *E* (FEM)
1	-0.0897	1.20	3.15
2	0.0012	0.958	6.58
4	-0.0318	1.45	9.47
5	-0.0126	2.85	12.0
8	-0.0343	12.5	73.7

All parameters used in the simulations were kept the same for the two methods.

comparison. The sum-squared errors of MSRPT and FEM with Ax = 0.5 cm (Pe = 50) are compared in Table 1, which also lists the mass balance errors of the MSRPT scheme at different times. Notice that they are less than 0.1% for all simulations. Calculated solute distributions obtained with the MSRPT, FEM and the refined FEM techniques are shown in Figure 8 at times of 2, 4, and 8 days. The results in Table 1 and Figure 8 clearly demonstrate that MSRPT provides for this example much more accurate results than the oscillation-prone FEM. While MSRPT yields distributions which compare closely with those simulated using the refined FEM, the MSRPT results required about 80 times less computer time as compared to the refined FEM.

Finally, Figure 9 presents the concentration profiles for a purely convective transport process ($\lambda = 0$) in a transient flow field as simulated with the MSRPT method. As for the uniform flow field (Figure 3 (top)), MSRPT gives an exact description of the sharp front without producing any numerical oscillation and artificial dispersion.

CONCLUSIONS

A computationally efficient Eulerian-Lagrangian method is presented for solving one-dimensional convection-dispersion problems in steady and transient flow fields.

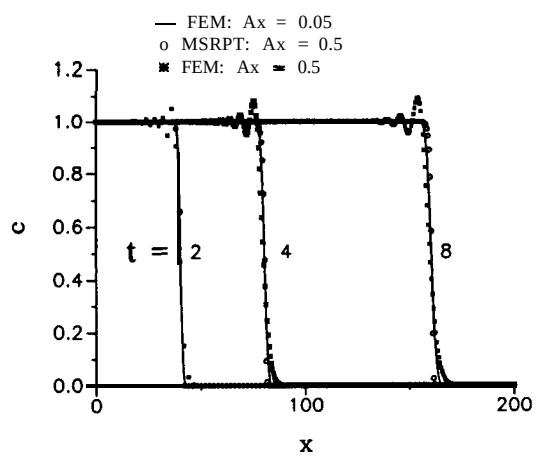

Fig. 8. Solute transport simulations at times $t = 2, 4,$ and 8 days for a transient flow field using the modified single-step reverse particle tracking method (Ax = 0.5), the finite element method with Ax = 0.5, and the FEM method using a more refined grid system (Ax = 0.05).

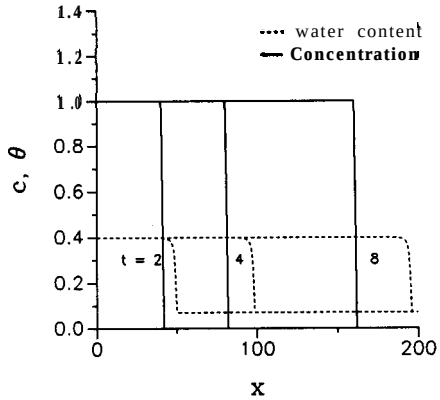

Fig. 9. Concentration profiles for a purely convective transport process simulated with the modified single-step reverse particle tracking (MSRPT) method at times of $t = 2$, 4, and 8 days in a transient flow field.

The relatively simple algorithm is a modification of the SRPT method. The method employs two weighting factors to control the particle tracking process. One weighting factor greater than unity is used in the upstream region, and another less than unity is used in the downstream region. The two weighting factors approach unity for dispersion-dominated problems, in which case MSRPT becomes the traditional SRPT method. A relatively pragmatic approach was followed by relating the weighting factors to the grid Peclet and Courant numbers by means of empirical equations. The weighting factors for transient flow fields were selected using an automatically adjustable procedure which minimizes mass balance errors at each time step.

Several problems were used to compare the MSRPT predictions against available analytical solutions and numerical results obtained with a linear finite element method assuming a more refined grid system. Results indicate that MSRPT is effective and accurate for a variety of problems. The method can handle solute transport problems over the entire range of Peclet numbers form zero to infinity for both steady and transient flow fields.

The MSRPT scheme was found to eliminate numerical oscillations and to reduce or virtually eliminate numerical dispersion in comparison to the finite element method, the single-step reverse particle tracking technique, and the upstream weighted method. MSRPT also dramatically reduced computational times as compared to the finite element method with a refined grid system. The MSRPT method appears especially useful for convection-dominated transport problems. The algorithm in this paper was formulated for one-dimensional problems and is currently limited to grid Courant numbers less than or equal to 1. Further research is being carried out to extend the MSRPT concept to problems with larger Courant numbers and multidimensional flow fields.

REFERENCES

Bear, J., ***Dynamics of Fluid in Porous Media,*** Elsevier, New York, 1972.

Cheng, R. T., V. Casulli, and S. N. Milford, Eulerian-Lagrangian solution of the convection-dispersion equation in natural coordinates, ***Water Resow. Res., 20, 944-952, 1984.***

Dimou, K. N., and E. E. Adams, Representation of sources in a 3-D Eulerian-Lagrangian mass transport model, in ***Water Pollution: Modelling, Measuring and Prediction,*** edited by L. C. Wrobel and C. A. Brebbia, pp. 251-264, Elsevier, New York, 1991.

Fujinawa, K. A., "Characteristic" finite element scheme for convective-dispersive transport with non-equilibrium reaction, Int. J. ***Numer. Methods Eng., 23, 1161-1178, 1986.***

Galeati, G., G. Gambolati, and S. P. Neuman, Coupled and partially coupled Eulerian-Lagrangian model of freshwater-seawater mixing, ***Water Resow. Res., 28(l), 149-165, 1992.***

Garder, A. O., D. W. Peaceman, and A. L. Pozzi, Numerical calculation of multidimensional miscible displacement by the method of characteristics, Soc. ***Pet. Eng. J., 4,*** 26-36, 1964.

Heinrich, J. E., P. S. Huyakom, 0. C. Zienkiewicz, and A. R. Mitchell, An "upwind" finite element scheme for two dimensional convective transport equation, ***Znt. J. Numer. Methods Eng., 11, 131-143, 1977.***

Huang, K., R. Zhang, and M. T. van Genuchten, A simple particle tracking technique for solving the convection-dispersion equation, in ***Computational Methods in Water Resources IX,*** vol. 1, ***Numerical Methods in Water Resources,*** edited by T. F. Russell, pp. 87-96, CMP, Boston, Mass., and Elsevier Science, New York, 1992.

Khaleel, R., and D. L. Reddell, Miscible displacement in porous media: MOC solution, ***J. Zrrig. Drain. Eng.,-1ll, 45-64, 1985.***

Konikow, L. F.. and J. D. Bredehoeft. Computer model of 2-D solute transport and dispersion in ground water, in ***Techniques of Water Resources Investigations of the United States Geological Survev.*** chap. C2. U.S. Government Printing Office, Washington. D.C., 1978.'

Kool, J. B., and M. T. van Genuchten, HYDRUS, one-dimensional variably saturated flow and transport model, including hysteresis and root water uptake, ***Res. Rep. 124,*** 101 pp., U.S. Salinity Lab., Riverside, Calif., 1991.

Leith, C. E., Numerical simulation of the earth's atmosphere, in ***Methods on Computational Physics,*** vol. 4, pp. 1-28, Academic, San Diego, Calif., 1965.

Leonard, B. P., The ULTIMATE conservative difference scheme applied to unsteady one-dimensional advection, ***Comput. Methods Appl. Mech.*** Eng., 88, 17-74, 1991.

Millington, R. J., and J. M. Quirk, Permeability of porous solids, ***Trans. Faraday Soc., 57, 1200-1207, 1961.***

Neuman, S. P., Adaptive Eulerian-Lagrangian finite element method for advection-dispersion, ***Znt. J. Numer. Methods*** Eng., 20, 321-337, 1984.

Neuman, S. P., and T. N. Narasimhan, Mixed explicit-implicit iterative finite element scheme for diffusion type problems, I, Theory, ***Znt. J. Numer. Methods Eng., 11, 309-323, 1977.***

Neuman, S. P., and S. Sorek, Eulerian-Lagrangian methods for advection-dispersion, in ***Finite Element in Water Resources,*** edited by K. P. Holz et al., pp. 14.41-14.68, Springer-Verlag, New York, 1982.

van Genuchten, M. T., A closed-form equation for predicting the hydraulic conductivity of unsaturated soils, ***Soil Sci. Soc.*** Am. ***J.,*** 44, 892-898, 1980.

van Genuchten, M. T. and W. J. Alves, Analytical solutions of the one-dimensional convective-dispersive solute transport equation, ***Tech. Bull. 1661, 151*** pp., Agric. Res. Serv., U.S. Dep. of Agric., Washington, D. C., 1982.

Varoglu, E., and W. D. L. Finn, A finite element method for the diffusion-convection equation with constant coefficients, ***Adv. Water Resour., 1, 337-343, 1978.***

Yeh, G. T., A Lagrangian-Eulerian method with zoomable hidden fine-mesh approach to solving advection-dispersion equations, ***Water Resour. Res., 26, 1133-1144, 1990.***

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