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ARE PARTICLE METHODS ONLY SUITED FOR MODELING ADVECTIVE TRANSPORT ? SOME COUNTER-EXAMPLES

Amvrossios C. Bagtzoglou[1]

Department of Civil Engineering
University of California
Irvine, California 92717, USA

David E. Dougherty

Department of Civil & Mechanical Engineering
University of Vermont
Burlington, Vermont 05405, USA

Andrew F. B. Tompson

Earth Sciences Department
Lawrence Livermore National Laboratory
Livermore, California 94551, USA

1. Abstract

"Particle models" is a generic term used for a broad class of simulation models in which the discrete representation of physical phenomena involves the use of interacting particles. Since this technique was first applied by Ahlstrom *et al.* (1977) to numerical studies of groundwater hydrology, many other researchers have used it with success. Unlike the conventional Eulerian methods, particle tracking methods (PTMs) have no grid Peclet number problems or grid orientation effects, and are traditionally considered as well suited for advection dominated simulations.

[1] Now at: *Center for Nuclear Waste Regulatory Analyses*
Southwest Research Institute
San Antonio, Texas 78228-0510, USA

The results presented in this paper indicate that PTMs are well suited for any type of solute transport modeling. Classical conservative transport test cases, such as the advancing front problem and the rectangular wave propagation problem are considered in this study. The grid-based random walk particle method (RWPM) behaves quite well for both high and low Peclet numbers, even for Peclet numbers as low as two, and compares exceptionally well with four conventional and two nonlinear, flux-limiting Eulerian schemes. Furthermore, two-dimensional results compare very well with analytically derived solutions. Finally, a challenging nonlinear diffusion-reaction problem, known as Fisher's equation, is tackled with success. The approach is based on an inconsistent interpolation that imposes on particles mass changes induced by grid-based reactions (Bagtzoglou, 1990; Bagtzoglou and Dougherty, 1990).

2. Particle-Grid Approach for Solute Transport Simulations

The balance of mass of a reactive, neutrally buoyant solute in a porous medium of constant porosity is

$$\frac{\partial c}{\partial t}+\nabla\cdot(uc)-\nabla\cdot(D\cdot\nabla c)=r(c,t) \tag{1}$$

where c is the solute concentration, u is the fluid velocity, D is the velocity-dependent dispersion coefficient, and r(c,t) is a net species production rate.

Neuman (1981) and Ewing (1988) have reported the application of an operator-splitting approach for the solution of (1). By integrating over small time intervals Δt, one can express the concentration change $\Delta c = c^{n+1} - c^n$ at a point x as $\Delta c = \Delta c_{AD} + \Delta c_R$. At a given time step, the approach proceeds by approximating the term Δc_{AD} and an "intermediate" solution $c^*(x)$. The intermediate solution is then used to compute Δc_R, on a grid, and from that the total change in concentration, Δc.

Particle methods have been extensively used to solve problems in fluid dynamics, plasma physics, astrophysical sciences, as well as heat transfer (Hockney and Eastwood, 1988). In the context of solute transport, particles represent elements of mass distributed in space. The particle representation for the concentration at some point in space and time may be expressed by

$$c(x_g,t)=\sum_{P\in N_p} m_P(t)\cdot\delta(x_g-X_P(t)) \tag{2}$$

where $\delta(x)$ is the Dirac function, x_g are the grid spatial coordinates, and X_P and m_P are the position and mass of particle P in a set of N_P particles.

In the particle-grid approach, the random walk particle method (RWPM) is employed to evaluate Δc_{AD} over a time step Δt by moving particles according to

$$X^{n+1}=X^n+A(X^n)\cdot\Delta t+B(X^n)\cdot Z^n\sqrt{\Delta t} \tag{3}$$

where X^n is the position of a particle at time t^n, and Z^n is a vector of independent random numbers of zero mean and unit variance. In the limit as the number of particles $N_P \to \infty$, it is shown (Kinzelbach, 1988; Tompson and Gelhar, 1990) that the mass density of the particle distribution converges to the solution of the nonreactive form of (1) if $A \equiv u + \nabla \cdot D$ and if $B \cdot B^T \equiv 2D$. Intermediate concentrations $c^*(x_g)$ are obtained by applying interpolation from the particle discrete distribution to a grid-based, concentration distribution with the help of projection functions (particle to grid projection). Many investigators have applied this algorithm for the solution of nonreactive groundwater contaminant problems (e.g., Ahlstrom *et al.*, 1977; Tompson and Dougherty, 1988). Unlike the conventional Eulerian methods, this method is not affected by grid orientation effects or conditions characterized by unacceptable grid Peclet numbers, and it is traditionally considered to be well suited for advection dominated simulations.

The most important errors in the RWPM formulation come from the finite particle "resolution" (a measure of the precision used in describing the spatial distribution of mass, $N_r = 1/m_p$), the truncation effects associated with the split operator, and mass balance discrepancies created from particle-grid interpolations. To account for the latter, and obtain smoothed concentration solutions, four one-dimensional forms of these projection functions were implemented and tested. They are: the NGP (nearest grid point; piecewise constant), CIC (cloud in cell; piecewise linear), TSC (triangular shaped cloud; bi-parabola), and TG (truncated gaussian) schemes. Their form and mathematical representation can be found in Bagtzoglou (1990).

3. Analysis of the Particle-Grid Method Behavior and Comparison with Other Schemes

The effectiveness of RWPM to accurately solve the nonreactive form of (1) is tested with the help of two well known one-dimensional problems. Monte Carlo experiments were conducted to study the effects of the type and support of projection functions used, the particle resolution (N_r), and the grid Peclet number ($P_e = u\Delta x/D$) on the accuracy and average variability of the results.

3.1 Advancing Front Problem

The advancing, one-dimensional, front problem can be mathematically stated as

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} - D\frac{\partial^2 c}{\partial x^2} = 0 \tag{4}$$

with $x \in [0,\infty]$ and initial and boundary conditions $c(x,0) = C_0 = 0 \ \forall\ x$, $c(0,t) = C_1 = 1 \ \forall\ t$, and $c(\infty,t) = C_0 = 0 \ \forall\ t$, where u and D, the flow velocity and dispersion coefficient, are constants. The analytical solution is given by (Van Genuchten and Alves, 1982)

$$c^a(x,t) = \frac{1}{2}\left[erfc\left(\frac{x-ut}{2\sqrt{Dt}}\right) + \exp\left(\frac{ux}{D}\right) \cdot erfc\left(\frac{x+ut}{2\sqrt{Dt}}\right)\right] \tag{5}$$

which for D=0 yields the well known first-order wave solution.

The numerical simulations are computed on $x \in [0,12800]$ with a grid spacing $\Delta x = 200$; a flow velocity $u = 0.5$; a time step $\Delta t = 96$, or 960; a total simulation time of 9600, and a dispersion coefficient D=0, 2, or 50. Grid Peclet numbers of ∞, 50, and 2 are thus considered. To see the effect of the noise associated with the concentration estimate of the RWPM, and account for its stochastic nature, several repeated simulations are averaged. Figure 1 shows the average profile <c(x,9600)> after 800 Monte Carlo runs when CIC (piecewise linear) interpolation is used, and N_r=64.

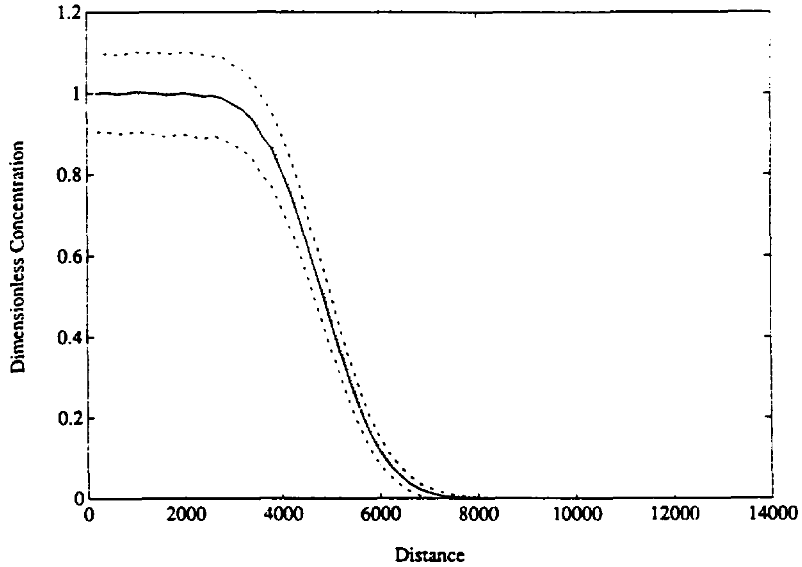

Figure 1 <c(x,9600)> (solid) after 800 Monte Carlo runs for P_e=2 and N_r=64; mean concentrations ± standard concentration errors (dashed); analytic solution (dotted).

The rough band around the mean is a measure of the average noise, σ(x,9600), above or below the signal. The mean concentration as measured over N_{MC} Monte Carlo runs is

$$<c(x,t)>=\frac{1}{N_{MC}}\sum_{n=1}^{N_{MC}} c^{n}(x,t) \tag{6}$$

where $c^n(x,t)$ is the numerical solution for realization n. The standard concentration variance as measured over N_{MC} Monte Carlo runs is

$$\sigma^2(x,t)=<c^2>-<c>^2 \tag{7}$$

The variability in σ and <c> is a function of the Monte Carlo runs, and diminishes with the number of runs being increased. In Figure 2 a plot of σ as a function of <c> is presented, for the four interpolation functions described in section 2. An approximate linear dependence on $<c>^{(1/2)}$ is observed, consistent with the random walk theory (Ahlstrom *et al.*, 1977) stating that

$$\sigma \approx \gamma\left(\frac{<c>}{N_r V}\right)^{\frac{1}{2}} \tag{8}$$

where γ is a constant and V is a measure of the volume over which concentration is computed.

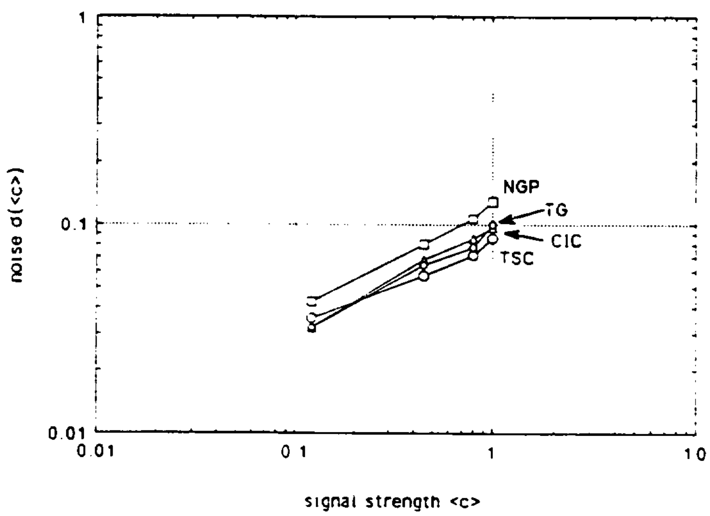

Figure 2 Standard concentration error vs. <c(x,t)> after 800 Monte Carlo runs for 4 advancing front problems based on four interpolation functions (all with P_e=2, N_r=64).

As seen in Figure 2, the simple NGP method (piecewise constant) yields the largest and most distinct noise error. This effect can be seen, also, in Figure 3 where the maximal values of σ (=σ_m, behind the front) are plotted for the cases of P_e=2, 50, and ∞. The largest errors occur, typically, when simple (conventionally used) interpolations are implemented and especially in more diffusive regimes. As the Peclet number approaches infinity, the differences between methods become negligible. Note that there is an approximate variation of σ with the $^{(-1/10)}$ power of P_e. Although this result is not explicitly expected from (8), we can include its effect by suggesting that $\gamma \propto P_e^{(-1/10)}$.

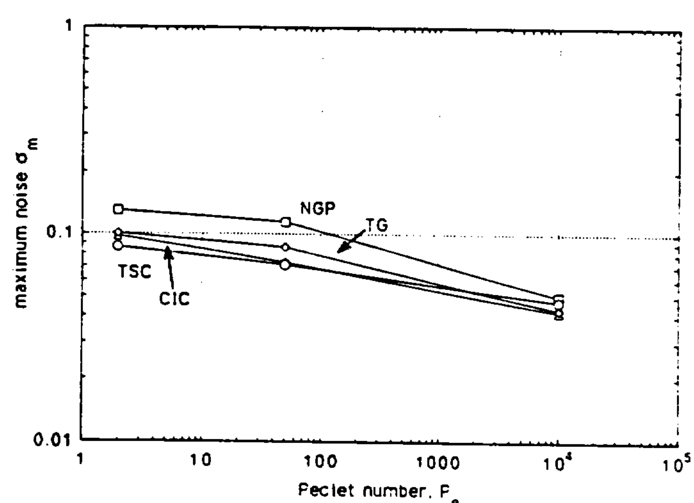

Figure 3 Maximum standard concentration error vs. P_e.

The effect of N_r on the size of σ_m, as well as a similar variation of σ with the (-1/10) power of P_e, is shown in Figure 4. These results are presented in a different way in Figure 5, where the maximal noise is plotted against N_r for each flow regime. The variation of σ_m

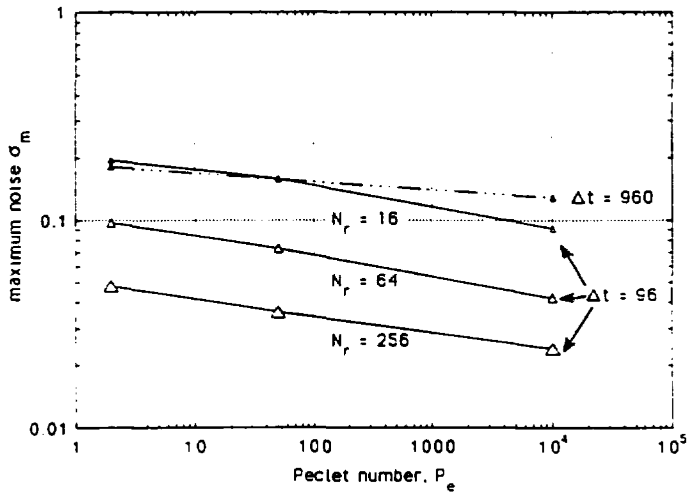

Figure 4 Maximum standard concentration error vs. P_e, N_r and Δt.

appears to go with the (-1/2) power of N_r as indicated in (8). Finally, some observations are made regarding the effects of the support of the interpolation function and the time step, Δt, used in the RWPM. It is worthwile noticing that in the less diffusive regimes (Figure 4) we see smaller errors associated with the smaller time step, a manifestation of the fundamental convergence of the random walk with Δt.

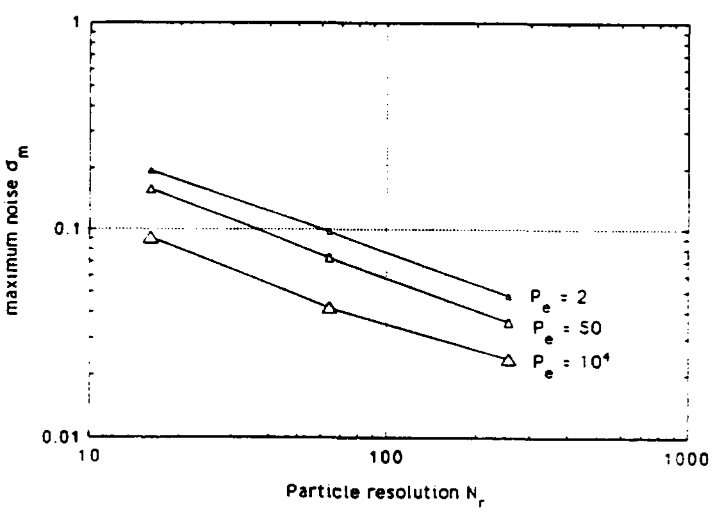

Figure 5 Maximum standard concentration error vs. N_r and P_e.

In Figure 6 we see an approximate (-1/2) power variation of σ_m with the support in the more diffusive regimes. Since the support is related to the volume V over which concentrations are estimated, then these results are also consistent with (8). Figure 6 shows also that the larger noise observed with P_e=2 can be reduced to that observed for $P_e=\infty$ by increasing the projetion support by a factor of five.

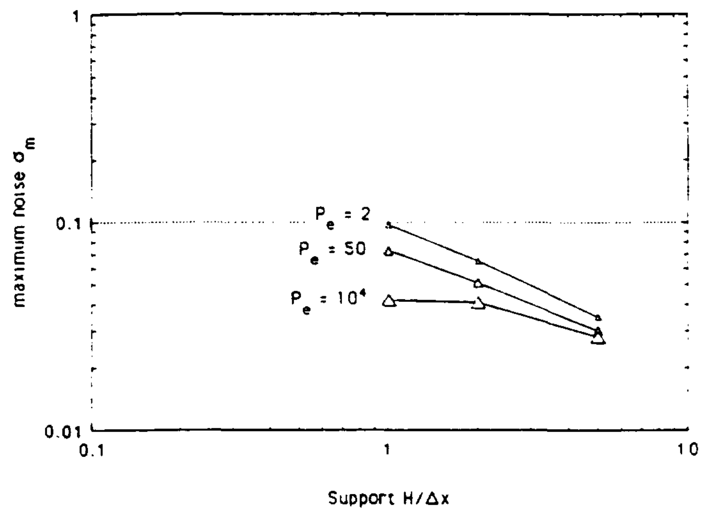

Figure 6 Maximum standard concentration error vs. interpolation function support and P_e.

Four classical numerical methods are used for comparisons with the piecewise linear CIC(RWPM): centered finite difference (CFD), upwind finite difference (UFD), Lax-Wendroff (LW), and Fromm (FR), all described by Roache (1976). In addition, two nonlinear flux-limiting schemes are employed: piecewise parabolic method (PPM) (Collela and Woodward, 1984), and flux corrected transport (FCT) (Borris and Book, 1973). It should be noted that the results correspond to single-realization simulations of the RWPM with 400 particles. Figure 7 shows that the particle method outperforms all six methods for the case of $P_e=\infty$, being graphically indistinguishable from the analytic solution. This was a well-expected result. Figure 8 exhibits the behavior of all seven numerical schemes for $P_e=2$. The noise of the particle method is now apparent. Nevertheless, it still approximates the analytic solution much better than the LW, UFD, and FR schemes. The dominating diffusion leads to a CFD scheme performing quite well. Finally, both PPM and FCT schemes are practically indistinguishable from the analytic solution.

3.2 Rectangular Wave Propagation Problem

The rectangular wave propagation problem is governed by (4) with $x \in [0,\infty]$ and initial and boundary conditions $c(x,0)=C_0=0\ \forall\ 0<x<1400$ and $2600<x<12800$, $c(x,0)=C_1=1\ \forall\ 1400<x<2600$, and $c(\infty,t)=C_0=0\ \forall\ t>0$. The analytic solution for this problem is given by (Neuman, 1981)

$$c^a(x,t)=\frac{1}{2}[erf(\frac{b-x+ut}{2\sqrt{Dt}})+erf(\frac{b+x-ut}{2\sqrt{Dt}})] \qquad (9)$$

Only CIC(RWPM), PPM, and FCT are tested for this model-problem. For the flow and discretization parameters described previously, the grid Courant number, $C_0=u\Delta t/\Delta x$, is equal to 0.24. Figure 9 depicts the concentration profile for $P_e=\infty$, and $P_e=2$. For the case of

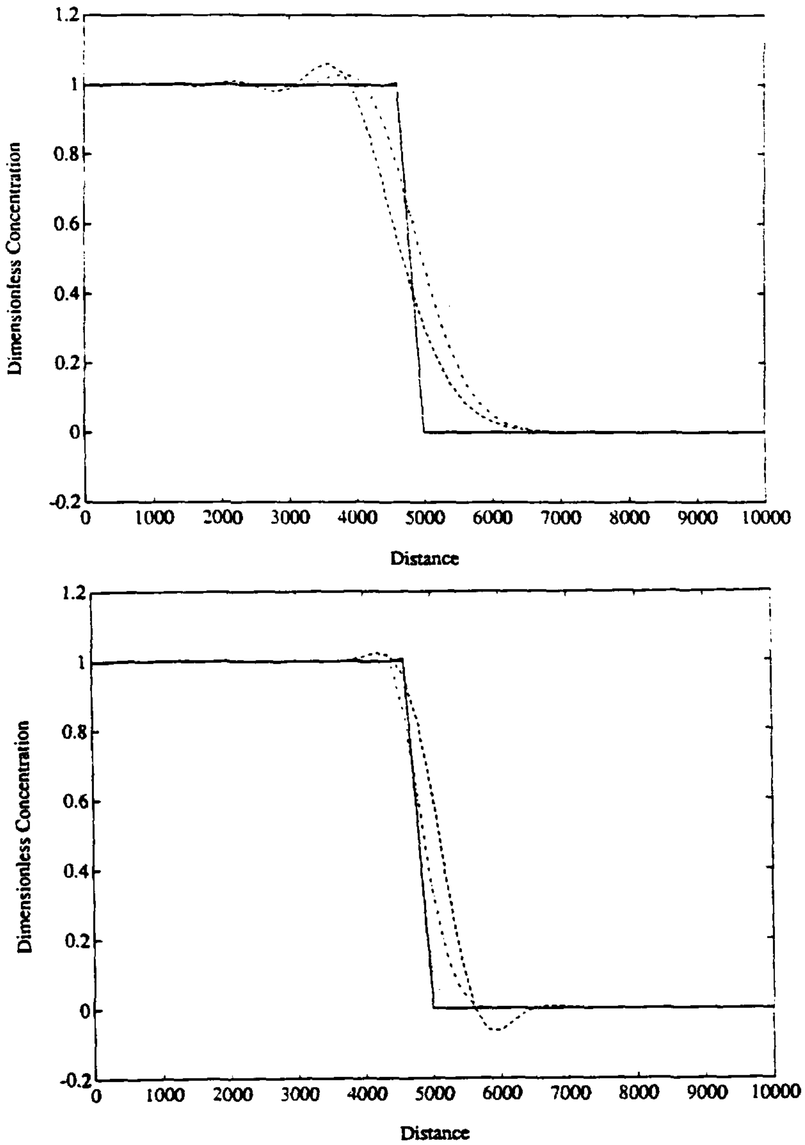

Figure 7 Analytic and particle method results (solid) for $P_e=\infty$, and a) CFD (dashed), UFD (dotted), LW (dashed-dotted) b) FR (dashed), PPM (dotted), FCT (dashed-dotted).

advection-dominated flow, the RWPM is subject to neither severe damping, nor oscillatory behavior. However, it produces a noisy solution at the maximum concentration region. PPM is characterized by both diffusive attenuation of the peak concentration, and undershoot wiggles at the toes of the wave. FCT performs better than PPM in that it satisfies positivity and shows less concentration peak errors. For the case of $P_e=2$, both PPM and FCT compare favorably to the analytic solution. The particle solution is noisy, clearly suggesting the need for either more than 400 particles or repeated realizations.

It should be re-emphasized that the RWPM results do not involve repeated simulations. This was found to be necessary in order to make its results comparable to the single-run, deterministic, standard numerical methods. As shown in the previous section, where projection functions were compared, the effect of repeated Monte Carlo simulations is significant for noise elimination and error minimization.

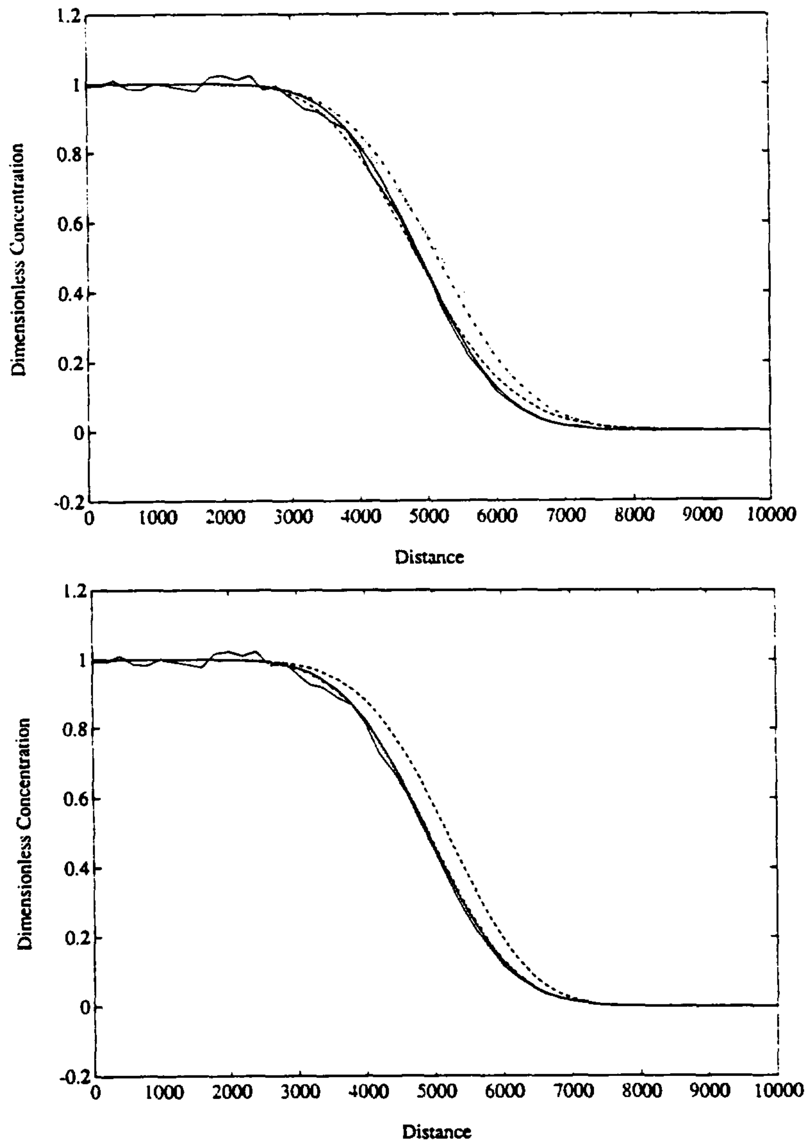

Figure 8 Analytic and particle method results (solid) for P_e=2, and a) CFD (dashed), UFD (dotted), LW (dashed-dotted) b) FR (dashed), PPM (dotted), FCT (dashed-dotted).

4. Extension to Two Dimensions

The two-dimensional form of (1), for a conservative solute is

$$\frac{\partial c}{\partial t}+u\frac{\partial c}{\partial x}-D_x\frac{\partial^2 c}{\partial x^2}-D_y\frac{\partial^2 c}{\partial y^2}=0 \tag{10}$$

where D_i (i=x,y) are the dispersion coefficients. This problem is associated with an infinite domain subject to the initial conditions c(x,y,0)=0, and an instantaneous point source of mass ΔM at time t=0 at x=10.5, y=25.0.

Analytic solutions for this solute transport problem have been reported by various

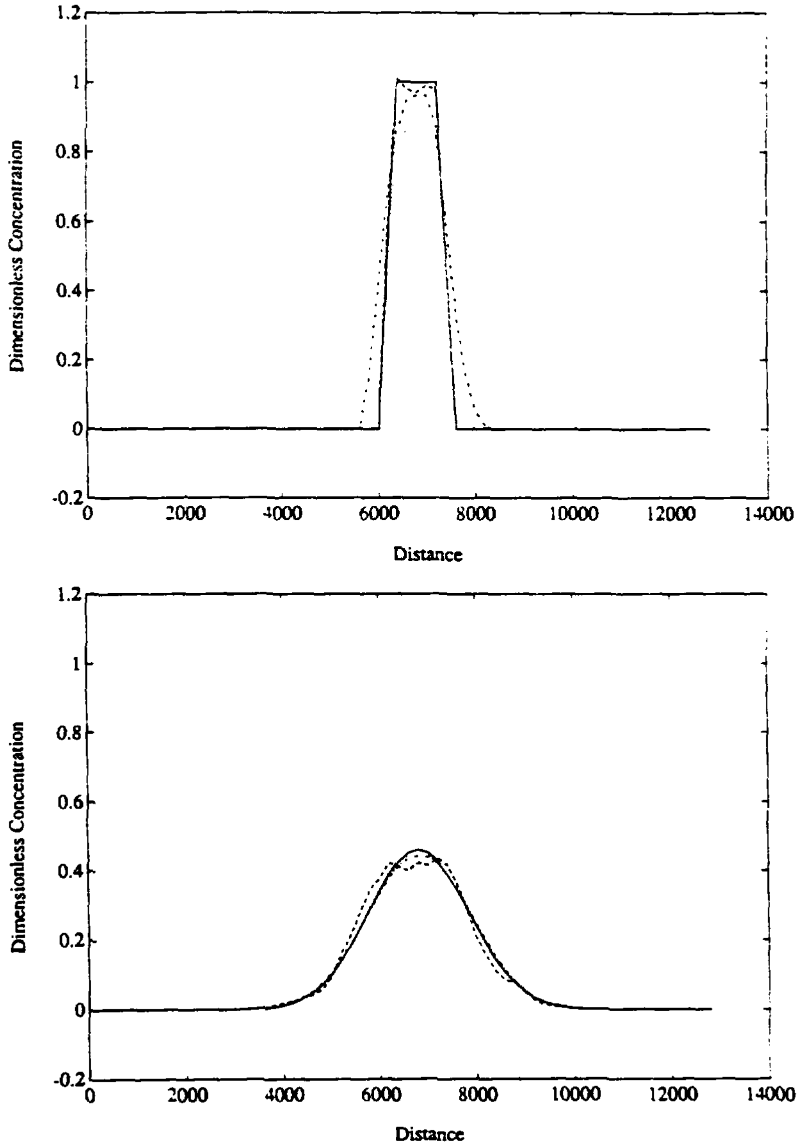

Figure 9 Rectangular wave results for a) $P_e=\infty$ and b) $P_e=2$. Analytic (solid), particle (dashed), FCT (dashed-dotted), PPM (dotted).

investigators. Wilson and Miller (1978) give the following solution

$$c(x,y,t)=\frac{\Delta M}{4\pi\eta t\sqrt{D_x D_y}}\exp\left[-\frac{(x-ut)^2}{4D_x t}-\frac{y^2}{4D_y t}\right] \tag{11}$$

In (11) η is the effective porosity. RWPM simulations of (10) are conducted in a domain size 50 × 50 × 1 with u=0.4, η=0.25, $\Delta x=\Delta y=1$, $\Delta M=200$, $\Delta t=0.25$ and a total simulation time of t=50. For these flow and discretization parameters $P_e^x=2$ and $P_e^y=20$. A typical contour plot of the CIC(RWPM) concentration field is shown in Figure 10 together with the two-dimensional analytic solution. Keeping in mind that the particle simulation involved 400 particles and 20 Monte Carlo runs, the agreement is considered satisfactory.

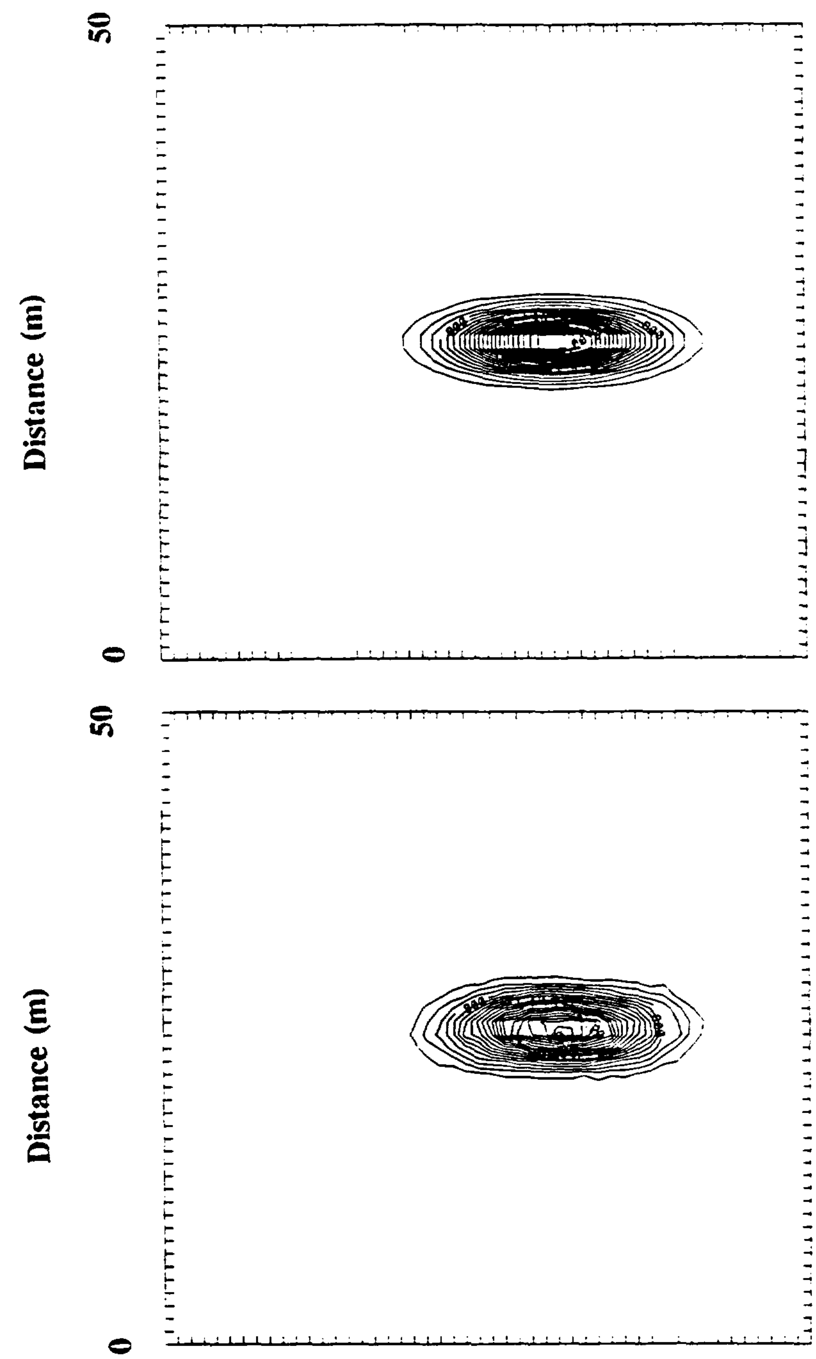

Figure 10 Two-dimensional transport results for P_e^x=2, a) analytic and b) particle method results.

In cases where longitudinal dispersion (colinear with velocity) dominates transverse dispersion, experimentation with two- and three-dimensional problems has shown that the use of ***streamline composite*** projection functions can improve the solutions. These projection functions involve the use of piecewise linear CIC (or any high order function) in the direction of prevailing flow and piecewise constant NGP (or any low order function) transverse to it. With this approach, sharp transverse fronts are better approximated by discontinuous functions rather than piecewise linear ones.

5. Reactive Transport Applications

The application of the operator splitting concept allows one to treat the advective-diffusive part of the solute transport independent of the reactive part. Within the context of the particle tracking method, reactions are modeled by modifying the mass at a point in space, that is, by either adjusting the number of particles or the mass per particle of a specific species. Since in most cases the reaction mechanisms are modeled in terms of mass densities, a grid-based approach is followed in the present work. This leads to the need for a method that performs *consistent backward interpolation* from concentration changes, on a grid, to mass changes on particles. Bagtzoglou (1990), Bagtzoglou and Dougherty (1990), and Bagtzoglou *et al.* (1991) present a thorough discussion of the problems associated with this methodology.

Consider the one-dimensional nonlinear reaction-diffusion equation

$$\frac{\partial c}{\partial t}=D\frac{\partial^2 c}{\partial x^2}+r(c,t) \tag{12}$$

with a second order reaction rate $r(c,t)=c(1-c)$, boundary conditions $c(\infty,t)=0$, and $c(-\infty,t)=1$ and initial condition

$$c(x,0)=[1+\exp(x/\sqrt{6})]^{-2} \tag{13}$$

Since this is an advection-free problem, particles are translated only by random Brownian motions. The leftmost boundary is treated as reflective, whereas the rightmost is treated as free (open). By definition the model equation requires that $0\leq c\leq 1$. Therefore, the reaction rates will always be positive and add new mass into the system. As mass diffuses to the right, the concentration becomes nonzero, and the reaction adds more mass in regions where $0<c<1$. Figure 11 demonstrates the solution of (12) for $D=0$ at $t=0$, 2.5, and 5. It can be seen that even though there is no particle movement (no advection, no diffusion), there exists a mass propagation from left to right because of reactions.

Due to the highly nonlinear reaction term, perturbations (errors) introduced into the solution can grow rapidly. These errors arise due to inaccurate representation of initial conditions, the stochastic nature of RWPM and loss of particle resolution during the course of simulation. The model equation (12) (known as Fisher's equation for $D=1$) is considered a challenging test problem for numerical studies because of the stiffness and nonlinearity of the reaction term. A balance between the reaction and diffusion processes in this system leads to a family of traveling wave solutions, sensitive to far field perturbations.

Our solution to the problem of resolution loss is to enhance the particle-grid algorithm with a particle redistribution procedure that reduces the noise propagation. Tompson and Dougherty (1990) presented an alternative approach that dynamically adjusts the particle resolution near the front, by splitting massive particles via a process they call *spawning*. Figure 12 shows results from a simulation involving 13500 particles. This figure indicates that the wave propagates to the right slightly ahead of the exact solution, but is in good agreement with what the theory predicts.

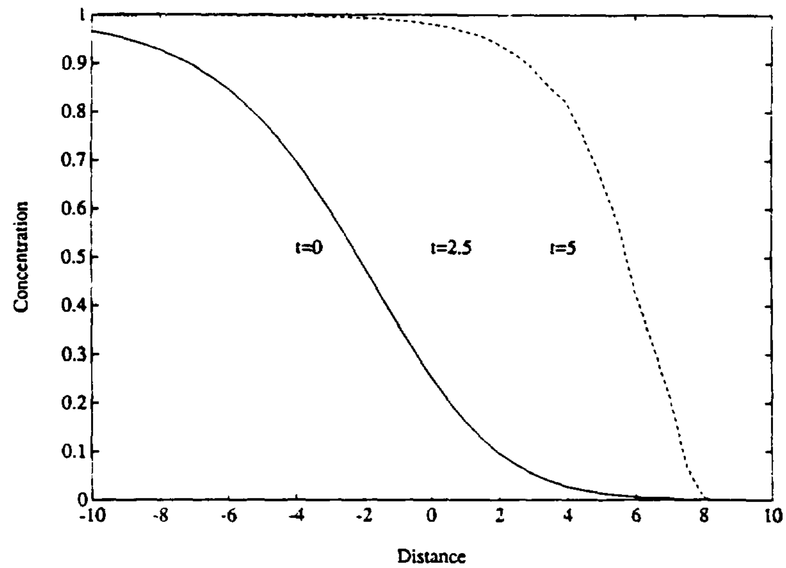

Figure 11 Particle method solution of equation (12) for D=0.

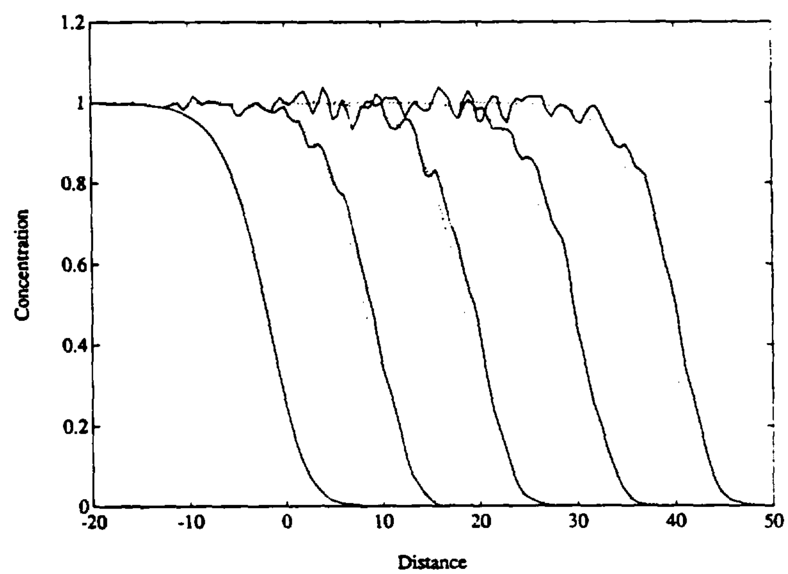

Figure 12 Particle method (solid) and analytic (dotted) solution of Fisher's equation.

6. Summary

This paper presented various results from a particle-grid methodology for the numerical solution of advection-diffusion-reaction problems. Within this approach, projection functions are used to transform particle-based masses to grid-based concentrations, and *vice versa.*

A series of one-dimensional tests confirmed that the point interpolation error $\sigma(x,t)$ is strongly dependent on the (1/2) power of the mean concentration, $\langle c(x,t) \rangle$, the (-1/2) power of the particle resolution, N_r, and the (-1/10) power of the grid Peclet number, P_e. Results from the RWPM were also compared to six numerical methods for solving the field equations of nonreactive transport. The RWPM performed quite satisfactorily compared to these methods in the one-dimensional test problems. Two-dimensional results matched closely the analytical solutions for cases with Peclet numbers as low as two. When reactions are present, the need for more sophisticated advection-diffusion solutions increases. We employed an inconsistent particle-grid method that yielded reasonable solutions and feasible computational requirements. The methodology was applied, with success, to the advection-free, nonlinear reaction-diffusion problem known as Fisher's equation.

These examples serve to dispel the commonly held belief that particle methods are best applied to, and only to, advection-dominated solute transport.

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