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A Comparative Study of Particle Tracking Techniques for Numerically Solving the Convection-Dispersion Equation

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Abstract

Characteristics-based particle tracking techniques combined with standard finite element or finite difference methods have been widely used for solving convection-dispersion type solute transport equations. The popularly-used single-step backward tracking technique (SRPT) and a mixed technique (HYBRID), obtained by combining SRPT with continuous forward tracking, were evaluated by means of a large number of numerical tests. Solutions obtained with SRPT and HYBRID were both found to be free of oscillations. Although HYBRID generally worked better than SRPT, both schemes suffered from numerical dispersion. Numerical dispersion always increased with increasing grid Peclet number, and usually with decreasing cell Courant number. The numerical problems were especially evident when sharp concentration peaks (local maxima) or valleys (local minima) existed. Numerical dispersion in these cases was found to result mainly from interpolation errors in the particle tracking techniques. We developed a modified SRPT method which continuously tracks the local maximum or minimum concentrations for use in the interpolation of the convective components. The modified SRPT was far more effective in eliminating numerical dispersion than current particle tracking methods.

Introduction

Convection-dispersion type equations (CDE's) are generally solved numerically using standard finite difference or finite element methods. Such methods are relatively accurate for dispersion-dominated transport problems, but often face numerical difficulties when convective transport dominates dispersion and the concentration fronts are steep. The numerical difficulties are manifested by artificial dispersion of sharp concentration fronts and/or numerical oscillations at or near the sharp fronts. Although some of the numerical dispersion and oscillation problems can be avoided by grid refinement, such an approach may greatly increase the computational effort.

Several alternative methods have been developed to avoid or limit numerical problems in the standard solution schemes. One of the more popular methods for

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this purpose is the Eulerian-Lagrangian approach which solves separately for the convective and dispersive components of the transport equation. The convective transport problem is solved on a moving coordinate system by tracking a moving particle along a characteristic line, while the dispersion problem is solved on a fixed Eulerian grid system *(Douglas and Russell,* 1982; *Neuman, 1984).* Several characteristics-based particle tracking techniques currently exist for calculating the convective component. Among these, the single-step reverse particle tracking (SRPT) is probably the more popular one because of its simplicity, whereas a mixed technique (HYBRID), obtained by combining SRPT with continuous forward tracking, is relatively more robust for handling the convection problem for any value of the grid Peclet number. Although SRPT effectively eliminates numerical oscillations, this scheme may still produce serious numerical dispersion for problems involving large Peclet numbers. Several approaches have been used to reduce numerical dispersion. For example, *Casulli* (1987) suggested reducing the spatial step, *Huang et al.* (1992) implemented a more precise method for tracking the concentration front, while Goblet and *Cordier* (1993) used a spectral element method to achieve a more accurate interpolation when the SRPT is implemented. Although some improvements were made, none of these schemes were completely successful in eliminating numerical dispersion. Whereas the HYBRID scheme at present seems to produce the most accurate results, its numerical problems (notably numerical dispersion) have still not been adequately addressed.

In this paper we evaluate the numerical behavior of the SRPT and HYBRID particle tracking techniques by means of several numerical tests. The SRPT scheme will be implemented using a modified numerical method which tracks the local extremes of a concentration profile.

The Eulerian-Lagrangian Approach

For simplicity, we consider here one-dimensional transport in a porous medium with uniform water flow and constant transport parameters as follows

$$R\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - v\frac{\partial c}{\partial x} - \mu c + \gamma \qquad (1)$$

where c is the solute concentration, t is time, x is distance, R is the retardation factor, v is the pore-water velocity, D is the dispersion coefficient, and μ and γ are rate constants for first-order decay and zero-order production, respectively. Equation (1) will be solved subject to the initial condition

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

The inlet boundary condition is taken to be

$$c(0, t) = C_0(t) \qquad (3)$$

while at the lower boundary, x = L, *a* zero-gradient is assumed:

$$\frac{\partial c}{\partial x}(L,t) = 0 \tag{4}$$

where $C_i(x)$ and C,,(t) are prescribed functions of x and t, respectively.

Equation (1) may be rewritten in Lagrangian form as

$$R\frac{Dc}{Dt} = D\frac{\partial^2 c}{\partial x^2} - \mu c + \gamma \tag{5}$$

where Dc/Dt is the Lagrangian derivative

$$\frac{Dc}{Dt} = \frac{\partial c}{\partial t} + v \cdot \frac{\partial c}{\partial x} \tag{6}$$

in which $v^* = v/R$, and where c now describes the concentration of a fluid particle moving along a characteristic path defined by the equation

$$\frac{dx}{dt} = v \tag{7}$$

According to Neuman's operator splitting approach, the transport problem is decoupled into two parts, one covering pure convection, and the other dispersion and all remaining transport processes. The split convection problem is required to satisfy the homogeneous Lagrangian derivative

$$\frac{D\bar{c}}{Dt} = 0 \tag{8}$$

along the characteristic line. The "convective component", $\bar{c}$, of the concentration c, is solved independently by the method of characteristics, and subsequently substituted into the discretized Lagrangian derivative of equation (6) as follows

$$R\frac{c - \bar{c}}{\Delta t} = D\frac{\partial^2 c}{\partial x^2} - \mu c + \gamma \tag{9}$$

where Δt is the time increment. The residual transport problem, Eq. (l0), can be solved for c using standard fixed-grid methods such as finite elements or finite differences.

Two different characteristics-based particle tracking methods are considered in this study. One method is the SRPT single-step reverse particle tracking (Neuman, 1981; ***Galeati et al.,*** 1992) in which the characteristic paths are traced backward. The other approach is the HYBRID scheme proposed by ***Neuman (1983)*** in which the convective components of steep concentration fronts are tracked forward with the help of moving particles clustered around each front. The convection problems away from the fronts are solved using backward particle tracking. When a front dissipates in time, its forward tracking stops automatically and the corresponding cloud of particles is eliminated.

Numerical Experiments

This section presents results of several numerical tests comparing the relative accuracy of the SRPT and HYBRID particle tracking methods. For the HYBRID method we initially (at t=0) introduced 60 particles (2 per element) in areas with large concentration gradients. The analytical solutions of (1) subject to (2), (3) and (4) were used to verify the numerical results of both particle tracking methods. Assuming v= 10 and Ax = 1.0 (any consistent set of units may be used), a conservative tracer (R = l), and no production or decay ($\mu=\gamma=0$) for all examples, concentration distributions were calculated for a variety of dispersion coefficients, D, and time steps, Δt, such that the values of the grid Peclet number, $Pe = v\Delta x/D$, and the grid Courant number, Cu = $v\Delta t/\Delta x$, differed from case to case. Comparisons with the analytical solutions provide stringent tests on the performance of the numerical methods, especially their ability to correctly track sharp fronts.

We first simulated concentration distributions for $C_0 = 1$ and $C_i = 0$ assuming a relatively small Peclet number of 10. Results indicated a fairly good match between the exact solution and the SRPT and HYBRID particle tracking methods. However, as shown in Figure 1, both methods suffered from numerical dispersion when the grid Peclet number, *Pe, was* increased to 100. The simulations were obtained with fractional Courant numbers of 1.5 (t = 2) and 0.5 (t = 4). When integer Courant numbers (e.g., Cu = 2) were used, the numerical results (dots in the figure) essentially duplicated the exact solution.

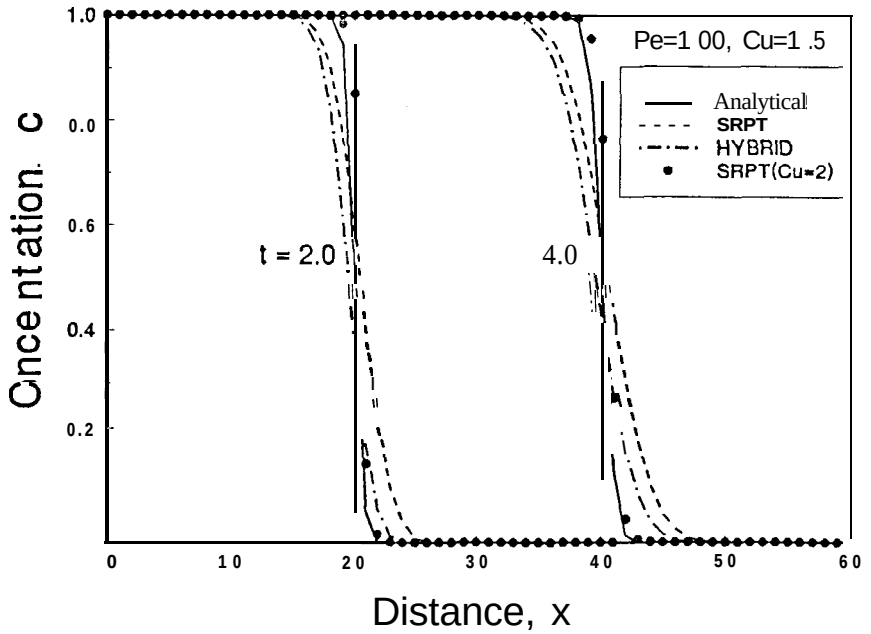

Fig. 1. Simulated single-front concentration distributions obtained with SRPT and HYBRID.

The above comparisons pertain to single-front concentration distributions. Simulations were also carried out for steep, multi-peak initial distributions assuming solute-free input ($C_0 = 0$). Figure 2 shows the simulated distributions using a fractional Courant number of 1.25 and a relatively large Peclet number of 100. Calculated concentrations obtained with both SRPT and HYBRID clearly suffered from numerical dispersion, especially near the concentration peaks and valleys. Notice that the numerical dispersion in Figure 2, increased with simulation time, or equivalently, with the number of time steps during which particle tracking was implemented. The HYBRID method in most cases was found to be more accurate than SRPT, especially for relatively high Peclet numbers.

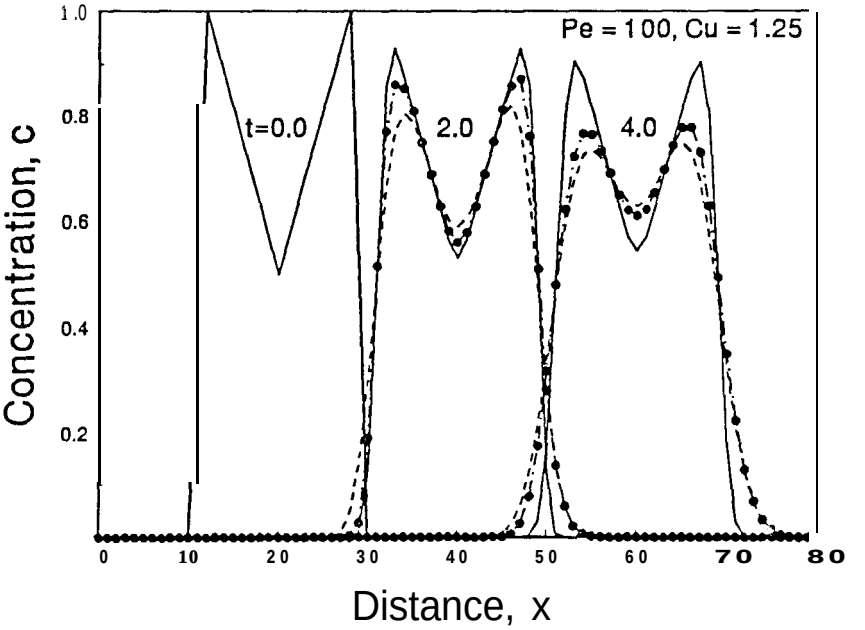

Fig. 2. Simulated multi-peak concentration distributions obtained with SRPT (dashed lines) and HYBRID (dot-dashed lines).

The grid Peclet number, *Pe,* is generally viewed as a major factor determining the extent of numerical dispersion (i.e., increasing *Pe* leads to more numerical dispersion). This finding is not necessarily true for transport problems having moderately steep concentration fronts. As an example, the SRPT was used to simulate the transport of a multi-peak concentration profile with relatively small gradients and assuming a value of 1000 for *Pe.* Such a high value for *Pe* often leads to serious numerical instabilities in numerical transport studies. The simulation was performed using fractional Courant numbers ranging from 0.044 to 1.3 1, values which usually produce serious numerical dispersion when particle tracking techniques are implemented. The simulated results (not shown here) were very accurate, even near the peaks. These results suggest that the performance of a numerical scheme is

affected not only by the Peclet number, but also by the spatial gradient. Actually, we found that the spatial gradient is often more important than the value of Pe because of potentially large interpolation errors near steep fronts.

Implementation

The numerical experiments above indicate that SRPT and HYBRID perform relatively poorly for transport problems involving steep concentration gradients. In general, particle tracking techniques become more dissipative when the Peclet number increases or the Courant number decreases. Our calculations indicate that the numerical problems, mainly numerical dispersion, in both schemes are likely a result of interpolation errors near sharp fronts, especially near concentration extremes. One should expect some errors of this type when simple linear interpolation schemes are used in SRPT to solve for the convective components near steep fronts. Figure 4 shows schematically how a steep concentration peak, ABC, is tracked using SRPT. According to the Lagrangian point of view, i.e., equation (9), the concentration of a particle moving along its characteristic path remains constant. Therefore, the shape of the concentration distribution at time $t_{k+1}=t_k+$ At should be the same as that at t_k because only convective transport is considered. However, the peak ABC has been flattened and smeared into $A'B'C'$ by the SRPT scheme.

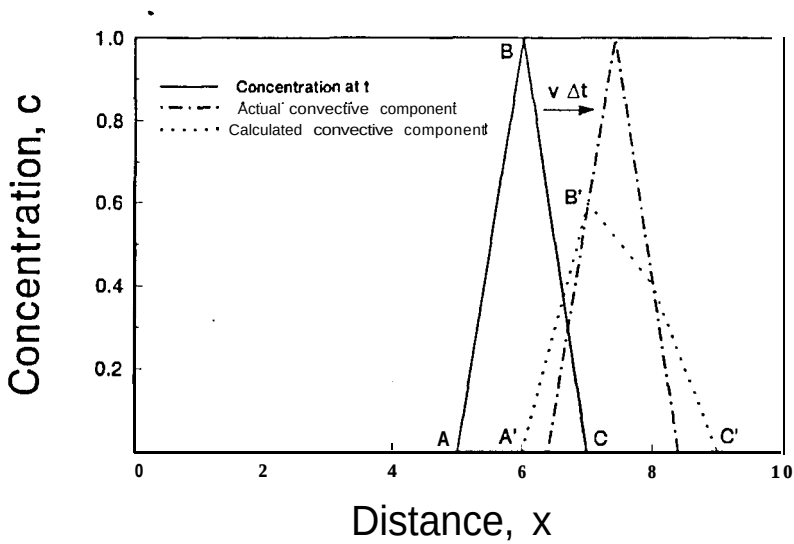

Fig. 3. Schematic illustration of the convective component as calculated with the SRPT technique.

Higher-order interpolation formula, such as cubic Hermitian equations, could possibly improve the accuracy. However, higher-order equations often involve spatial

derivatives which may be difficult to determine accurately. Alternatively, small spatial steps should also reduce the interpolation errors. The additional forward-moving particles introduced with the HYBRID scheme then serve primarily to add extra interpolation points in areas with steep fronts, thus making HYBRID more accurate than SRPT. Although the moving particles used in HYBRID help to reduce artificial damping of the numerical results as compared to SRPT, they are not useful if they can not trace the exact paths of the local extremes. To reduce the interpolation errors near the peaks, which are key points dominating the shape of a concentration distribution, we propose a modified SRPT scheme as described below.

Assume that the concentration c^k at time t_k is known. Equation (6) subject to auxiliary conditions (2) through (4) will be used to solve for c^{k+1} at time step $t_{k+1} = t_k + \Delta t$ using the following consecutive steps:

1. *Determine the Local Maximum/Minimum Concentrations.* At the beginning of the simulation, determine the local maximum and minimum concentrations, C^p at x^p $(p = 1,...,P)$, from the initial concentration distribution and the inlet boundary condition at $x = 0$ (P represents the number of the selected concentration extremes). The inlet boundary must also be viewed as an extreme if the inlet concentration differs significantly from the first nodal concentration.

2. Continuous Forward Tracking. Once determined, the local minimum and maximum concentration points are considered to be moving particles and tracked continuously forward along the characteristic path. Assume x_p^k is the position of particle p at t_k. Position x_p^{k+1} of this particle at $t_{k+1} = t_k + \Delta t$ can then be calculated from equation (8) as follows

$$x_p^{k+1} = x_p^k + \int_{t_k}^{t_{k+1}} v^* dt \qquad (p = 1,2,...,P) \tag{10}$$

3. *Single-Step Reverse Tracking (Modified Method of Characteristics).* Consider a fictitious particle that moves during time step Δt from location x_n' at t to a new location x_n which is the fixed Eulerian coordinate of the finite element node n. Based on equation (8), the initial particle location x_n' can be tracked backward as *(Neuman,* 1984)

$$x_n' = x_n - \int_{t_k}^{t_{k+1}} v \cdot dt \tag{11}$$

Once the backward position x_n' has been determined, the corresponding concentration, i.e., the convective component c_n for node n, can be computed by interpolating between nodal values using the finite element formulation

$$\bar{c}_n = \sum_{i=1}^{N_p} c_i(t)\varphi_i(x_n') \qquad (N_p = N + P) \tag{12}$$

where the $\varphi_i(x)$ are the usual finite element basis functions. The $c_i(t)$ in equation

(13) represent concentrations of all nodes (N) and moving particles (P). The concentrations of the moving particles are used in (13) to increase the number of interpolation points in areas having high concentration gradients, thus improving the accuracy of the interpolations in these areas. Concentrations of the moving particles, c_p, are generally more accurate than those of the nodes, c_n, since they are calculated independently from the characteristics approach as will be discussed later.

4. *Finite Element Approximation.* Solutions for c^{k+1} are subsequently obtained by applying the Galerkin finite element method with linear basis functions to (6). Since the Galerkin method is relatively standard, we do not further review here its application to the solution of equation (6). However, we emphasize that the Lagrangian derivative should be approximated by

$$\frac{Dc_n}{Dt} \approx \frac{c_n^{k+1} - \bar{c}_n}{\Delta t} \tag{13}$$

This discretization is based on the view that node n is a fictitious particle reaching x_n at t_{k+1}.

5. Dispersion Correction for Moving Particles. Finally, the concentration of moving particle p at time t_{k+1} is corrected by the dispersive component which is estimated from the finite element interpolation as follows

$$c_p^{k+1} = c_p^{k} + \sum_{i=1}^{N} (c_i^{k+1} - \bar{c}_i)\varphi_i(x_p) \tag{14}$$

Note that the term $(c_i^{k+1} - \bar{c}_i)$ is the dispersive component of the concentration at node i. Repeating steps 2 to 5 yields the complete solution at the next time step.

Examples

The modified SRPT scheme was found to produce encouraging results which agreed well with the analytical solution for several test cases. Figure 4 shows simulated results for a steep-peak initial distribution assuming *Pe* = 1000 and Cu = 0.9. The proposed modified scheme yielded accurate solutions, whereas SRPT and HYBRID produced considerable numerical dispersion.

Figure 5 shows that the modified SRPT scheme generated also more accurate results than either SRPT or HYBRID for a multi-peak initial distribution. In particular, the sharp concentration peaks and valleys were more accurately simulated with the modified scheme. Accurate simulation of local concentration minima or maxima is sometimes important when predicting contaminant transport in the subsurface. As opposed to the modified SRPT scheme, SRPT and HYBRID both generated serious numerical dispersion. For this simulation we assumed a Peclet number of 100, and a Courant number of 1.25.

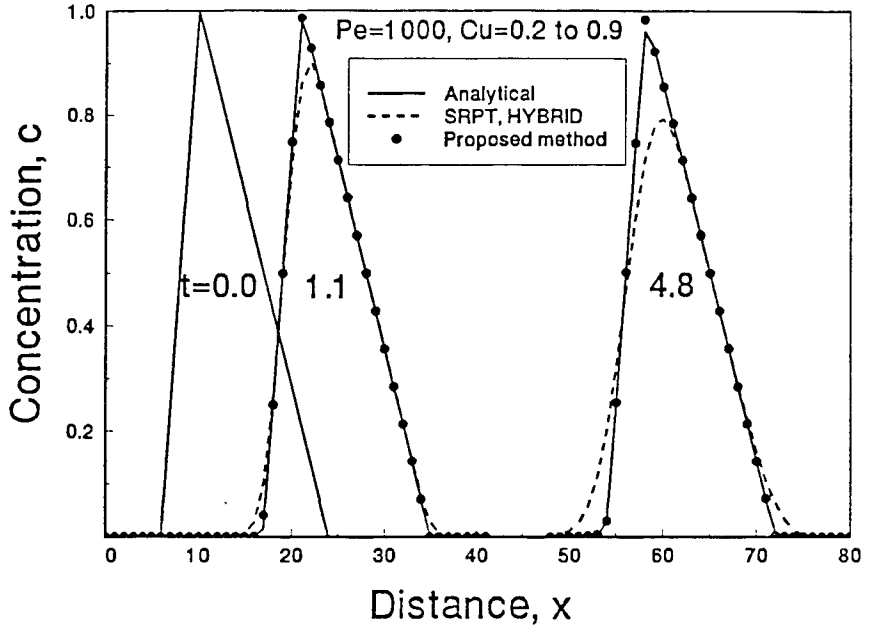

Fig. 4. Calculated concentration distributions for a single-peak using SRPT, HYBRID, and the proposed modified SRPT method.

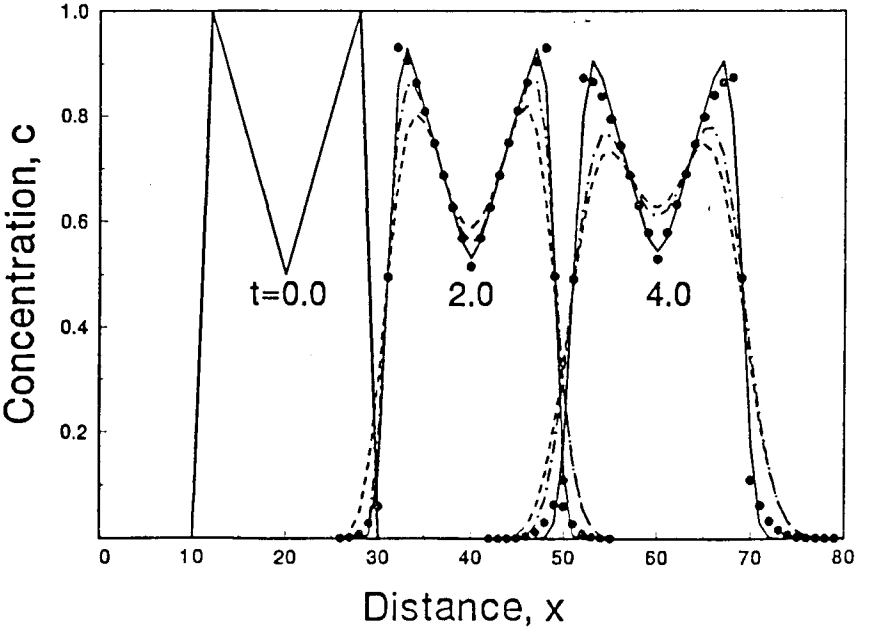

Fig. 5. Simulated multi-peak concentration distributions obtained with SRPT (dashed lines), HYBRID (dot-dashed lines), and the proposed modified SRPT method (dots) using Pe = 100, $Cu = 1.25$.

Conclusions

The SRPT and HYBRID particle tracking methods were both found to be free of numerical oscillations. HYBRID generally gave somewhat better results than SRPT, especially for relatively high *Pe values.* Both particle tracking techniques suffered from numerical dispersion when *Pe was* relatively large and sharp concentration fronts existed. Numerical dispersion produced with SRPT and HYBRID increased when smaller time steps (relatively small fractional Courant numbers) were used. Still, SRPT and HYBRID both gave satisfactory results for transport problems involving moderate gradients in the concentration distributions, even for relatively high *Pe* values (e.g., *Pe as* high as 1000). This fact indicates that the Peclet number is not the only factor determining the performance of a numerical scheme; the results are also affected by the concentration gradient.

Our results indicate that numerical dispersion is caused primarily by inaccurate determination of the convective components because of interpolation errors, especially in areas having large concentration gradients. The proposed modified SRPT virtually eliminated these interpolation errors. Preliminary tests showed that the modified SRPT scheme is accurate and very robust for solving transport problems involving sharp multi-peak concentration distributions and relatively high Peclet numbers.

References

1. Casulli, V. (1987) "Eulerian-Lagrangian methods for hyperbolic and convection dominated parabolic problems", in C. Taylor et al. (eds.), *Computational Methods for Nonlinear Problems,* Pineridge, Swansea, Wales, pp. 239-269, Chap. 8.
2. Douglas, J., Jr., and Russell, T.F. (1982) "Numerical methods for convection-dominated diffusion problems based on combining the method of characteristics with finite element or finite difference procedures", *SLAM J. NumericalAnalysis.* 19, 871-885.
3. Galeati, G., Gambolati, G., and Neuman S. P. (1992) "Coupled and partially coupled Eulerian-Lagrangian model of freshwater-seawater mixing", *WaterResourcesResearch 28(l),* 149-165.
4. Goblet, P., and Cordier, E. (1993) "Solution of flow and mass transport equations by means of spectral elements", *Water Resources Research 29(9), 3135-3144.*
5. Huang, K., Zhang, R., and van Genuchten, M. Th. (1992) "A simple particle tracking technique for solving the convection-dispersion equation", in T. F. Russel et al. (eds.), *Numerical Methods in Water Resources, Proc., Ninth International Conference on Computational Methods in Water Resources,* Elsevier, New York, pp. *86-97.*
6. Neuman, S. P. (1981) "An Eulerian-Lagrangian numerical scheme for the dispersion-convection equation using conjugate space-time grids", J. *of Computational Physics 41, 270-294.*
7. Neuman, S. P. (1984) "Adaptive Eulerian-Lagrangian finite element method for advection-dispersion", Int. J. *for Numerical Methods in Engineering 20, 321-337.*