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## A Lagrangian-Eulerian Finite Element Method with Adaptive Gridding for Advection-Dispersion Problems

Y. Ijiri and K. Karasaki

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*Yuji Ijiri and Kenzi Karasaki*

Earth Sciences Division
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

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# A Lagrangian-Eulerian Finite Element Method with Adaptive Gridding for Advection-Dispersion Problems

YUJI IJIRI[1] AND KENZI KARASAKI

Earth Sciences Division, Lawrence Berkeley Laboratory
University of California, Berkeley, California 94720

ABSTRACT

In the present paper, a Lagrangian-Eulerian finite element method with adaptive gridding for solving advection-dispersion equations is described. The code creates new grid points in the vicinity of sharp fronts at every time step in order to reduce numerical dispersion. The code yields quite accurate solutions for a wide range of mesh Peclet numbers and for mesh Courant numbers well in excess of 1.

## INTRODUCTION

The advection-dispersion equation used for simulating subsurface transport of solutes has been solved by a number of numerical methods including Eulerian, Lagrangian and Lagrangian-Eulerian methods. In recent years, many attempts have been made to eliminate numerical oscillation and dispersion, which are especially troublesome for advection-dominated problems. The mixed Lagrangian-Eulerian methods have been gaining popularity for solving these problems.

[1]In the mixed Lagrangian-Eulerian methods, the advection-dispersion equation is decomposed into two parts, one controlled by pure advection and the other by dispersion (Neuman, 1981,1984). The advected concentration profiles are calculated by Lagrangian approaches such as particle tracking methods, whereas the dispersed concentration profiles are numerically solved by conventional techniques such as the finite difference method or finite element method on fixed Eulerian grids.

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[1] Now at Taisei Corporation, Technology Research Center, 344-1 Nasemachi, Totsukaku, Yokohama 245, Japan.

Neuman (1984) proposed an adaptive scheme for calculating the advected profile. In his paper, continuous forward particle tracking is used for nodes in the vicinity of sharp fronts and single-step reverse particle tracking is used for nodes away from sharp fronts. However, his method still suffers from some numerical dispersion due to the interpolation scheme used in the tracking methods. Furthermore, the accuracy of the results is highly dependent on the number of particles introduced in the model.

The interpolation scheme of Neuman (1984) was improved by Cady and Neuman (1988). In their scheme, the fixed grid is covered by a cloud of front-tracking particles, the concentration at the grid is calculated from the concentrations of the cloud particles by triangulating these cloud particles according to the algorithm of Sloan and Houlsby (1984) and then the residual dispersion finite element equations are solved on this local grid using linear functions. They noted that their approach is based on a mesh refinement idea.

Another mesh refinement approach with a Lagrangian-Eulerian method has been developed by Yeh (1990). His approach successfully reduces numerical dispersion by zooming the sharp-front elements in which the gradients of concentration are steep, and activating hidden fine-mesh nodes in the elements.

Karasaki (1987,1988) developed a numerical code that employs a mixed Lagrangian-Eulerian scheme with adaptive gridding, which is called TRINET, for three-dimensional fracture networks of channels. This approach avoids numerical dispersion by creating new Eulerian grid points instead of interpolating the advected profile back to the fixed Eulerian grid. Another important feature of his approach is that he used tracking methods not for particles but for nodes. Therefore, the number of particle introduced in the model is not an issue.

In the present paper, the scheme used in TRINET is extended and applied to a two-dimensional porous medium model, TRIPOR. In addition to the ability to handle a two-dimensional continuous medium, the main advantage of TRIPOR is its capability to create new nodes anywhere in a two-dimensional domain while TRINET creates new nodes only along existing channels. The present paper describes the numerical approach and some applications for one- and two-dimensional problems in order to demonstrate the capability of the method. Comparing results of the preliminary studies against analytical solutions suggests that the present method gives accurate results for a wide range of Peclet numbers and for Courant numbers well in excess of 1.

## NUMERICAL APPROACH

The flow field is first solved by a simple Galerkin finite element method in order to calculate the velocity profile for the entire domain. Since linear shape functions are currently used to calculate the flow field, the velocity is assumed to be uniform within a given element. The code then solves the solute transport problem expressed by the advection-dispersion equation written as

$$\frac{\partial c}{\partial t} = \nabla\,(D \cdot \nabla c \; - vc\,) + q \tag{1}$$

where $c$ is solute concentration, $D$ is dispersion coefficient, $v$ is pore water velocity, $q$ is a source term and $\nabla$ is the gradient operator. Since the equation is decomposed into two parts as mentioned earlier, advection and dispersion problems are calculated separately. The advection part is solved by tracking methods and the dispersion part is solved by a Galerkin finite element method with fixed Eulerian grids. Triangular elements are used for finite element discretization in TRIPOR.

### *Tracking Methods for Advection*

The tracking methods used in this approach are done in the same manner as described in Neuman (1984) except that they are applied not to particles but to nodes. Therefore, no particles are introduced in the model. First, backward tracking is applied to obtain an advected concentration for all nodes (Figure 1(a)). The advected concentration of node $j$ at time $t+\Delta t$, $\bar{c}_j^{\,t+\Delta t}$, is given by that of the point $x_j^*$, which is tracked backward along the streamline from node $j$.

$$x_j^* = x_j - \int_t^{t+\Delta t} v \, \mathrm{d}t \qquad\qquad j=1,2,\cdots,N \tag{2}$$

$$\bar{c}_j^{\,t+\Delta t} = \bar{c}\,(x_j, t+\Delta t) = c\,(x_j^*, t\,) \tag{3}$$

where $x_j$ is the location of node $j$, $c\,(x_j^*, t\,)$ is the concentration of $x_j^*$ at time $t$, $\Delta t$ is time step size and $N$ is the number of nodes.

If the tracked point, $x_j^*$, does not correspond to a fixed node, $\bar{c}_j^{\,t+\Delta t}$ is calculated by a finite element interpolation scheme written as

$$\bar{c}_j^{\,t+\Delta t} = \sum_{m=1}^{3} c\,(x_m, t\,)\,\phi_m(x_j^*) \tag{4}$$

where $\phi_m(x_j^*)$ is the basis function evaluated at $x_j^*$ and $x_m$ denotes the vertex of the triangular element surrounding $x_j^*$.

Second, forward tracking is used for nodes where concentration gradient is greater than a user-defined tolerance, or for nodes defined by the user as moving nodes. The node $j$ is tracked forward along the streamline to the point $x_j'$, and the concentration of the point at time $t+\Delta t$, $\mathring{c}_j^{\,t+\Delta t}$, is given by that of node $j$ at time $t$.

$$x_j' = x_j + \int_t^{t+\Delta t} v \, \mathrm{d}t \qquad j=1,2,\cdots,N \tag{5}$$

$$\mathring{c}_j^{\,t+\Delta t} = \mathring{c}\,(x_j', t+\Delta t) = c\,(x_j, t) \tag{6}$$

If the tracked point, $x_j'$, does not correspond to a fixed node, a new node is created at the point as shown in Figure 1(b). In this manner, sharp fronts are kept at exact positions during the simulation. If the sharp front has passed through the area, the created nodes in the area are not necessary and are eliminated.

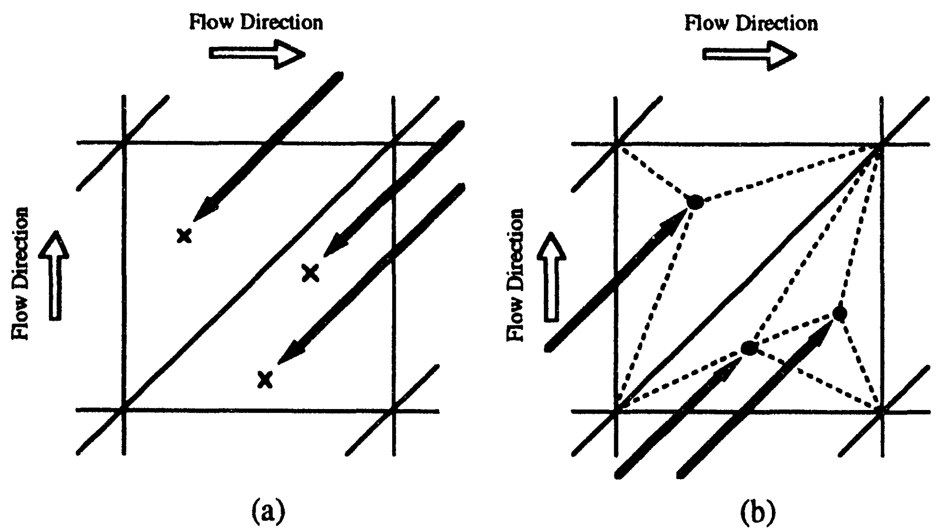



Figure 1. Tracking methods in TRIPOR: (a) backward tracking method, (b) forward tracking method: Cross denotes the point tracked backward. Solid circle and dotted line denote the new node and element, respectively, created by forward tracking method.

*Finite Element Method for Dispersion*

As a Galerkin finite element method is used for discretization in space, the dispersion part of equation (1) can be written in matrix form as

$$[R]\left\{\frac{\partial c}{\partial t}\right\} + [P]\{c\} = \{F\} \tag{7}$$

$[R]$, $[P]$ and $\{F\}$ are given by

$$R_{ij} = \sum_{e=1}^{N} \int_{V^e} \phi_i^e \, \phi_j^e \, dV^e \tag{8}$$

$$P_{ij} = \sum_{e=1}^{N} \int_{V^e} (\nabla \phi_i^e) \cdot D \cdot (\nabla \phi_j^e) \, dV^e \tag{9}$$

$$F_i = \sum_{e=1}^{M} \int_{\Gamma^e} \phi_i^e \, \boldsymbol{n} \cdot [D \cdot (\nabla c)] \, d\Gamma^e \tag{10}$$

where $\phi_i^e$ is the basis function of element $e$ associated with node $i$, $V^e$ is the region of the element, $N$ is the set of elements connected to side $i$-$j$, $\Gamma^e$ is the boundary of element $e$, $M$ is the set of boundaries connected to node $i$ and $\boldsymbol{n}$ is the unit vector normal to $\Gamma^e$ and pointing outward. As a finite difference approximation is used for the time derivative, equation (7) can be written as

$$\left(\frac{R_{ij}}{\Delta t} + \theta P_{ij}\right) c_j^{t+\Delta t} = \left[\frac{R_{ij}}{\Delta t} - (1-\theta) P_{ij}\right] c_j^t + F_i \tag{11}$$

where $c_j^{t+\Delta t}$ and $c_j^t$ are the concentrations of node $j$ at time $t+\Delta t$ and $t$, respectively and $\theta$ is the weighting function for time and is 2/3 in this paper.

*The Complete Mixing Method in TRINET*

Here, we briefly describe the complete mixing method which is currently assumed at intersections of channels in TRINET. All the fixed nodes are tracked backward for $\Delta t$ along the possible channels as shown in Figure 2(a). The nodes in the vicinity of sharp fronts are also tracked forward for $\Delta t$ along the possible channels as shown in Figure 2(b). In these procedures, if the grid is tracked more than one channel, the concentration at intersections are calculated by the complete mixing method. In the method, the concentrations in downstream channels, $c_d$, are given by

$$c_d = \sum_{i=1}^{I} c_u q_u \Big/ \sum_{j=1}^{J} q_d \quad (12)$$

where $q$ is flux and subscripts $u$ and $d$ denote upstream and downstream of intersection, respectively. Therefore, the concentration of a fixed node is calculated from the concentrations of upstream points tracked backward by applying equation (12) to each intersection. In the forward tracking method, the concentrations of created points are calculated in the same manner. The complete mixing method is also used in TRIPOR if flow is converging into the same node from more than one position.

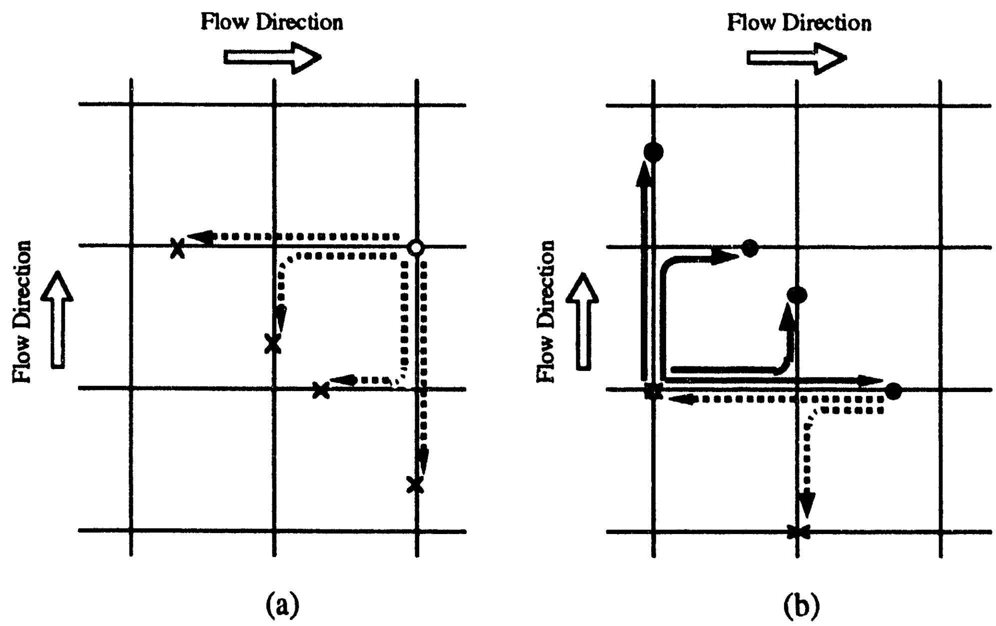



Figure 2. Tracking methods in TRINET: (a) backward tracking method, (b) forward tracking method: Open circle denotes the node being tracked. Cross denotes the point tracked backward. Solid circle denotes the new node created by forward tracking method.

## APPLICATIONS

In the following preliminary studies, TRINET is used to model a porous medium by setting appropriate value of apertures for channels in a lattice configuration.

### *One-Dimensional Problem*

The one-dimensional problem concerns the solution of the following advection-dispersion equation in a uniform velocity field.

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - v\frac{\partial c}{\partial x} \qquad 0 \le x < \infty \tag{13}$$

subject to

$$c(x, 0) = 0 \qquad 0 \le x < \infty$$

$$c(0, t) = 1 \qquad t > 0$$

$$c(x, t) \to 0 \qquad t > 0, x \to \infty$$

The analytical solution is given by Carslaw and Jaeger (1946) and can be written as

$$c(x, t) = \frac{1}{2}\,\mathrm{erfc}\left(\frac{x-vt}{\sqrt{4Dt}}\right) + \frac{1}{2}\exp\left(\frac{vx}{D}\right)\mathrm{erfc}\left(\frac{x+vt}{\sqrt{4Dt}}\right) \tag{14}$$

First, we solve the problem using a fine grid system [$\Delta x$=0.01($0 \le x \le 1$)]. Figure 3 and 4 show the results of our methods at $t$=50 for case A ($D=10^{-5}$, $v=10^{-2}$, $\Delta t$=5, Peclet number:$Pe=v\Delta x/D=10$, Courant number:$Cr=v\Delta t/\Delta x=5$) and case B ($D=10^{-6}$, $v=10^{-2}$, $\Delta t$=5, $Pe$=100, $Cr$=5), respectively. In both cases, no nodes are defined as moving nodes. As can be seen in these figures, the results of both TRINET and TRIPOR agree very well with the analytical solution for a wide range of Peclet numbers and for Courant numbers well in excess of 1.

In order to demonstrate the capability of our methods, an irregular grid system is also used for solving this problem (case C). In this grid system, only the vicinity of the concentration boundary is discretized [$\Delta x$=0.01($0 \le x \le 0.2$), no discretization for $0.2 < x < 1$], and the nodes for $0 \le x \le 0.2$ are defined as moving nodes. The parameters used here are the same as in case A except $Pe$ and $Cr$. The results of TRIPOR at $t$=50 are shown in Figure 5. Although no nodes are initially set for $0.2 < x < 1$, the code yields quite accurate results by creating new nodes in the vicinity of the concentration front. This result suggests that hardly any attention has to be paid to discretizing the domain away from the concentration boundary.

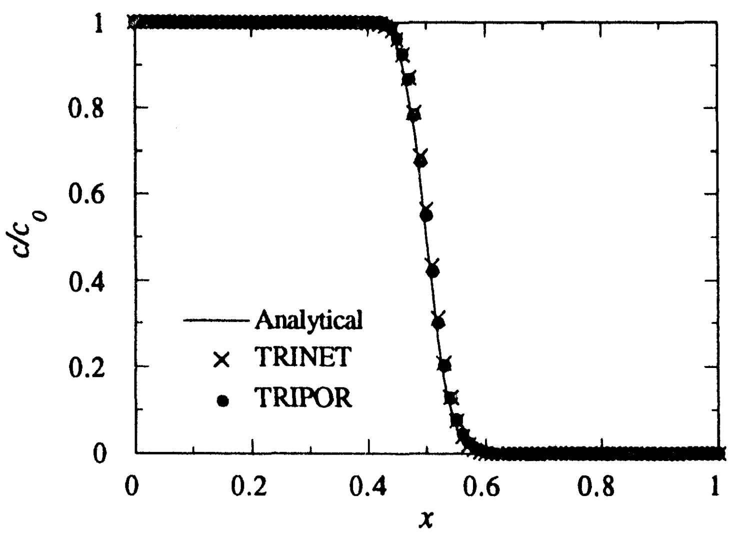



Figure 3. Results obtained with TRINET and TRIPOR, and analytical solution for one-dimensional problem at $t$=50 for case A ($Pe$=10, $Cr$=5).

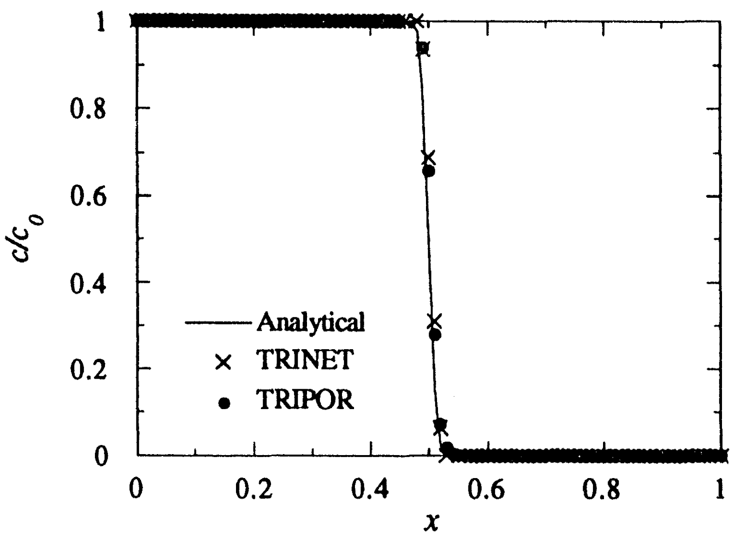



Figure 4. Results obtained with TRINET and TRIPOR, and analytical solution for one-dimensional problem at $t$=50 for case B ($Pe$=100, $Cr$=5).

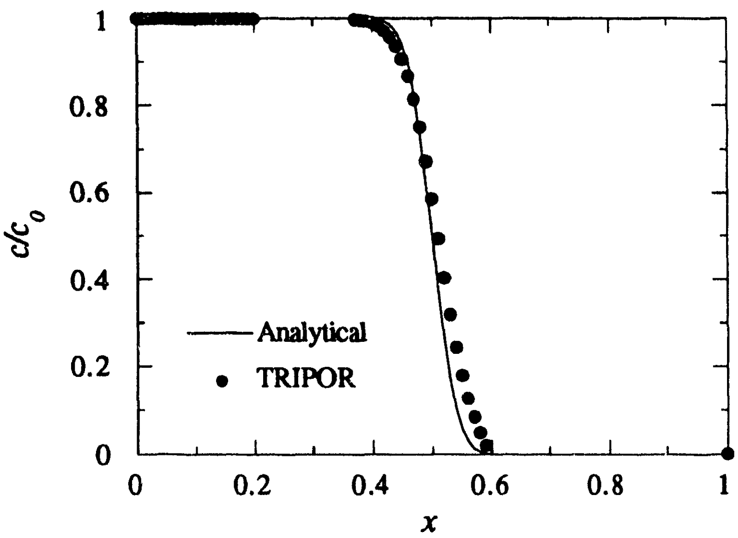



Figure 5. Results obtained with TRIPOR and analytical solution for one-dimensional problem at $t$=50 for case C [$\Delta x$=0.01 ($0 \leq x \leq 0.2$), no grid for $0.2 < x < 1$].

*Two-Dimensional Problem*

The two-dimensional problem concerns the solution of the advection-dispersion equation in a uniform velocity field, which is written as

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

subject to the following initial and boundary conditions

$$c\,(0, y, t) = 1 \qquad -a \leq y \leq a$$

$$c\,(0, y, t) = 0 \qquad y < -a, \; y > a$$

$$\lim_{y \to \pm\infty} \frac{\partial c}{\partial y} = 0, \quad \lim_{x \to \infty} \frac{\partial c}{\partial x} = 0$$

where $D_L$ and $D_T$ are longitudinal and transverse dispersion coefficient, respectively, and $a$ is half length of a line source. The direction of flow is along the $x$-axis. The analytical solution of this problem is given by Javandel et al. (1984) and can be written as

$$c(x, y, t) = \frac{x}{4\sqrt{\pi D_L}} \exp\left(\frac{vx}{2D_L}\right) \int_0^t \exp\left[-\frac{v^2\tau}{4D_L} - \frac{x^2}{4D_L\tau}\right]\tau^{-3/2}$$
$$\cdot \left[\mathrm{erf}\left(\frac{a-y}{2\sqrt{D_T\tau}}\right) + \mathrm{erf}\left(\frac{a+y}{2\sqrt{D_T\tau}}\right)\right] d\tau \qquad (16)$$

A schematic view of this problem is shown in Figure 6. The parameters used in this problem are $D_L=10^{-2}$, $D_T=2.5\times10^{-3}$, $v=0.1$ and $a=0.5$. Two cases using different grid systems are analyzed. The geometric parameters for case D are $\Delta x=0.2$, $\Delta y=0.1$, $\Delta t=2(Pe=2, Cr=2)$ and those for case E are $\Delta x=0.5$, $\Delta y=0.1$, $\Delta t=5(Pe=5, Cr=1)$. The concentration distribution obtained with TRIPOR for case D, which is almost identical to that of the analytical solution, is shown in Figure 7. The concentration profiles obtained with TRINET and TRIPOR at different coordinates are shown in Figure 8. Although a smaller Peclet number (case D) yields better results, the results of all cases agree favorably well with the analytical solution.

Because the domain is discretized along the flow direction, new nodes are created along elements in TRINET and along the sides of elements in TRIPOR. Therefore, not much difference is seen between the results of the two codes. Further study is needed where the flow direction is variable in space to demonstrate the advantage of TRIPOR over TRINET for two-dimensional problems.

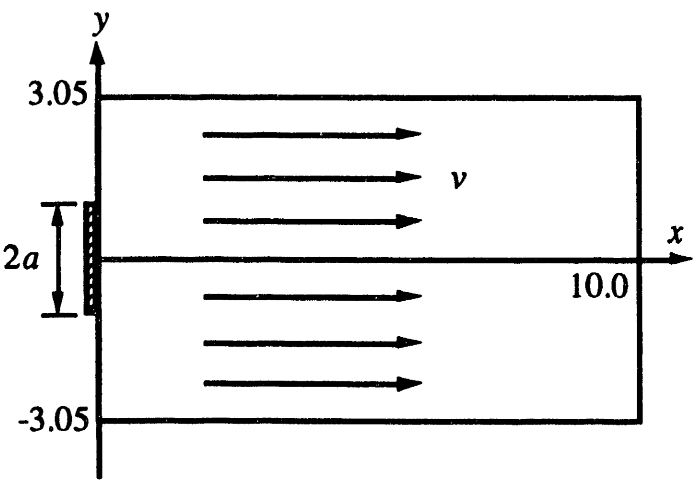



Figure 6. A schematic view of the two-dimensional model.

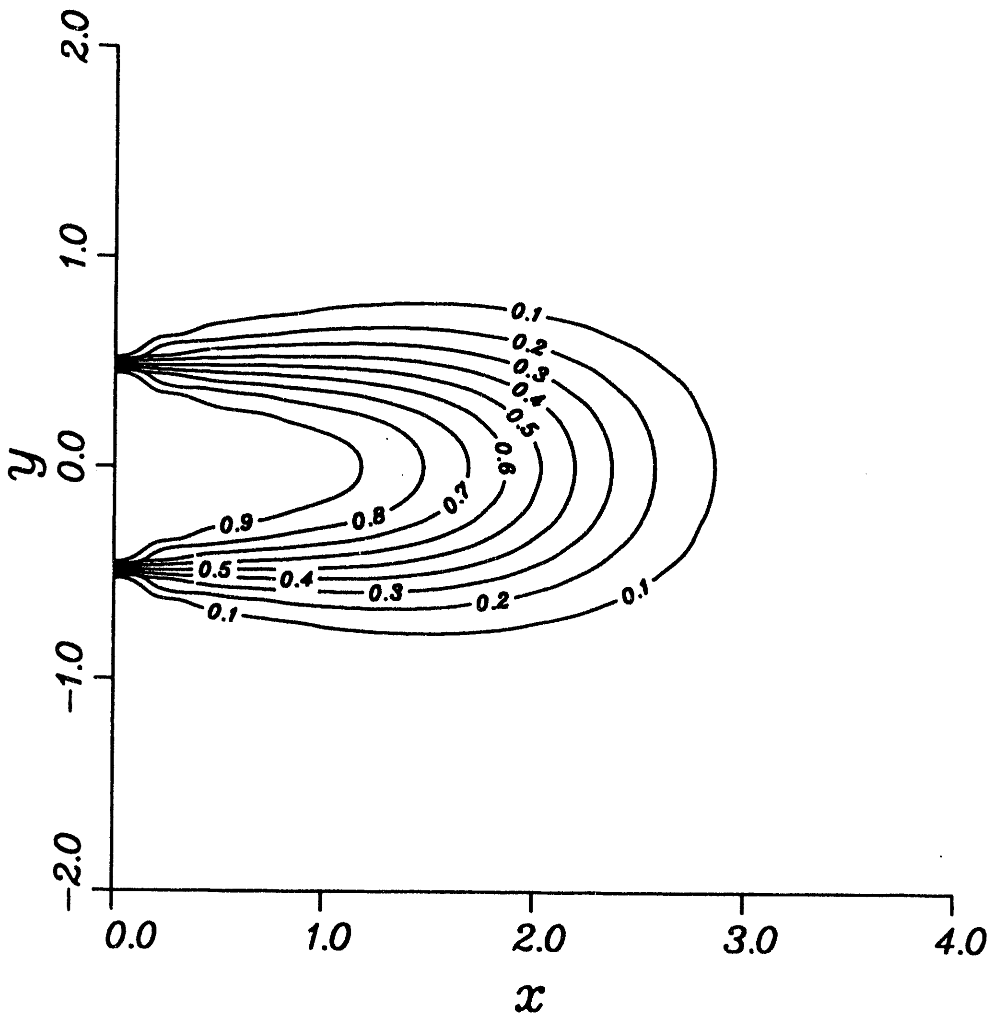
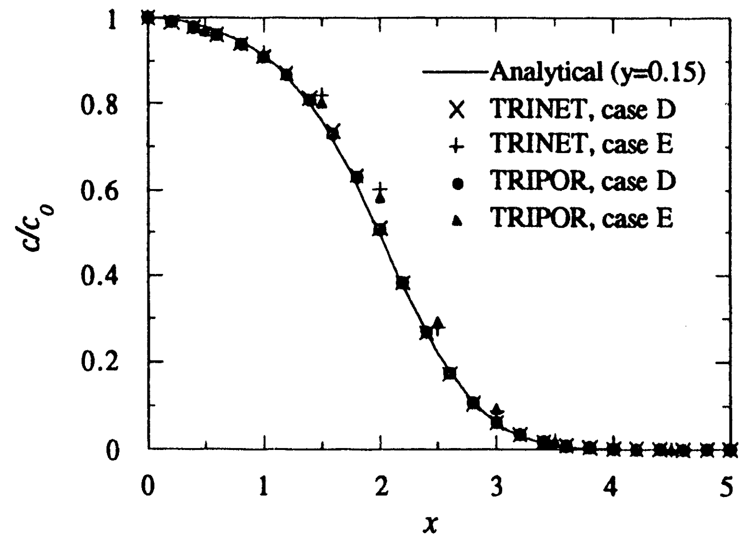
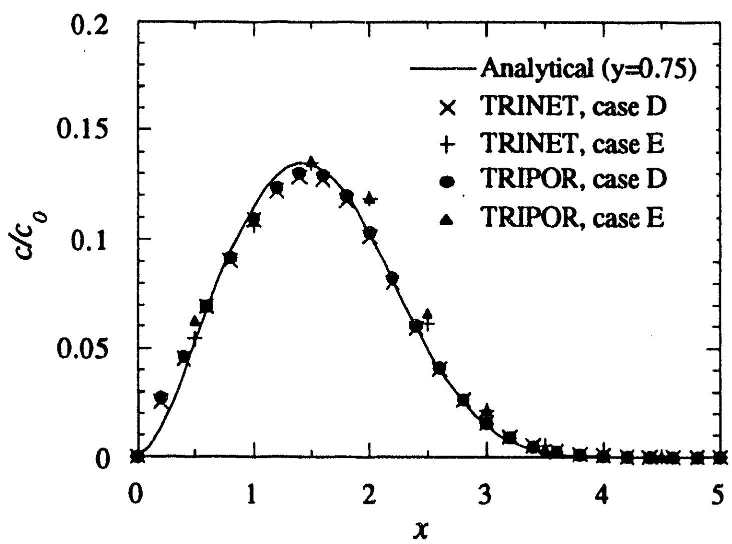



Figure 7. Concentration distribution obtained with TRIPOR at $t$=20 for case D.

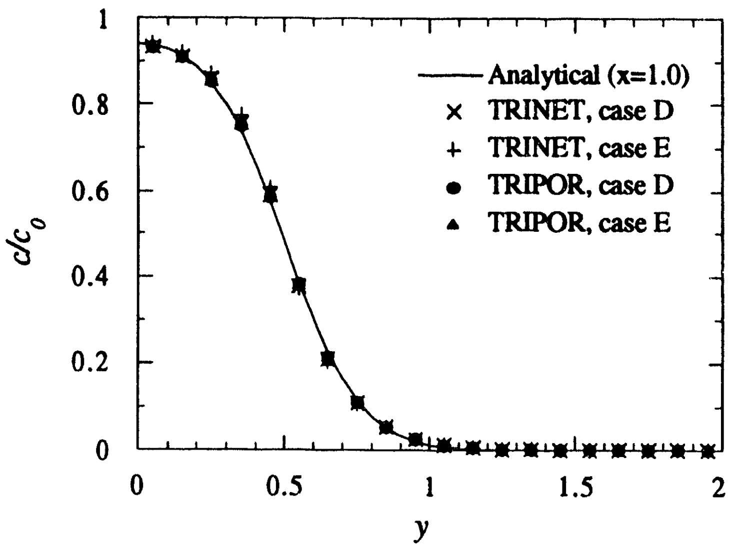



(a)

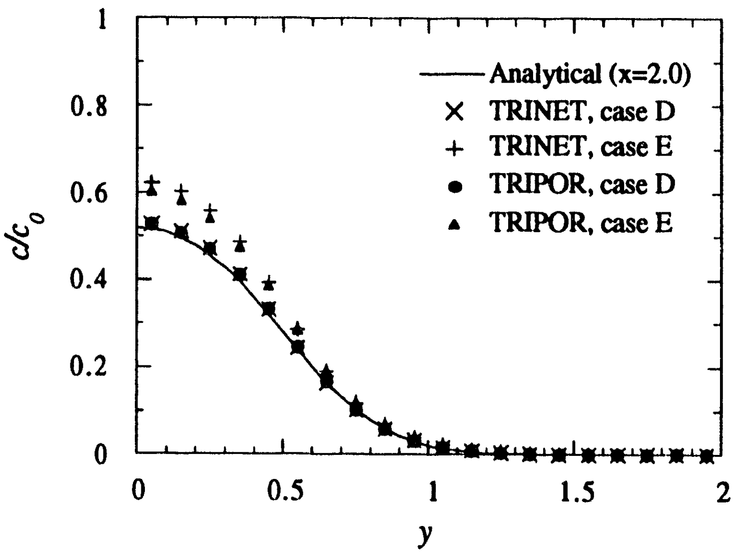



(b)

Figure 8. Concentration profiles obtained with TRINET and TRIPOR, and analytical solution for two-dimensional problem at $t$=20 for case D and E: (a) $y$=0.15, (b) $y$=0.75, (c) $x$=1.0, (d) $x$=2.0.




(c)




(d)

Figure 8. Concentration profiles obtained with TRINET and TRIPOR, and analytical solution for two-dimensional problem at $t$=20 for case D and E (continued): (a) $y$=0.15, (b) $y$=0.75, (c) $x$=1.0, (d) $x$=2.0.

## CONCLUSIONS

Our preliminary studies suggest that our method is capable of accurately solving advection-dispersion problems for a wide range of Peclet numbers and for Courant numbers well in excess of 1. Since the codes create new nodes in the vicinity of the concentration fronts at each time step, hardly any attention has to be paid to the discretization of space away from the concentration boundary.

The code, however, sometimes creates flat elements (high aspect ratio elements) when the tracked points are close to the sides of elements. These flat elements will affect the convergence of the matrices and the accuracy of the results will be decreased. Further studies are necessary in this respect.

## ACKNOWLEDGMENT

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