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Computer Prediction of Subsurface Radionuclide Transport: An Adaptive Numerical Method

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ABSTRACT

Radionuclide transport in the subsurface is often modeled with the aid of the advection-dispersion equation. A review of existing computer methods for the solution of this equation shows that there is need for improvement. To answer this need, a new adaptive numerical method is proposed based on an Eulerian-Lagrangian formulation. The method is based on a decomposition of the concentration field into two parts, one advective and one dispersive, in a rigorous manner that does not leave room for ambiguity. The advective component of steep concentration fronts is tracked forward with the aid of moving particles clustered around each front. Away from such fronts the advection problem is handled by an efficient modified method of characteristics called single-step reverse particle tracking. When a front dissipates with time, its forward tracking stops automatically and the corresponding cloud of particles is eliminated. The dispersion problem is solved by an unconventional Lagrangian finite element formulation on a fixed grid which involves only symmetric and diagonal matrices. Preliminary tests against analytical solutions of one- and two-dimensional dispersion in a uniform steady state velocity field suggest that the proposed adaptive method can handle the entire range of Peclet numbers from 0 to ∞, with Courant numbers well in excess of 1.

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PREFACE

Most existing computer models for the prediction of subsurface mass transport are founded on the advection-dispersion equation. According to this equation, a tracer or contaminant is transported by means of two principal mechanisms: advection with the mean groundwater velocity, and hydrodynamic dispersion. The hydrodynamic dispersion term in the equation is said to account for molecular diffusion and deviations of the actual groundwater velocity from its mean value. In analogy to Fick's first law of molecular diffusion, mass flux of a given chemical species due to hydrodynamic dispersion is commonly assumed proportional to the gradient of its concentration. Other phenomena such as radioactive decay and sorption are superimposed on the advective-dispersive process as source or sink terms.

In recent years, many questions have been raised regarding the applicability of the Fickian analogy to fractured and porous rocks. One important aspect of our own research work, under the auspices of the Nuclear Regulatory Commission, has been to determine the degree to which the traditional Fickian form of the advection-dispersion equation applies to fractured rocks. Our work as well as that of others suggest that the traditional form has serious shortcomings and as such, is less than a perfect predictive tool. Efforts are underway to modify the existing form, or develop alternative mathematical models, so as to improve our ability to predict contaminant transport. These efforts not withstanding, the Fickian advection-dispersion equation will most probably remain the chief tool of subsurface transport analysis at least for the immediate future.

Our recognition that the traditional equation will remain the mainstay of contaminant transport modeling in the coming years has prompted us to examine the numerical methods currently used to solve this equation on the computer. Numerical difficulties arise due to the complex three-dimensional flow patterns often encountered in the subsurface, the anisotropic nature of hydrodynamic dispersion, and other complicating factors such as radioactive decay, sorption, and chemical reactions. However, a more fundamental numerical difficulty stems from the very nature of the advection-dispersion equation which may be predominantly parabolic in some parts of the flow field, and hyperbolic in other parts, depending on the local Peclet number. Most numerical methods are tailored to handle one of these situations, but not both simultaneously. Consequently, many existing numerical models of subsurface transport are prone to errors that may manifest themselves in the form of unwarranted oscillations or the smearing of steep concentration gradients. One aspect of our work for the Nuclear Regulatory Commission is to evaluate these numerical methods and suggest possible improvements.

This report includes a critical review of existing numerical methods for advection-dispersion. Our review reveals fundamental weaknesses in most of the modeling techniques that have been described in the literature. To overcome some of these weaknesses, we propose a new adaptive Eulerian-Lagrangian method that can be used in conjunction with any well-established grid technique such as finite differences, integral finite differences, point collocation, or finite elements; we currently work with the latter.

The proposed method is based on a formal decoupling of the concentration field into an "advective" part and a "dispersive" part. This makes it possible to automatically adapt the method of solution to the nature of the problem. When sharp concentration fronts are present, their advective component is tracked forward with the aid of moving particles. Away from such fronts, the advection problem is handled by an efficient modified method of characteristics referred to here as "single-step reverse particle tracking." When a front becomes sufficiently smooth to be handled by the single-step reverse particle tracking method, its forward tracking stops automatically and the corresponding particles are eliminated. The residual dispersion problem is solved by finite elements in each case. Since advection is handled separately, the matrices arising from the finite element formulation are either symmetric or diagonal. Most conventional finite element schemes lead to nonsymmetric matrices. Preliminary tests with one- and two-dimensional dispersion in a uniform velocity field suggest that the method is capable of handling Peclet numbers from 0 to ∞ without oscillations and numerical dispersion, while using large time steps with Courant numbers well in excess of 1.

1. INTRODUCTION

The nature of the advection-dispersion equation can be conveniently characterized by the dimensionless Peclet number

$$Pe = \frac{|\underline{v}|L}{\|\underline{\underline{D}}\|} \tag{1-1}$$

where $\underline{v}$ is velocity vector, L is a characteristic length, and $\underline{\underline{D}}$ is dispersion tensor. For example, in the case where an inert chemical species is spreading due to molecular diffusion in a one-dimensional velocity field, the governing equation can be written as

$$\frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial x^2} - Pe \frac{\partial c}{\partial x} \tag{1-2}$$

where c is concentration, t is time, x is spatial coordinate defined relative to L, and Pe = vL/Dm, v being velocity and Dm molecular diffusion coefficient. Clearly, when Pe is small, diffusion dominates, and the equation is parabolic in character. When Pe is large, advection dominates, and the character of the equation changes to hyperbolic. In nonuniform and nonsteady flow fields where the velocity is not constant, the character of the advection-dispersion equation may vary in space and time, being predominantly parabolic in some regions and hyperbolic in others.

Most conventional numerical methods for solving the advection-dispersion equation can be classified into two major categories, Eulerian or Lagrangian, depending on the emphasis that they place on the parabolic or hyperbolic nature of the problem. In the Eulerian method, the equation is discretized by a finite difference or finite element grid fixed in space. Lagrangian methods utilize either a deforming grid, or a fixed grid in deforming coordinates. A review of these methods, together with a discussion of their relative advantages and disadvantages, is given in the next chapter.

A third approach that has been gaining popularity in recent years is the mixed Eulerian-Lagrangian method. As will be shown below, this method combines the simplicity of the fixed Eulerian grid with the computational power of the Lagrangian approach, both of which are essential when relatively sharp concentration fronts are traveling through complex geologic environments. Existing Eulerian-Lagrangian numerical schemes are reviewed in the next chapter. Unfortunately, the review points to several shortcomings. In an effort to overcome these shortcomings, we proposed earlier a new technique consisting of two steps (Ref. 1): 1. Formal decomposition of the concentration field into two parts, one controlled by pure advection, the other essentially by dispersion, and 2. Solution of the resulting advection problem by the method of characteristics on a fixed space-time grid, coupled with a finite element solution of the dispersion problem on another fixed grid. Our formal decomposition of the concentration field is rigorous and differs from previous such attempts in that it leaves no room for ambiguity.

However, the particular numerical implementation of this idea described in Neuman's paper (Ref. 1) suffers from some artificial dispersion.

This report describes an alternative numerical scheme based on Neuman's theory (Ref. 1). The fundamental new idea behind the proposed scheme is automatic adaptation of the solution process to the nature of the problem. When sharp concentration fronts are present, their advective component is tracked forward with the aid of moving particles. Away from such fronts, the advection problem is handled by an efficient method called "single-step reverse particle tracking." When a front becomes sufficiently smooth to be treated by the single-step reverse particle tracking method, its forward tracking stops automatically and the corresponding particles are eliminated. The residual dispersion problem is solved by finite elements in each case. Since advection is considered separately, the matrices arising from the finite element formulation are either symmetric or diagonal. Most conventional finite element schemes lead to nonsymmetric matrices. Preliminary tests with one- and two-dimensional dispersion in a uniform velocity field suggest that the method is capable of handling the entire range of Peclet numbers from 0 to ∞ while using large time steps with Courant numbers well in excess of 1.

2. STATE OF THE ART

Most numerical methods for solving the advection-dispersion equation can be categorized as Eulerian, Lagrangian, or Eulerian-Lagrangian.

2.1 Eulerian Methods

The most common Eulerian method is that based on finite differences. Early experiments with this approach (Refs. 2-4) have shown that this technique performs well in dispersion-dominated situations at low Peclet numbers where the concentration function is relatively smooth. However, when the gradient of concentration is steep due to the prevalence of advection at high Pe, methods based on central difference approximations for the advection term may suffer from oscillations resulting in overshoot, undershoot and negative concentrations. Price et al. (Ref. 5) proved that such oscillations can be eliminated by restricting the size of the spatial grid increments; in the case of Eq. 1-2, the increments must satisfy $\Delta x \leq 2/Pe$. Since this is not always practical, the alternative is to use upstream difference approximations (also known as upstream weighting or upwinding) that are able to eliminate oscillations, but also introduce large truncation errors which are equivalent to a numerical (as opposed to physical) dispersion term (Refs. 6, 7). The effect of this numerical dispersion term is to smear sharp concentration fronts. Lantz (Ref. 7) showed that for many practical problems, reducing numerical dispersion sufficiently so as to prevent masking physical dispersion may require an extremely fine grid. Another way to reduce numerical dispersion in upstream schemes is to cancel part of the truncation error by using higher-order approximations in space (Refs. 8-11), time (Refs. 6,12-14), or both (Ref. 15). Most of these have the effect of adding a negative correction term to the dispersion coefficient. A similar effect

can also be achieved by means of flux corrections (Ref. 16), variable upstream/downstream weighting (Ref. 17), variably timed flux updating (Refs. 18,19), or on the basis of physical considerations (Ref. 20).

During the last decade, there has been a growing belief that an alternative Eulerian approach for handling sharp fronts may be provided by high order finite element techniques (Refs. 21-23). Price et al. (Ref. 21) showed that high-order Galerkin approximations using smooth and non-smooth Hermite polynomials are potentially far more accurate for a given amount of computational effort than standard finite difference techniques. Low-order Galerkin finite element schemes also appear to be more accurate than standard finite differences (Refs. 24-26). However, in dealing with advection-dominated problems (especially the translation of square waves), the former are sometimes inferior when compared to the lowest-order flux-corrected finite difference scheme of Book et al. (Refs. 16,27). Furthermore, time-centered finite element schemes suffer from oscillations, and backward difference schemes exhibit numerical dispersion (Refs. 25,26). So far, neither higher-order interpolations in space (Ref. 26) nor in time (Ref. 28) have proven capable of entirely and efficiently eliminating both problems.

The use of upstream weighting on finite elements reduces oscillations only at the expense of numerical smearing (Refs. 29-31). More promising is the idea of adding an anisotropic correction to the dispersion term as postulated for steady state problems by various authors (Refs. 32-34). Both approaches can be cast in the more general context of Petrov-Galerkin methods which alter the symmetry of terms resulting from standard Galerkin approximations by using interpolation functions that differ from the basis functions. A review of the most recent advances in this area shows that the Petrov-Galerkin method holds promise for steady state problems (Refs. 35,36) but its extension to transient advection-dispersion requires further development (Ref. 37).

Another recent trend in the development of Eulerian techniques is the use of point collocation, often in conjunction with ADI (Refs. 38,39). While the combination of collocation with ADI appears to be computationally efficient, one must recognize that a similar effect can be achieved by combining ADI with finite elements (Ref. 40). There seems to be no indication in the literature that collocation is superior to conventional finite elements of comparable polynomial degree in dealing with oscillations and numerical dispersion.

2.2 Lagrangian Methods

Since standard Eulerian techniques are unsatisfactory while the more complex techniques may not always be easily adapted to difficult problems, and since some of the more promising new ideas are in an early stage of development, it is of interest to examine methods founded on the Lagrangian approach. Such methods are based either on a deforming grid or on a fixed grid in deforming coordinates. Varoğlu and Finn (Refs. 41-44) use space-time finite elements in one and two spatial dimensions with sides paralleling either

surfaces of constant time, or surfaces defined by characteristics. In this manner, the finite element equations become free of advective terms, resulting in a relatively well-behaved diffusion-type problem. The idea is based on earlier uses of space-time finite elements in connection with the Stefan problem (Refs. 45,46) and equations representing conservation laws (Ref. 47). The method was tested by the authors on various problems ranging from dispersion-dominated cases to the pure advection of a rectangular wave. Their results did not show any oscillations and exhibited only a small amount of numerical dispersion in the case of pure advection. Another closely related approach is one in which the nodal points of a one-dimensional Hermitian finite element grid are shifted during each time step parallel to the characteristics (Refs. 48,49). The resulting finite element equations, which are coupled with finite differences in time, are thus devoid of advective terms and can be solved without difficulty. The authors demonstrated that when the grid is made fine enough in the vicinity of a sharp front, the results can be entirely free of oscillations or numerical dispersion. Not only are both methods highly accurate but, when advection dominates, both are also able to use large time steps such that the distance traveled by a fluid particle, say, Δs, is well in excess of the distance between contiguous nodal points, say, Δx. The same is probably true about the more complex moving Petrov-Galerkin method described in a recent paper by Botha et al. (Ref. 50). In Eulerian schemes, stability and convergence often require that time step size be small enough to satisfy the Courant-Friedrichs-Lewy condition

$$\Delta s \leq \alpha \Delta x \tag{2-1}$$

where α, the Courant number, is at most 1 (Ref. 51). Practical experience with various Eulerian schemes, including Hermitian finite elements, suggests that it is prudent to set α equal to 1/3 (Ref. 48).

Jensen and Finlayson (Refs. 52,53) proposed a scheme in which the advection-dispersion equation is written in Lagrangian coordinates with origin at the center of a moving front. When the velocity field is uniform, the equation becomes free of advective terms; otherwise, some residual first-order space derivatives remain. By using orthogonal collocation on finite elements, the authors were able to obtain good results that showed no oscillations and only a minute amount of numerical dispersion at high Peclet numbers.

2.3 Eulerian-Lagrangian Methods

Even though the above Lagrangian methods are more powerful than most Eulerian techniques, they suffer from several limitations which may become serious when one considers difficult problems such as groundwater contamination in complex subsurface environments. Since geologic environments are often characterized by highly nonuniform material properties, the movement of nodal points across material interfaces may cause difficulties in the handling of equation parameters, especially if sorption and chemical reactions are important. Such movement may also result in severe grid

deformations due to the refraction of streamlines across material interfaces, leading to numerical errors. When multiple sources exist, as in the case of chemical injection into the subsurface through several wells, concentration fronts may propagate in opposite directions and cross each other at various angles, causing mesh tangling. This type of transport cannot be handled with the aid of deforming meshes or moving coordinates of the kind described above. Since velocities are usually computed independently of the transport problem by using a fixed Eulerian grid, it would be most convenient if the advection-dispersion equation could be solved on a grid compatible with the latter, especially when the velocity field varies with time. Finally, when the grid or the coordinates deform, the finite element matrices must be reevaluated and/or decomposed anew at every time step (in the case of Lagrangian coordinates, this is so because the boundary location varies with time); in linear problems solved on an Eulerian grid, the matrices remain constant, and if the time increment is fixed, a single LU-decomposition is enough.

The purpose of Eulerian-Lagrangian methods is to combine the simplicity of the fixed Eulerian grid with the computational power of the Lagrangian approach. Runca and Sardei (Ref. 54) proposed to do this for horizontal advection and vertical eddy diffusion of air pollution by discretizing the vertical wind profile in a stepwise fashion. They then used different time intervals for each step so as to translate the concentration field to positions coincident with fixed Eulerian grid points during each time increment. Melli (Ref. 55) solved the same problem with an irregular grid adapted to the wind profile so that the horizontal distance between nodes at each elevation is exactly equal to the distance traveled by a particle due to advection during a time step. Although his technique yielded good results for relatively large eddy diffusivities, attempts to propagate a sharp front met only with marginal success. On the other hand, Sauty (Ref. 56) reported success in using a similar idea to analyze the movement of groundwater tracers between wells.

More general than the former is the continuous forward particle tracking method originally suggested by Garder et al. (Ref. 57) and later used extensively for subsurface transport (Refs. 58-61). In this method, advection is handled by the method of characteristics applied to a set of moving particles. The dispersion part of the problem is solved by explicit finite differences on a fixed grid. Although the method is virtually free of numerical dispersion, it suffers from instability when the time step size exceeds a certain limit. Existing theory behind this version of particle tracking is vague and, therefore, it cannot be shown to converge. The treatment of complex boundary conditions and nonlinearities is not straightforward, and the constant handling of numerous particles is time consuming. In another version of particle tracking developed by Ahlstrom et al. (Ref. 62) and recently popularized among subsurface hydrologists by Prickett et al. (Ref. 63), dispersion is effected by means of a random walk process applied to each particle. The method is conceptually simple and relatively easy to program. Its main drawback is that concentrations are computed by sampling the mass concentration of particles, a process that is strongly dependent on sample size. Experience shows that many thousands of particles

may be required for the sample size to be large enough to provide accurate solutions in simple two-dimensional flow fields.

To avoid the need for a large number of moving particles, Hinstrup et al. (Ref. 64) suggested redefining the particles at discrete time intervals so as to make them coincide with the nodes of a fixed finite difference grid at the end of each time step. The position of each particle at the beginning of a time step is obtained by polynomial interpolation between concentration values at neighboring grid points. Neuman and Sorek (Ref. 65) used a similar approach in conjunction with finite elements and referred to it as "single-step reverse particle tracking." The same approach was termed "modified method of characteristics" by Russell, Ewing, and Douglass (Refs. 66-70) who studied some of their theoretical properties. In particular, Ref. 70 shows that, for advection-dominated problems, the approach has much smaller time-truncation errors than some purely Eulerian methods. According to Russell (Ref. 67), the method is free of grid orientation effects, numerical dispersion, and overshoot.

Our own work demonstrates that single-step reverse particle tracking indeed possesses some very attractive features: It is simple, numerically efficient, leads to symmetric matrices, and can handle large time steps with Courant numbers well in excess of 1. Contrary to Russell (Ref. 67), however, our results show that at high Pe, the method is not free of numerical dispersion and overshoot unless the spatial grid is made very fine. When a reasonably coarse grid is used, the results deteriorate as the time interval, Δt, is reduced, due to the accumulation of interpolation errors.

3. ADAPTIVE EULERIAN-LAGRANGIAN METHOD

We saw that Eulerian methods have many advantages stemming from a fixed grid, but they are not well suited for the handling of sharp fronts, and their time step size is often limited by the Courant-Friedrichs-Lewy condition. Lagrangian methods are able to deal with steep concentration gradients while utilizing relatively large time steps, but the lack of a fixed grid, or fixed coordinates, causes difficulties in dealing with complex subsurface conditions. Mixing the Eulerian and Lagrangian methods provides an opportunity to benefit from the best of both worlds by being able to handle sharp fronts while maintaining a fixed grid.

Unfortunately, none of the existing Eulerian-Lagrangian methods takes full advantage of this opportunity. The particle tracking method of Garder et al. (Refs. 57-61) lacks a firm theoretical foundation and requires excessive computer time. The single-step reverse particle tracking method suffers from numerical dispersion which becomes worse as the time discretization interval goes down. We propose to resolve these difficulties by supplying a rigorous theory in support of the Eulerian-Lagrangian approach, and by enhancing its computational power through an adaptive scheme.

Our theory, developed originally by Neuman (Ref. 1), is presented below. It allows for a formal decoupling of advection from dispersion in a manner

which, contrary to previous such attempts (Refs. 57, 64, 71) does not leave room for ambiguity. Since the advection and dispersion problems require different treatments, they are solved separately, one by a Lagrangian method and the other by an Eulerian method.

Our adaptive scheme rests on the recognition that many problems involve sharp fronts which dissipate with time. The tracking of such fronts is accomplished most efficiently with the aid of forward moving particles clustered around each front (Ref. 72). However, there is no need to track particles away from such fronts, and there is no need to continue tracking a front after it has become sufficiently smooth due to dispersion, sorption, or decay. Instead, the solution away from sharp fronts is handled much more efficiently by single-step reverse particle tracking. In short, we propose to adapt the method of solution to the manner in which the concentration field evolves in space and time. Preliminary results will demonstrate that our proposed adaptive scheme leads to a considerable improvement in accuracy and computational efficiency.

4. THEORY

Consider the advection-dispersion equation

$$(1 + s)\frac{\partial c}{\partial t} = \nabla\cdot(\underline{\underline{D}}\nabla c - \underline{v}c) - \lambda c + q \qquad (4\text{-}1)$$

where c is concentration, s is retardation coefficient (some reserve this term for $1 + s$), t is time, ∇ is gradient operator, $\underline{\underline{D}}$ is dispersion tensor, $\underline{v}$ is seepage velocity vector, λ is radioactive decay coefficient, and q is source term. The parameters of Eq. 4-1 satisfy $s \geq 0$, $\lambda \geq 0$, and $\underline{\underline{D}}$ is symmetric positive-semidefinite. The equation is to be solved for c, subject to the initial and boundary conditions

$$c(\underline{x},0) = C_0(\underline{x}) \qquad (4\text{-}2)$$

$$(-\underline{\underline{D}}\nabla c + \underline{v}c)\cdot\underline{n} + \alpha(c-C) = Q \qquad \text{on } \Gamma \qquad (4\text{-}3)$$

Here $\underline{x}$ is position vector; Γ is boundary; $\underline{n}$ is unit vector normal to Γ and pointing outward; C_0, C, and Q are prescribed functions; and α controls the type of boundary condition prevailing on Γ: If $\alpha \to \infty$, Eq. 4-3 is a prescribed concentration condition; if $\alpha = 0$, it is a prescribed mass flux condition; otherwise, it is a mixed condition. Eq. 4-3 applies to inflow and noflow boundaries. Along outflow boundaries, it is common to assume that

$$\underline{\underline{D}}\nabla c\cdot\underline{n} = 0 \qquad \text{on } \Gamma \qquad (4\text{-}4)$$

Using the hydrodynamic derivative

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \frac{\underline{v}\cdot\nabla}{1+s} \tag{4-5}$$

we can rewrite Eq. 4-1 in Lagrangian form as

$$(1+s)\frac{Dc}{Dt} = \nabla\cdot(\underline{\underline{D}}\nabla c) - fc + q \tag{4-6}$$

where $f = \nabla\cdot\underline{v} + \lambda$. Here c no longer represents concentration at a point in space-time, but rather the concentration of a fluid particle moving at the velocity $\underline{v}^* = \underline{v}/(1+s)$. The pathline of this particle is described by the hydrodynamic derivative of $\underline{x}$, which leads to the characteristic equation

$$\frac{D\underline{x}}{Dt} = \underline{v}^* \tag{4-7}$$

Neuman (Ref. 1) has shown that Eqs. 4-6 and 4-7 subject to Eqs. 4-2 through 4-4 can be replaced by two sets of equations, one in terms of $\bar{c}$, the other in terms of $\overset{\circ}{c}$, where

$$c = \bar{c} + \overset{\circ}{c} \tag{4-8}$$

One way to perform such a decomposition is to let c satisfy the homogeneous first-order partial differential equation

$$\frac{D\bar{c}}{Dt} = \frac{\partial\bar{c}}{\partial t} + \underline{v}^*\cdot\nabla\bar{c} = 0 \tag{4-9}$$

subject to the initial condition

$$\bar{c}(\underline{x},0) = C_0(\underline{x}), \tag{4-10}$$

and the Cauchy condition along inflow boundaries

$$\underline{v}\bar{c}\cdot\underline{n} + \alpha(\bar{c}-C) = Q \qquad \text{on } \Gamma \tag{4-11}$$

and along noflow boundaries

$$\underline{v}\bar{c}\cdot\underline{n} = 0 \qquad \text{on } \Gamma \tag{4-12}$$

Conditions along outflow boundaries have no effect on $\bar{c}$ and are thus irrelevant. Clearly, the $\bar{c}$ value of a given fluid particle remains constant as the latter is advected through the flow field. Thus, the "advection problem" defined by Eqs. 4-9 through 4-12 can be solved independently of $\overset{\circ}{c}$.

The residual concentration, $\overset{\circ}{c}$, must satisfy

$$(1+s)\frac{D\overset{\circ}{c}}{Dt} = \nabla\cdot(\underline{\underline{D}}\nabla\overset{\circ}{c}) - f\overset{\circ}{c} + q + \bar{g} \qquad (4\text{-}13)$$

where

$$\bar{g} = \nabla\cdot(\underline{\underline{D}}\nabla\bar{c}) - f\bar{c}$$

subject to the homogeneous initial condition

$$\overset{\circ}{c}(\underline{x},0) = 0 \qquad (4\text{-}14)$$

and the conditions along inflow boundaries

$$(-\underline{\underline{D}}\nabla\overset{\circ}{c} + \underline{v}\overset{\circ}{c})\cdot\underline{n} + \alpha\overset{\circ}{c} = \bar{h} \qquad \text{on } \Gamma \qquad (4\text{-}15)$$

where $\bar{h} = \underline{\underline{D}}\nabla\bar{c}\cdot\underline{n}$, along noflow boundaries

$$-\underline{\underline{D}}\nabla\overset{\circ}{c}\cdot\underline{n} + \alpha(\overset{\circ}{c}-C) = \bar{u} \qquad \text{on } \Gamma \qquad (4\text{-}16)$$

where $\bar{u} = Q - \alpha\bar{c} + \bar{h}$, and along outflow boundaries

$$-\underline{\underline{D}}\nabla\overset{\circ}{c}\cdot\underline{n} = \bar{h} \qquad \text{on } \Gamma \qquad (4\text{-}17)$$

Note that $\bar{g}$, $\bar{h}$, and $\bar{u}$ play the role of prescribed source functions when $\bar{c}$ is known. We will refer to Eqs. 4-13 through 4-17 as the residual "dispersion problem."

We see that the hyperbolic-parabolic advection-dispersion problem defined by Eqs. 4-1 through 4-4 can be formally decoupled into a purely hyperbolic "advection problem" defined in terms of $\bar{c}$, and another predominantly parabolic residual "dispersion problem" defined in terms of $\overset{\circ}{c}$. The approach

is to first solve the advection problem for $\bar{c}$, as the latter is independent of $\mathring{c}$, and then solve the residual dispersion problem for $\mathring{c}$. Another alternative is to solve Eq. 4-6 in its Lagrangian form without decomposing c into $\bar{c}$ and $\mathring{c}$; this is what the single-step reverse particle tracking method does. Our proposed numerical method utilizes both of these alternatives jointly in an adaptive manner.

5. NUMERICAL APPROACH

In Neuman's original paper on this subject (Ref. 1), the one-dimensional advection problem was solved on a fixed space-time grid by the method of characteristics, and the residual one-dimensional dispersion problem was solved on a different fixed space-time grid by finite elements. The use of such conjugate space-time grids required projecting results from one grid to another, which led to some numerical dispersion. Neuman and Sorek (Ref. 65) investigated the possibility of eliminating such numerical dispersion by solving the advection problem with moving particles instead of a fixed grid. Their results were encouraging, but showed slight oscillations. We now know how to eliminate such oscillations, and we have also developed an adaptive scheme that is much more efficient than conventional particle tracking.

Our adaptive method can be described briefly as follows. Suppose that c is known at time t_k, and we wish to compute it at $t_{k+1} = t_k + \Delta t$. First, we set

$$\begin{aligned} \bar{c}(\underline{x},t_k) &\equiv c(\underline{x},t_k) \\ \mathring{c}(\underline{x},t_k) &\equiv 0 \end{aligned} \qquad (5\text{-}1)$$

We then solve the advection problem for $\bar{c}(\underline{x},t_{k+1})$ by using continuous forparticle tracking in the vicinity of steep fronts, and single-step reverse particle tracking away from such fronts. The residual dispersion problem is solved for c, or $\mathring{c}$, by finite elements.

In this report, we develop the finite element equations in terms of c (for a development in terms of $\mathring{c}$, see Ref. 65). Thus, $c(\underline{x},t)$ is approximated by a finite element function, $c^N(\underline{x},t)$, defined as

$$\begin{aligned} c(\underline{x},t) &\approx c^N(\underline{x},t) \\ &= \sum_{n=1}^{N} c_n(t)\, \xi_n(\underline{x}) \end{aligned} \qquad (5\text{-}2)$$

Here N is number of grid points or nodes, c_n is concentration at node n, and ξ_n is a basis function satisfying

$$\xi_n(\underline{x}_m) = \delta_{nm} \tag{5-3}$$

$\underline{x}_m$ being $\underline{x}$ at node m, and δ_{nm} being the kronecker delta (i.e., $\delta_{nm} = 1$ if $n = m$ and $\delta_{nm} = 0$ if $n \neq m$).

5.1 Continuous Forward Particle Tracking

If there is a steep concentration front, the approach is to introduce moving particles at strategic points around the front and continuously track their positions along the pathlines. Any existing particle, p, located at point $\underline{x}_p$ at time t_k, is assigned a $\bar{c}$ value equal to $\bar{c}_p^k = \bar{c}(\underline{x}_p, t_k)$ for the duration of the time interval (t_k, t_{k+1}). By virtue of Eqs. 5-1 and 5-2, we have

$$\bar{c}_p^k = c(\underline{x}_p, t_k)$$

$$\approx \sum_{m=1}^{N} c_m^k \, \xi_m(\underline{x}_p) \tag{5-4}$$

Any new particle, r, introduced at $(\underline{x}_r, t_k)$ is assigned a $\bar{c}$ value equal to $\bar{c}_r^k = \bar{c}(\underline{x}_r, t_k)$. A new particle introduced along an inflow boundary is assigned the $\bar{c}$ value

$$\bar{c}_r^k = \left. \frac{\alpha C + Q}{\underline{v} \cdot \underline{n} + \alpha} \right|_{\underline{x}_r, t_k} \tag{5-5}$$

according to Eq. 4-11 for the duration of the time interval.

At the end of the time step, each particle, p, reaches a new position

$$\underline{x}_p^{k+1} = \underline{x}_p^k + \int_{t_k}^{t_{k+1}} \underline{v}^* \, Dt \tag{5-6}$$

At this stage, there is a need to project $\bar{c}$ onto the nodes, n, of the finite element grid. In the examples shown later, we use bilinear interpolation between particles arranged in a rectangular pattern.

The projected values of $\bar{c}$ are designated by ${}^k c_n$ such that

$$ {}^{k}c_n \equiv \bar{c}(\underline{x}_n, t_{k+1}) \tag{5-7} $$

Clearly, ${}^{k}c_n$ can be viewed as c at t_k of a fictitious moving particle which reaches node n at time t_{k+1}.

5.2 Single-Step Reverse Particle Tracking

In areas where the concentration gradients are mild, ${}^{k}c_n$ is computed by sending a fictitious particle from each node, n, backward to the point

$$ {}^{k}\underline{x}_n \equiv \underline{x}_n - \int_{t_k}^{t_{k+1}} \underline{v}^* \, Dt \tag{5-8} $$

during each time step. This means that a particle leaving ${}^{k}\underline{x}_n$ at t_k will reach the grid point location, $\underline{x}_n$, exactly at t_{k+1}. If the velocity field does not change with time and Δt is fixed, then ${}^{k}\underline{x}_n$ remains constant for each n and needs to be computed only once.

By virtue of Eqs. 5-1 and 5-2, we can express ${}^{k}c_n$ as

$$ \begin{aligned} {}^{k}c_n &\equiv \bar{c}({}^{k}\underline{x}_n, t_k) \\ &= c({}^{k}\underline{x}_n, t_k) \\ &\approx \sum_{m=1}^{N} {}^{k}c_m \, \xi_m({}^{k}\underline{x}_n) \end{aligned} \tag{5-9} $$

This requires much less computer time and storage than continuous forward particle tracking. However, the method cannot be used near sharp fronts because it exhibits numerical dispersion near such fronts.

5.3 Dispersion by Finite Elements

Applying the Galerkin orthogonalization procedure to Eq. 4-6 leads to

$$ \int_R \left[(1+s) \frac{Dc}{Dt} - \nabla \cdot (\underline{D} \nabla c^N) + f c^N - q \right] \xi_n \, dR = 0 \qquad n=1,2,\ldots,N \tag{5-10} $$

where R is the flow region bounded by Γ (for the moment, we will treat the time derivatives as known functions). Application of Green's first identity gives

$$\int_R [(1+s)\frac{Dc}{Dt} + fc^N - q]\,\xi_n\,dR + \int_R \underline{\underline{D}}\nabla c^N \cdot \nabla \xi_n\,dR$$

$$- \int_\Gamma \underline{\underline{D}}\nabla c^N \cdot \underline{n}\,\xi_n\,d\Gamma = 0 \qquad n=1,2,\ldots,N \qquad (5\text{-}11)$$

In what follows, we treat each node of the fixed finite element grid as a moving particle having reached $\underline{x}_n$ at t_{k+1}. This unconventional approach renders the problem purely parabolic. It has been shown by Neuman and Narasimhan (Ref. 73) that for such parabolic problems, there is often an advantage in using a lumped-mass finite element approach which is eqivalent to approximating the first term in Eq. 5-11 by

$$\int_R (1+s)\,\frac{Dc}{Dt}\,\xi_n\,dR \approx \frac{Dc_n}{Dt}\int_R (1+s)\xi_n\,dR \qquad (5\text{-}12)$$

Note that this is analogous to what one does in most conventional finite difference schemes. To approximate the time derivative by finite differences we write

$$\frac{Dc_n}{Dt} \approx \frac{c_n^{k+1} - {}^k c_n}{\Delta t} \qquad (5\text{-}13)$$

Since n is viewed as a particle reaching $\underline{x}_n$ at t_{k+1}, we must use a backward difference scheme.

From Eqs. 4-3 and 4-4, along inflow and noflow boundaries

$$\int_\Gamma \underline{\underline{D}}\nabla c^N \cdot \underline{n}\,\xi_n\,d\Gamma = \int_\Gamma [\underline{v}\cdot\underline{n}c^N + \alpha(c^N - C) - Q]\xi_n\,d\Gamma$$

and along outflow boundaries

$$\int_\Gamma \underline{\underline{D}}\nabla c^N \cdot \underline{n}\,\xi_n\,d\Gamma = 0$$

Substituting these together with Eqs. 5-2, 5-12, and 5-13 into Eq. 5-11 leads to the matrix equation

$$[\underline{\underline{A}} + \underline{\underline{B}} + \underline{\underline{F}} + \frac{1}{\Delta t}(\underline{\underline{W}} + \underline{\underline{S}})]\,\underline{c}^{k+1} = \underline{Q} + \frac{1}{\Delta t}(\underline{\underline{W}} + \underline{\underline{S}})^k \underline{c} \qquad (5\text{-}14)$$

Here $\underline{A}$ is a symmetric positive-semidefinite "dispersion matrix" of order N defined as

$$A_{nm} = \int_R \underline{D}\nabla\xi_n \cdot \nabla\xi_m \, dR \tag{5-15}$$

$\underline{B}$ is a symmetric "boundary matrix" of order N, whose terms are

$$B_{nm} = -\int_\Gamma (\underline{v} \cdot \underline{n} + \alpha) \, \xi_n \, \xi_m \, d\Gamma ; \qquad \alpha < \infty \tag{5-16}$$

if n and m are both on an inflow or noflow boundary, and

$$B_{nm} = 0 \tag{5-17}$$

otherwise. When $\alpha \to \infty$ at $\underline{x}_n$, c_n is known, and B_{nm} is not needed. $\underline{F}$ is a symmetric matrix of order N defined as

$$F_{nm} = \int_R f \, \xi_n \, \xi_m \, dR \tag{5-18}$$

$\underline{W}$ is a diagonal "capacity matrix" of order N,

$$W_{nm} = \delta_{nm} \int_R \xi_n \, dR \tag{5-19}$$

$\underline{S}$ is a diagonal "retardation matrix" whose terms are

$$S_{nm} = \delta_{nm} \int_R s \, \xi_n \, dR \tag{5-20}$$

$\underline{Q}$ is an N-dimensional "source vector" defined as

$$Q_n = \psi_n + \int_R q \, \xi_n \, dR \tag{5-21}$$

where

$$\psi_n = -\int_\Gamma (\alpha C + Q) \, \xi_n \, d\Gamma ; \qquad \alpha < \infty$$

if N is on an inflow or noflow boundary, and

$$\psi_n = 0$$

otherwise. As before, ψ_n is not needed if $\alpha \to \infty$ at n. $\underline{c}^{k+1}$ is the N-dimensional vector of c^{k+1} values, and $^k\underline{c}$ is the corresponding vector of ^kc_n values.

Eq. 5-14 differs from most other finite element, finite difference, or collocation schemes for the advection-dispersion equation in two important ways: 1) It is based on a Lagrangian formulation of the governing equation, involving the unconventional vector $^k\underline{c}$ that is obtained (independently) from a solution of the advection problem, and 2) it involves a symmetric matrix (bracketed term) in front of the unknown vector $\underline{c}^{k+1}$. Clearly, the symmetric nature of the matrix stems from the Lagrangian formulation which has eliminated advection from Eq. 5-14. It provides the advantage of reduced computer storage and time.

Eq. 5-14 can be solved for $\underline{c}^{k+1}$ by point iterative, block iterative (including ADI), or direct methods. We use either Cholesky decomposition or a direct solver due to Duff (Ref. 74). This solver permutes the matrix into block-diagonal form, decomposes it into factors, and solves the problem by a compact variant of Gaussian elimination. The solver decomposes a new matrix having the same sparsity pattern as a previous one by using the same pivotal sequence, which takes much less processing time than the original factorization. This is extremely useful when Δt varies from one step to another, or in nonlinear problems where the matrix components $\underline{A}$, $\underline{B}$, $\underline{F}$, and $\underline{S}$ can also vary.

The final step is to project c^{k+1} onto moving particles if such particles exist in the flow field. Let p be such a particle. Then c_p^{k+1} is computed according to

$$c_p^{k+1} = \bar{c}_p^k + \overset{\circ}{c}^N(\underline{x}_p, t_{k+1})$$

$$= \bar{c}_p^k + \sum_{m=1}^{N} (c_m^{k+1} - {}^kc_m)\, \xi_m(\underline{x}_p) \qquad (5\text{-}22)$$

where $c_m^{k+1} - {}^kc_m$ is equivalent to $\overset{\circ}{c}{}_m^{k+1}$ by virtue of Eq. 5-7. Eq. 5-22 utilizes a finite element interpolation scheme for $\overset{\circ}{c}$ which is similar to that used for c in Eq. 5-2. For the next time step, $\bar{c}_p$ is set equal to the above value of c_p in accordance with Eq. 5-1; this supercedes the use of Eq. 5-4.

5.4 Adaptive Mechanism

In our proposed scheme, forward moving particles are introduced only in the vicinity of sharp fronts and time-varying sources. The term ^kc_n is computed by continuous forward particle tracking if node n is covered by a cloud of

such particles, and by single-step reverse particle tracking otherwise. When a particular front, covered by a cloud of particles, becomes smooth enough due to dispersion, retardation, or decay, the corresponding cloud is eliminated. This results in significant savings of computer time and storage.

One important consideration in developing an adaptive mechanism of this kind is an appropriate criterion for particle elimination. How sharp is sharp, and how flat is flat? How should one decide at what point in time a front becomes smooth enough to justify eliminating the particles?

Our current answer to this question is empirical. We found that the oscillations reported by Neuman and Sorek (Ref. 65) can be eliminated by adopting the following smoothing criterion. Consider a moving particle, p, inside a particular element. Eq. 5-22 provides a c_p^{k+1} value for p. If this value satisfies the criterion

$$\min_n \; c_n^{k+1} \leq c_p^{k+1} \leq \max_n \; c_n^{k+1} \tag{5-23}$$

where $\min_n c_n^{k+1}$ is the minimum c_n^{k+1} value of all nodes n in the element, and $\max_n c_n^{k+1}$ is the corresponding maximum value, then we adopt the c_p^{k+1} value from Eq. 5-22. On the other hand, if Eq. 5-23 is violated, then c_p^{k+1} is redefined according to

$$c_p^{k+1} = \sum_{n=1}^{N} c_m^{k+1} \, \xi_m \, (\underline{x}_p) \tag{5-24}$$

Our experience shows that as long as Eq. 5-23 is violated by any particle in a cloud, the front covered by that cloud is too steep to allow elimination of the particles. On the other hand, when Eq. 5-23 is satisfied by all the particles in a cloud during two or three consecutive time steps, the cloud can be safely eliminated.

6. EXAMPLES

The following five examples show preliminary results obtained with linear chapeau basis functions for one- and two-dimensional dispersion in a uniform steady state velocity field. One-dimensional versions of similar examples were used earlier by Lam (Ref. 27) to show how poorly methods existing at the time worked when there were sharp fronts and high rates of advection.

Example 1 concerns the one-dimensional problem of solving

$$\frac{\partial c}{\partial t} = D_x \frac{\partial^2 c}{\partial x^2} - v_x \frac{\partial c}{\partial x} \qquad \text{on} \quad 0 \leq x \leq x_R \tag{6-1}$$

subject to

$$c(x,0) = 0$$

$$c(0,t) = 1 \tag{6-2}$$

$$c(x_R,t) = 0$$

The physical and grid parameters, in an arbitrary system of consistent units, are $D_x = 0.01$, $v_x = 0.05$, $x_R = 2.5$, and $\Delta x = 0.05$, Δx being the distance between neighboring grid points. The problem is strongly dispersion-dominated with a Peclet number $Pe_x = v_x \Delta x / D_x = 0.25$. One would therefore expect to obtain good results without continuous forward particle tracking, merely by using the single-step reverse particle tracking method. To test this, we introduced a cloud of 20 particles, 2 per element of length Δx, centered about $x = 0$ at $t = 0$ (the cloud initially consisted of 10 particles to the right of $x = 0$, but additional particles were added gradually as the front advanced to the right). Fig. 1 shows the results at $t = 10$ when $\Delta t = t/100$ (Courant number $\alpha_x = v_x \Delta t / \Delta x = 0.10$) and $\Delta t = t/11$ ($\alpha_x = 0.91$). In the first case, the particle cloud was automatically eliminated after 23 time steps, in the second case after 5 time steps. In both cases, the results agree very well with the analytical solution

$$c(x,t) = \frac{1}{2} \operatorname{erfc}\left(\frac{x - v_x t}{\sqrt{4 D_x t}} \right) + \frac{1}{2} \exp\left(\frac{v_x x}{D_x} \right) \operatorname{erfc}\left(\frac{x + v_x t}{\sqrt{4 D_x t}} \right) \tag{6-3}$$

which is valid for $x_R \to \infty$. However, we were able to obtain similar results by not using any forward moving particles at all. This suggests that our empirical criterion for the elimination of particles may be too conservative.

Example 2 is similar to the previous one except that now $D_x = 1.0$, $v_x = 10^4$, $x_R = 1.0$, $\Delta x = 0.02$, and $t = 5 \times 10^{-5}$. The problem is strongly advection-dominated with $Pe_x = v_x \Delta x / D_x = 200$. Fig. 2 shows the results when $\Delta t = t/50$ (Courant number $\alpha_x = 0.5$) and $\Delta t = t/11$ ($\alpha_x = 2.27$). When there are no moving particles, the single-step reverse particle tracking method suffers from numerical dispersion. The amount of this dispersion diminishes as Δt increases. This is expected because numerical smearing occurs due to the smoothing effect of the interpolation formula Eq. 5-9. The smaller the number of time steps, the fewer times this formula is applied, and thus cumulative interpolation error is smaller. This leads to the paradoxical result that instead of converging to the true solution as Δt decreases, the numerical scheme appears to diverge. The scheme is clearly deficient.

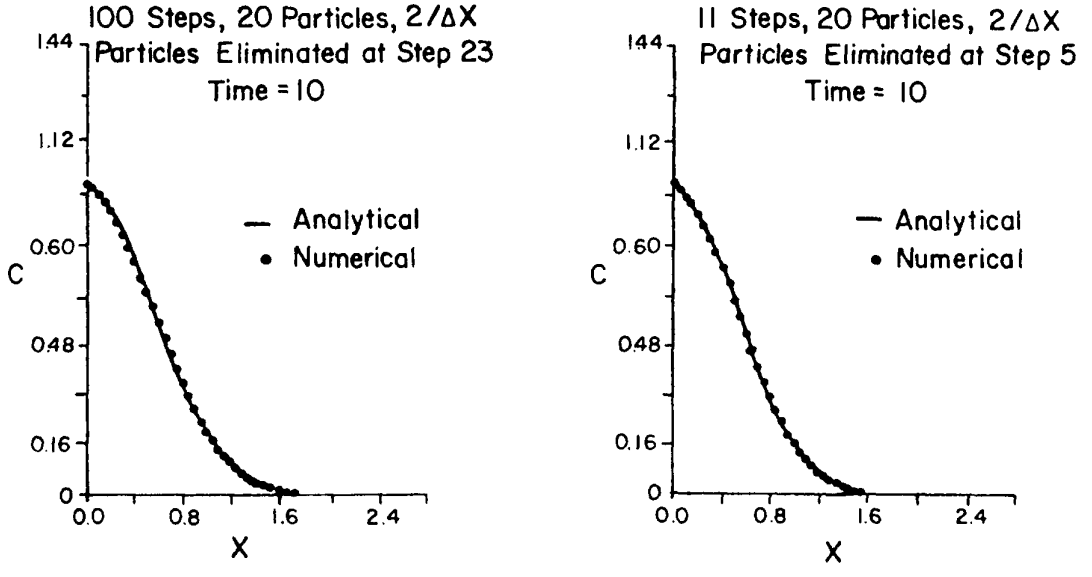

Fig. 1. Results of Example 1.

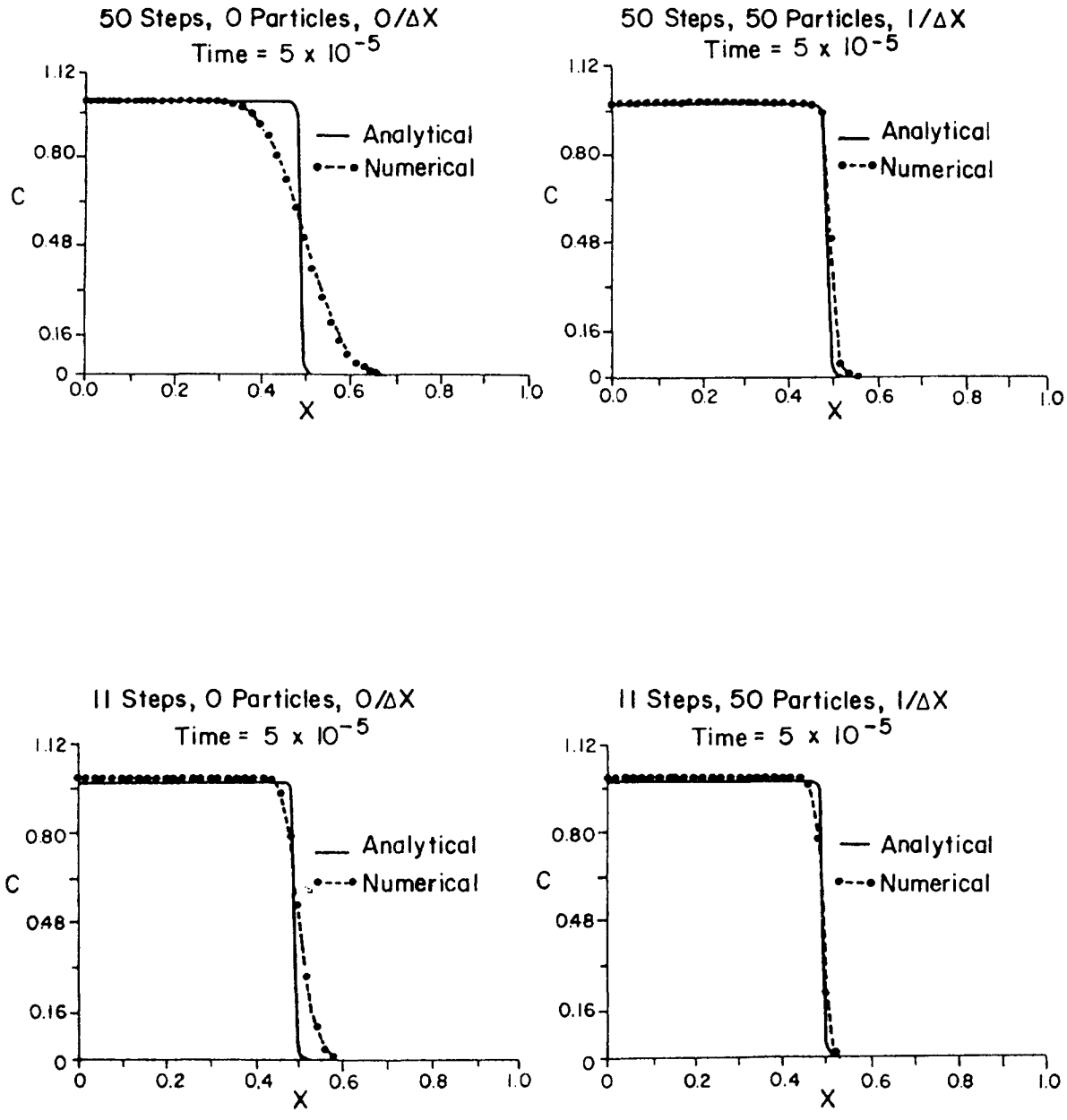

Fig. 2. Results of Example 2.

The picture changes drastically when the front is tracked with a cloud of 50 particles with a density of one particle per element, Δx. As shown in Fig. 2, here the solution is excellent whether the Courant number is less than 1 ($\alpha_x = 0.5$ for 50 time steps) or greater than 1 ($\alpha_x = 2.27$ for 11 time steps). The ability to work with Courant numbers in excess of 1 is an extremely important feature of our proposed method. The reader may do well to compare our results with those of other methods as shown by Lam (Ref. 27) and Varoğlu and Finn (Ref. 42).

The size of the cloud in Example 2 appears to be much larger than necessary; we suspect that 10-20 particles would probably perform as well as 50. Clearly, the question of the relationship between the number of particles in a cloud, their density, and the quality of the solution requires further study.

Note that since the front in Example 2 remains steep at all times of interest, the cloud of particles is not eliminated by the adaptive mechanism.

Example 3 deals with two-dimensional dispersion of a rectangular wave in a uniform velocity field. The governing equation is

$$D_x \frac{\partial^2 c}{\partial x^2} + D_y \frac{\partial^2 c}{\partial y^2} - v_x c - v_y c = \frac{\partial c}{\partial x}\ ; \quad -\infty < x < \infty;\ -\infty < y < \infty \tag{6-4}$$

subject to

$$\begin{aligned} c(x,y,0) &= 1 && \text{when } 0.1 \leq x \leq 0.2,\ -0.01 \leq y \leq 0.01 \\ c(x,y,0) &= 0 && \text{otherwise} \\ c(x_L,y,t) &= c(x_R,y,t) = c(x,y_B,t) = c(x,y_T,t) = 0 \end{aligned} \tag{6-5}$$

When $x_L = y_B = -\infty$ and $x_R = y_T = \infty$, the analytical solution is

$$c(x,y,t) = \frac{1}{4}\left[\operatorname{erf}\left(\frac{a-x+v_x t}{\sqrt{4D_x t}}\right) + \operatorname{erf}\left(\frac{a+x-v_x t}{\sqrt{4D_x t}}\right)\right] \cdot \left[\operatorname{erf}\left(\frac{b-y+v_y t}{\sqrt{4D_y t}}\right) + \operatorname{erf}\left(\frac{b+y-v_y t}{\sqrt{4D_y t}}\right)\right] \tag{6-6}$$

where $a = 0.05$ (half the length of the rectangle in the x direction) and $b = 0.01$ (half its length in the y direction). The results at $t = 6 \times 10^{-4}$ with

$D_x = 1$, $D_y = 0.1$, $v_x = 10^3$, $v_y = 0$, $\Delta x = 0.01$, $\Delta y = 0.004$, $x_L = 0$, $x_R = 1$, $y_B = -0.04$, $y_T = 0.04$, are shown in Fig. 3 for 100 time steps ($\alpha_x = 0.6$) and in Fig. 4 for 11 time steps ($\alpha_x = 5.45$). The left hand side of each figure corresponds to y = 0, the right hand side to x = 0.75, the position of the peak. The Peclet numbers are $Pe_x = v_x\Delta x/D_x = 10$ and $Pe_y = v_y\Delta y/D_y = 0$.

A comparison of Figs. 3 and 4 shows that if there are no moving particles, the solution suffers from numerical dispersion when Δt is small (100 time steps), but such dispersion disappears when Δt becomes large (11 time steps). This paradoxical phenomenon is similar to that observed in Example 2. Here, however, the solution is further afflicted by a clipping of the peak which does not disappear entirely even when Δt is large.

When the propagating rectangular wave is covered by a cloud of 80 x 60 moving particles, numerical dispersion disappears completely. Clipping occurs when Δt is large, but tends to disappear as Δt diminishes. This may show that the current numerical solution (with moving particles) has a convergence property which was lacking in the previous solution (without such particles).

Since there exists a sharp peak, the particle cloud was not eliminated by the program but persisted throughout the time of interest. Results obtained for an identical one-dimensional problem by other methods can be found in Lam (Ref. 27) and Varoğlu and Finn (Ref. 41).

Example 4 differs from Example 3 in that the velocity in the y-direction is no longer zero. Instead, $v_y = 33.33$ so that $Pe_y = v_y\Delta y/D_y = 1.33$ and advection takes place at an angle to the grid lines. In addition, the unit step of concentration is now placed at $0.01 \leq y \leq 0.03$ instead of $-0.01 \leq y \leq 0.01$ as in Example 3.

The results at $t = 6 \times 10^{-4}$ are shown in Fig. 5 for 30 time steps ($\alpha_x = v_x\Delta t/\Delta x = 2$ and $\alpha_y = v_y\Delta t/\Delta y = 0.17$) and in Fig. 6 for 11 time steps ($\alpha_x = 5.45$ and $\alpha_y = 0.45$). The left-hand side of each figure corresponds to y = 0.04, the right-hand side to x = 0.75, the position of the peak. As before, the solution suffers from inaccuracies in the absence of moving particles. Contrary to the previous example, however, there is no improvement as Δt increases from 0.0006/30 to 0.0006/11.

When the propagating rectangular wave is covered by a cloud of 80 x 60 moving particles, the solution remains unsatisfactory if Δt is large (11 time steps), but becomes virtually perfect as Δt diminishes (30 time steps).

Example 5 deals with the pure advection of a rectangular wave identical to that in Example 4. The problem is described by Eqs. 6-4 and 6-5 (except that $c(x,y,0) = 1$ when $0.01 \leq y \leq 0.03$ instead of $-0.01 \leq y \leq 0.01$) with $D_x = D_y = 0$ so that $Pe_x = Pe_y = \infty$. All other parameters are as in Example 4. Fig. 7 shows the results at t = 0.0006 using 11 time steps ($\alpha_x = 5.45$ and $\alpha_y = 0.45$), and Fig. 8 shows what happens at t = 0.0006 when 100 time steps are used ($\alpha_x = 0.6$ and $\alpha_y = 0.05$). As expected, the single-step reverse

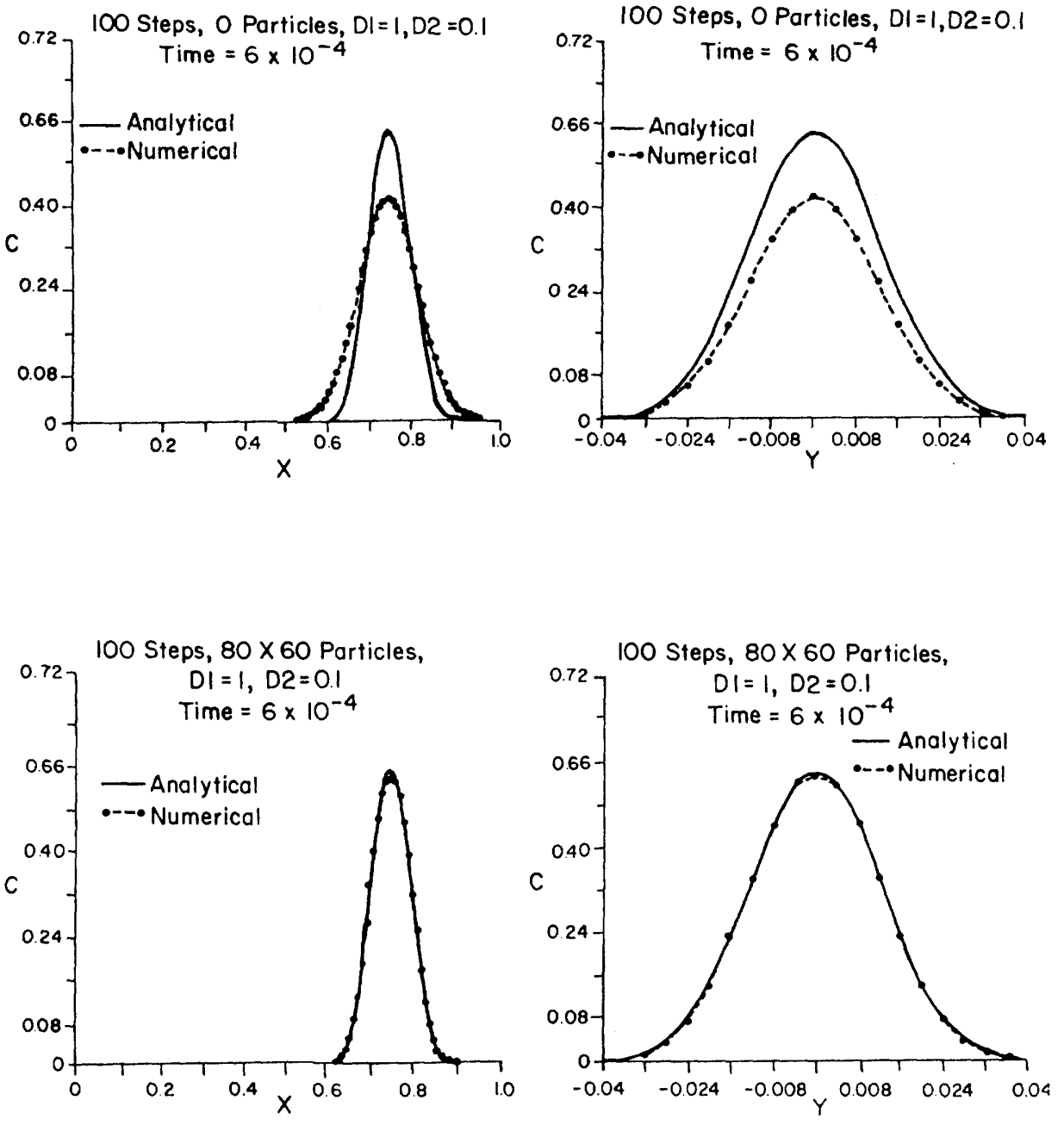

Fig. 3. Results of Example 3 with 100 time steps.

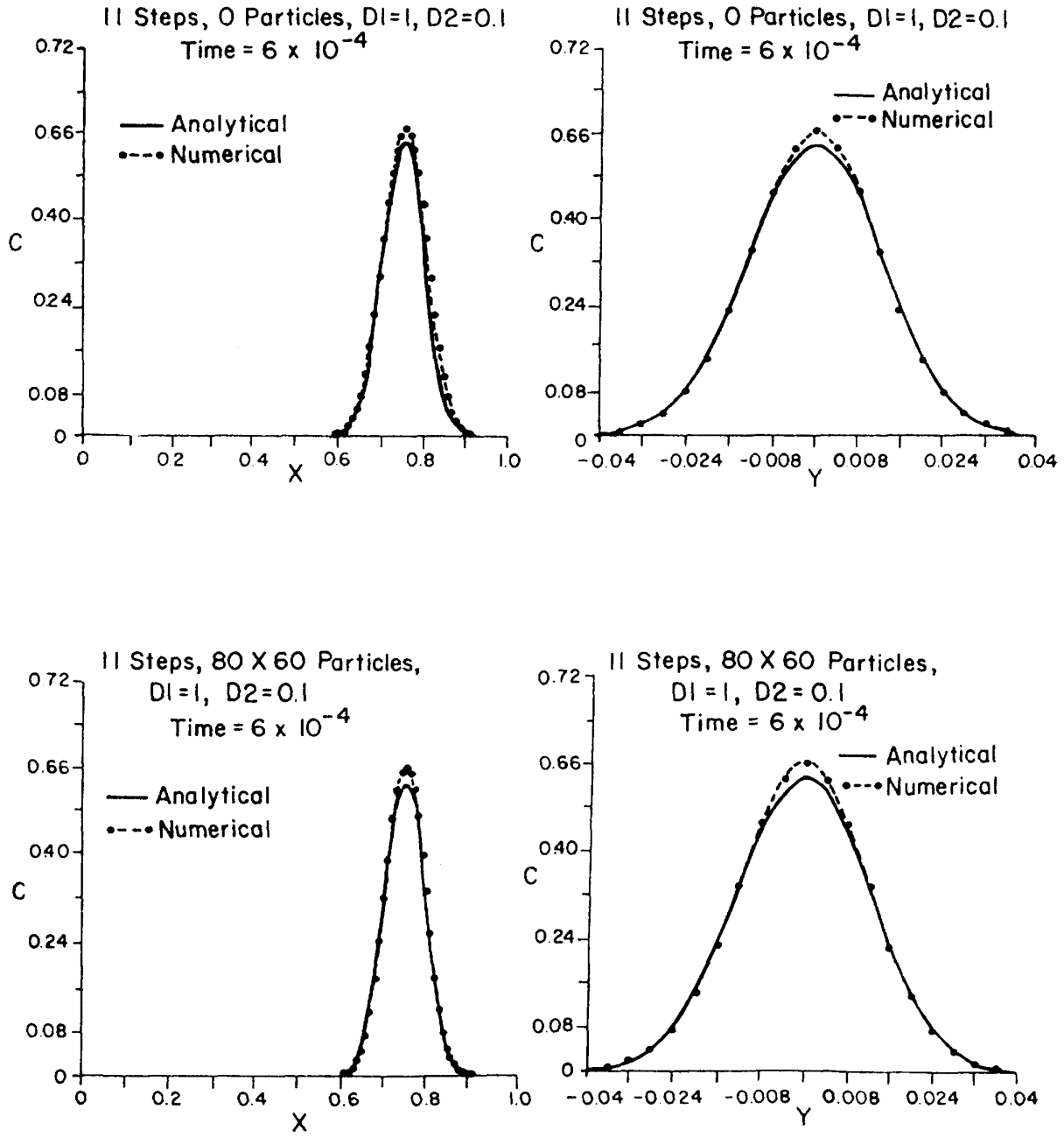

Fig. 4. Results of Example 3 with 11 time steps.

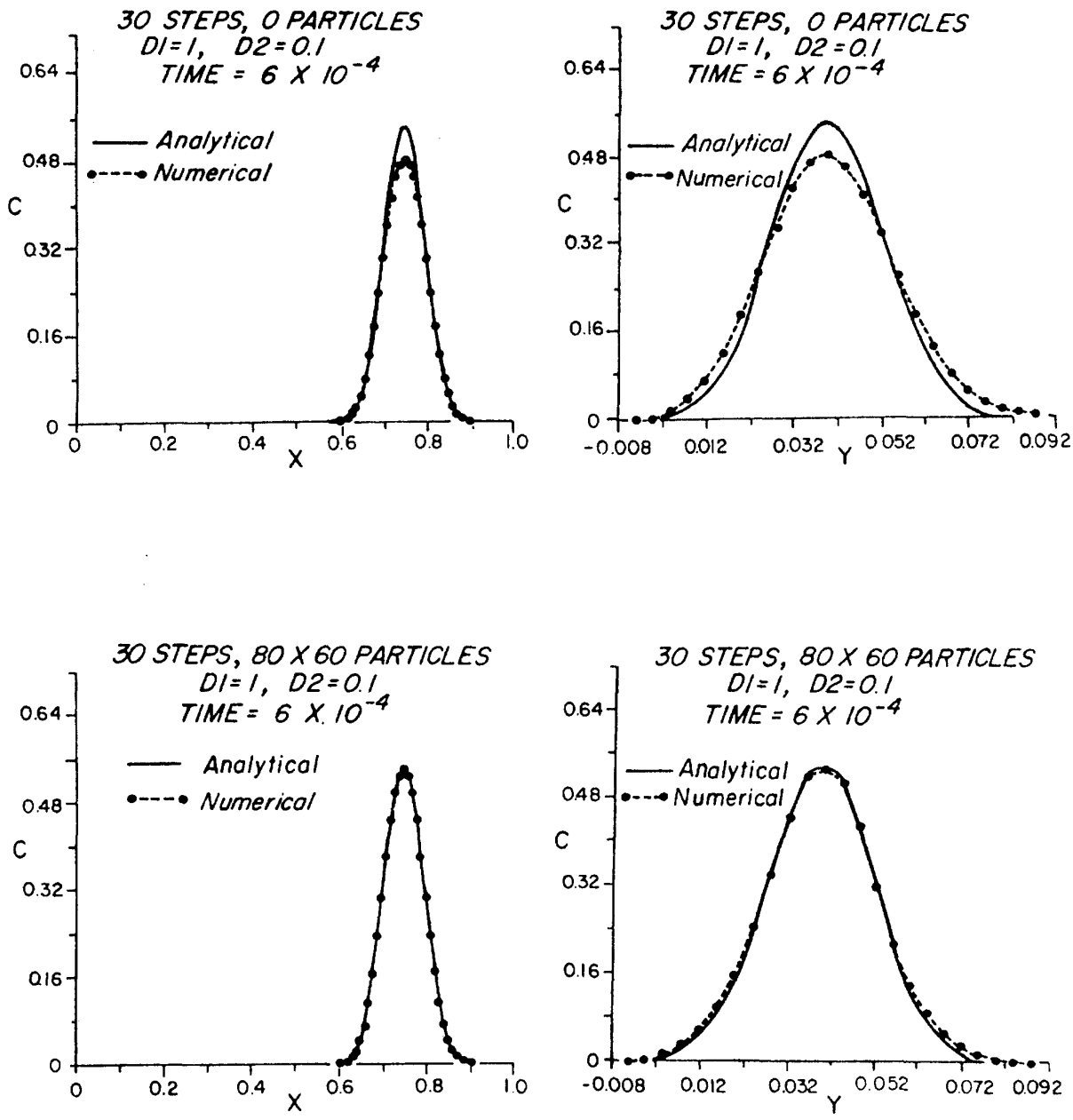

Fig. 5. Results of Example 4 with 30 time steps.

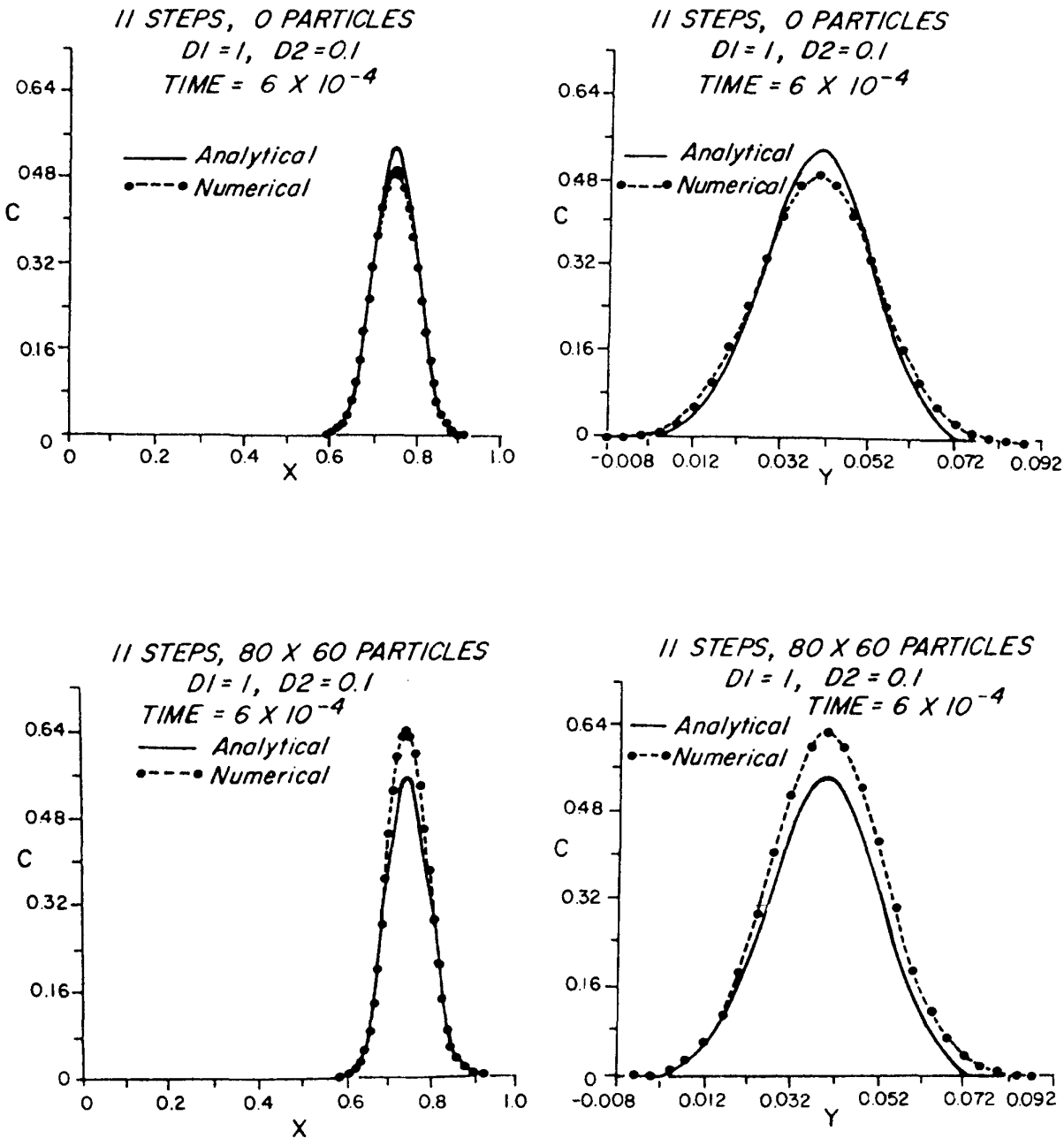

Fig. 6. Results of Example 4 with 11 time steps.

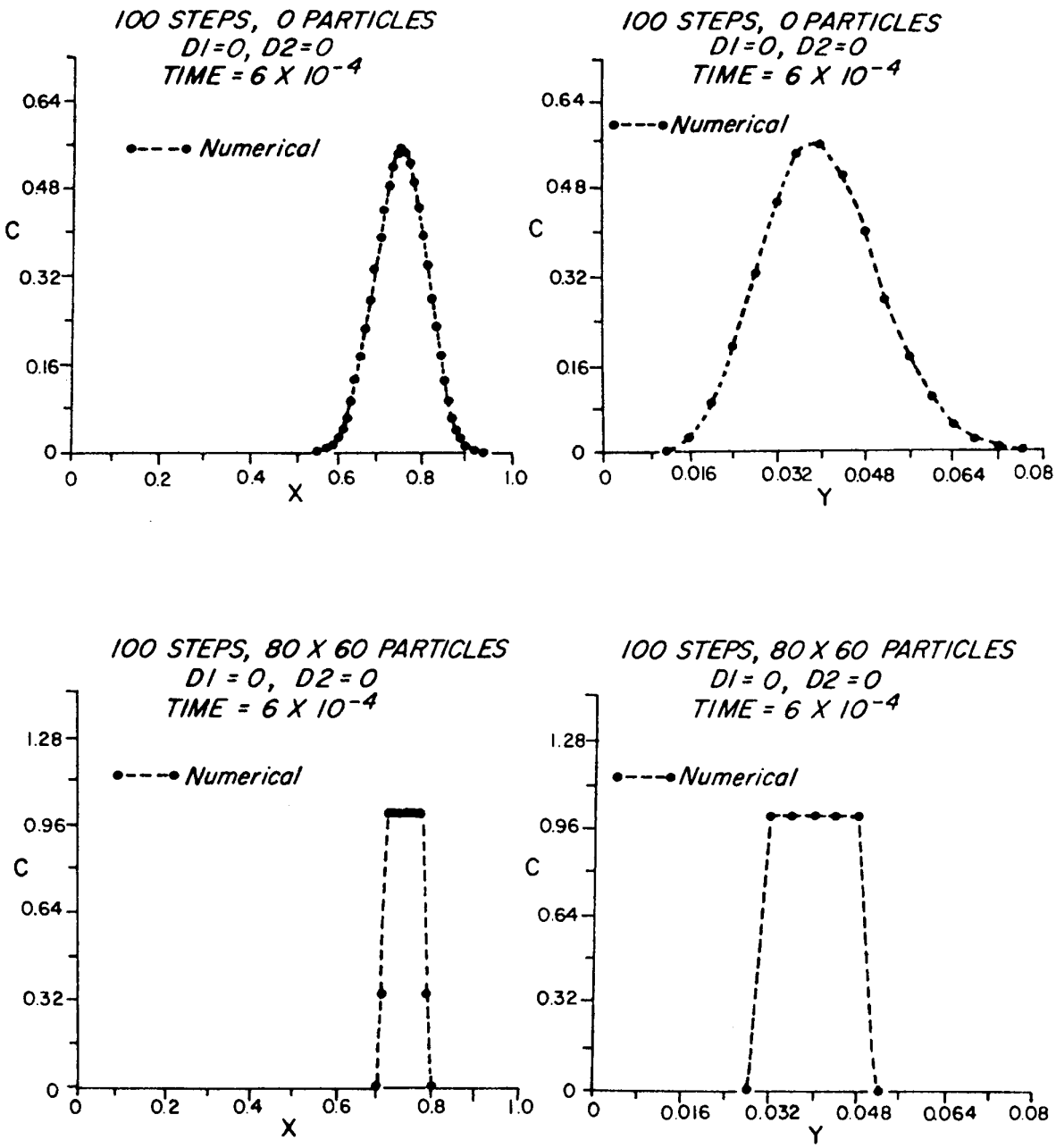

Fig. 7. Results of Example 5 with 100 time steps.

particle tracking method without moving particles suffers from numerical dispersion and clipping. When a cloud of 80 x 60 moving particles is allowed to hover over the front, the solution is virtually perfect whether the Courant number is less than 1 (α_x = 0.6 with 100 time steps) or greater than 1 (α_x = 5.45 with 11 time steps). The reader is urged to compare our results with those of Lam (Ref. 27) and Varoğlu and Finn (Refs. 41,42) for the equivalent one-dimensional case.

7. CONCLUSIONS

The following conclusions can be drawn from our study:

1. The advection-dispersion equation, together with the associated initial and boundary conditions, can be formally decomposed into two problems, one involving pure advection, the other involving primarily dispersion, in a manner which does not leave room for ambiguity. The advection problem can be solved independently at each time step by an adaptive combination of two methods: continuous forward particle tracking and single-step reverse particle tracking. The residual dispersion problem can be treated by a Lagrangian version of finite elements on a fixed grid.

2. Our adaptive method consists of tracking steep concentration fronts with the aid of forward-moving particles, while using the more economical single-step reverse particle tracking method away from such fronts. When the front flattens, the moving particles are eliminated. The use of moving particles around steep fronts is necessary to avoid numerical dispersion and clipping or exaggeration of concentration peaks. However, such particles may consume significant computer storage and time. The proposed adaptive scheme maximizes computational efficiency by eliminating moving particles when and where these are not needed.

3. Our unconventional Lagrangian formulation of the finite element equations eliminates advective terms so that these equations take on a purely parabolic appearance. This has two advantages: First, all finite element matrices are symmetric, and second, one is justified in using mass-lumping which further reduces matrices in front of time derivatives to a diagonal form. The result is an increase in accuracy and computational efficiency.

4. Preliminary results for two-dimensional dispersion in a uniform velocity field suggest that our adaptive method is capable of handling the entire range of Peclet numbers from zero to infinity, and large time steps with Courant numbers well in excess of 1.

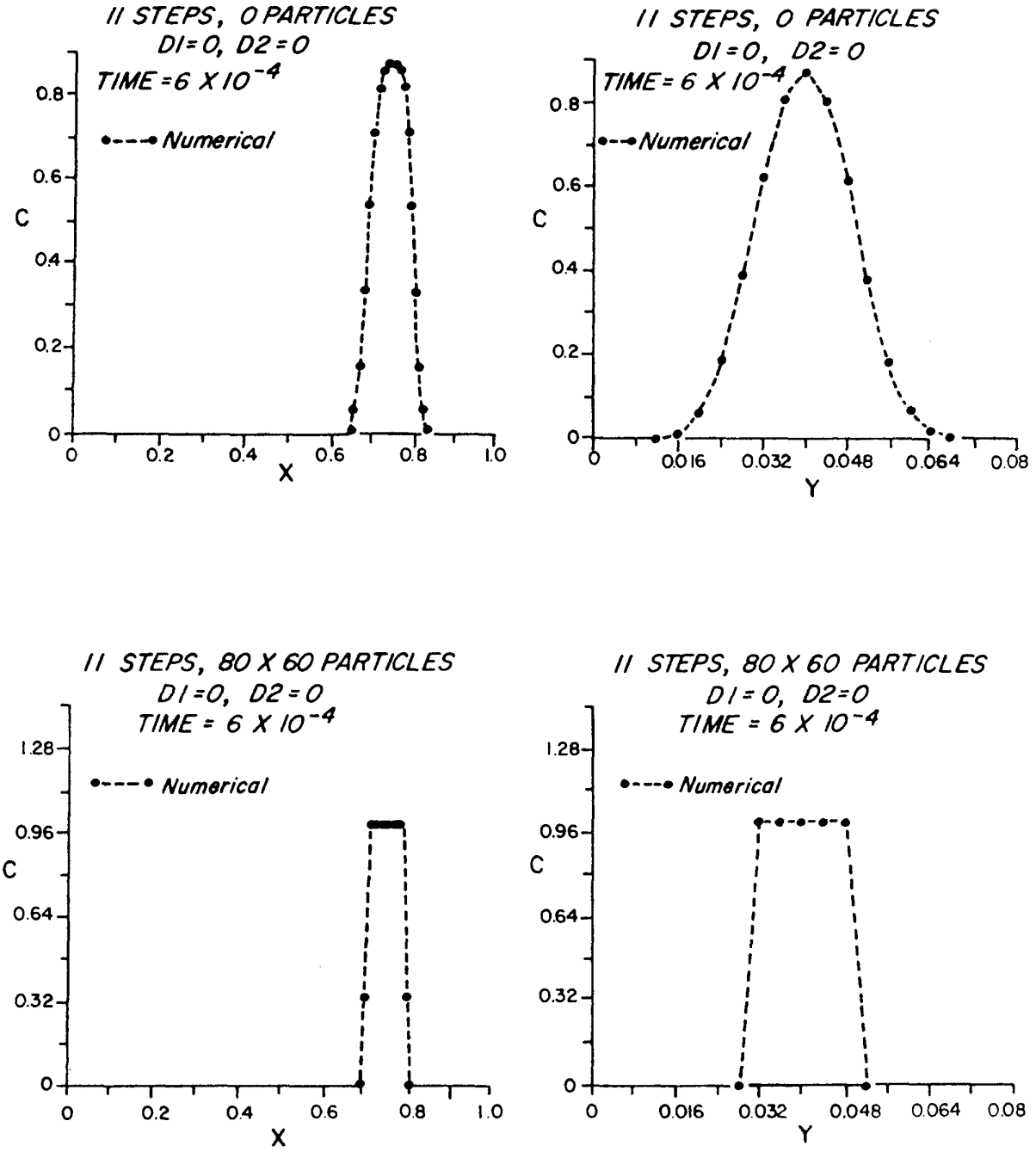

Fig. 8. Results of Example 5 with 11 time steps.

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