

Analysis of numerical dispersion in finite difference approximation of solute transport equation

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Abstract

Numerical solution of the ADE by traditional finite difference/finite element techniques poses serious difficulties, which stem from the truncation of Taylor's series while approximating both the spatial and temporal first-order derivatives occurring in the ADE. In a pure advection problem, this truncation error manifests as an additional term, described as numerical dispersion. Presence of this term renders the finite difference solution of the pure advection problem mathematically equivalent to that of an advection-dispersion problem. The paper analyzes and looks into the mathematical quantification of numerical dispersion originating from the truncation of Taylor's series. Techniques that have been adopted by researchers to remedy this problem to various degrees are also briefly discussed highlighting their advantages and limitations.

INTRODUCTION

During the last two decades, there have been an increasing number of attempts to develop suitable and efficient numerical schemes for approximating the transient advective-dispersive equation (ADE) governing solute transport in porous media. The sustained interest in this equation arises from the need to minimize/eliminate numerical difficulties encountered while solving ADE.

For a conservative solute, the basic transport mechanism is due to the coupled action of advection and dispersion. Solutes are displaced from one location to another in the form of plug due to advection and spread in all possible directions thereby occupying ever increasing volume of groundwater due to dispersion. A solute being advected travels at the same rate as average linear velocity of groundwater. As the contaminated fluid flows through a porous medium, it mixes with fresh groundwater due to dispersion. This results in a lowering of solute concentration. To describe 1-D non-reactive solute transport, the ADE is written as (Bear, 1979)

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} \quad (1)$$

where c = solute concentration; t = time; x = distance; D = longitudinal dispersion coefficient; and v = average seepage velocity.

Analytical solutions of ADE which are accurate are however applicable to certain idealistic situations only. In real life problems, due to irregular boundaries and inhomogeneous aquifer parameters, numerical techniques viz., finite differences (FD)/finite elements

(FE), are employed to arrive at an approximate solution of ADE. These techniques solve the ADE by discretizing the equation over a fixed grid.

The efficacy of most of the numerical schemes is governed by two dimensionless parameters - Peclet number (Pe) and Courant number (α). The grid Peclet number reflects the ratio between the rate of transport by advection to the rate of transport by dispersion and is expressed as follows:

$$P_e = v\Delta x/D \quad (2)$$

where Δx is the spacing between grid nodes.

For small values of P_e , Eq. (1) becomes parabolic and dispersion dominates. For larger values of P_e , the equation acquires a hyperbolic character and advection dominates. Thus, the nature of the equation may vary from parabolic to hyperbolic over space and time depending on the variation of velocity or dispersion.

The Courant number reflects the distance travelled by advection during one time step relative to grid spacing (Frind, 1982) and is expressed as

$$\alpha = v\Delta t/\Delta x \quad (3)$$

where Δt is the time step size.

The traditional FD/FE methods perform quite well when dispersion dominates the transport and the distribution of concentration is relatively smooth. However, in transport problems where advection dominates, the FD/FE solution exhibits a combination of numerical dispersion and oscillation. Numerical dispersion is an artificial, grid-dependent smearing of sharp solute concentration fronts while numerical oscillation is manifested by overshoot and undershoot about the true solution. Peaceman (1977) analyzed the artificial dispersion term appearing in the numerical solution. This paper discusses the origin and mathematical quantification of numerical dispersion for different schemes of FD method.

NUMERICAL DISPERSION

Origin

Numerical dispersion is basically a truncation error, which is incurred by replacing a differential equation by a finite difference approximation. Due to this error, the exact solution of a difference equation differs from the solution of the corresponding differential equation. The term *truncation error* derives from the fact that the replacement of a derivative by a difference quotient is equivalent to using a truncated Taylor's series. The local truncation error (δ) of a finite difference approximation can be defined as

$$\delta = |c_d - c_p| \quad (4)$$

where c_d and c_p are the exact solutions of the difference equation and the partial differential equation, respectively.

Analysis

Consider the case of pure advection problem where $D = 0$. Here, the 1-D transport equation is written as

$$\frac{\partial c}{\partial t} = -v \frac{\partial c}{\partial x} \quad (5)$$

The objective is to analyse the associated truncation error in the FD solution of the above equation. The general finite difference approximation of Eq. (5) is

$$\frac{c_{ik+1} - c_{ik}}{\Delta t} = -\frac{v}{\Delta x} \left[\tau \left\{ (1-\omega)c_{i+1k+1} + (2\omega-1)c_{ik+1} - \omega c_{i-1k+1} \right\} + (1-\tau) \left\{ (1-\omega)c_{i+1k} + (2\omega-1)c_{ik} - \omega c_{i-1k} \right\} \right] \quad (6)$$

where ω = weighting parameter with values 1, $\frac{1}{2}$ and 0 for upstream, mid-point and downstream weighting, respectively; τ = time-weighting parameter with values 1, $\frac{1}{2}$ and 0 for implicit, centered-in-time and explicit finite difference equations, respectively; c_{ik} = discrete concentration at node x_i at time t_k .

The expression $[(1-\omega)c_{i+1k+1} + (2\omega-1)c_{ik+1} - \omega c_{i-1k+1}]$ in Eq. (6) can be written as $\left[\frac{1}{2}(c_{i+1k+1} - c_{i-1k+1}) + \left(\frac{1}{2} - \omega \right) (c_{i+1k+1} - 2c_{ik+1} + c_{i-1k+1}) \right]$.

Thus, substituting Eqs. (5) and (6) into Eq. (4), the truncation error is obtained as

$$\delta = -v \left[\tau \left\{ \frac{c_{i+1k+1} - c_{i-1k+1}}{2\Delta x} + \Delta x \left(\frac{1}{2} - \omega \right) \frac{c_{i+1k+1} - 2c_{ik+1} + c_{i-1k+1}}{\Delta x^2} \right\} + (1-\tau) \left\{ \frac{c_{i+1k} - c_{i-1k}}{2\Delta x} + \Delta x \left(\frac{1}{2} - \omega \right) \frac{c_{i+1k} - 2c_{ik} + c_{i-1k}}{\Delta x^2} \right\} \right] - \frac{c_{ik+1} - c_{ik}}{\Delta t} + v \left(\frac{\partial c}{\partial x} \right)_{im} + \left(\frac{\partial c}{\partial t} \right)_{im} \quad (7)$$

where $m = (1-\tau)k + \tau(k+1)$

Using central difference approximations for the first four terms on RHS, Eq. (7) is rewritten as

$$\delta = -v \left[\tau \left(\frac{\partial c}{\partial x} \right)_{ik+1} + \tau \Delta x \left(\frac{1}{2} - \omega \right) \left(\frac{\partial^2 c}{\partial x^2} \right)_{ik+1} + (1-\tau) \left(\frac{\partial c}{\partial x} \right)_{ik} + (1-\tau) \Delta x \left(\frac{1}{2} - \omega \right) \left(\frac{\partial^2 c}{\partial x^2} \right)_{ik} \right] - \frac{c_{ik+1} - c_{ik}}{\Delta t} + v \left(\frac{\partial c}{\partial x} \right)_{im} + \left(\frac{\partial c}{\partial t} \right)_{im} + O(\Delta x^2) \quad (8)$$

where $O(\Delta x^2)$ represents the error term.

From Taylor series expansion of $c(x,t)$ and its first and second order derivatives, about time t , the following expressions are obtained:

$$\frac{c_{ik+1} - c_{ik}}{\Delta t} = \left(\frac{\partial c}{\partial t} \right)_{im} + \left(\frac{1}{2} - \tau \right) \Delta t \left(\frac{\partial^2 c}{\partial t^2} \right)_{im} + O(\Delta t^2) \quad (9)$$

$$\tau \left(\frac{\partial c}{\partial x} \right)_{ik+1} + (1 - \tau) \left(\frac{\partial c}{\partial x} \right)_{ik} = \left(\frac{\partial c}{\partial x} \right)_{im} + O(\Delta t^2) \quad (10)$$

$$\tau \left(\frac{\partial^2 c}{\partial x^2} \right)_{ik+1} + (1 - \tau) \left(\frac{\partial^2 c}{\partial x^2} \right)_{ik} = \left(\frac{\partial^2 c}{\partial x^2} \right)_{im} + O(\Delta t^2) \quad (11)$$

Substituting Eqs. (9), (10) and (11) into Eq. (8)

$$\delta = -v \Delta x \left(\frac{1}{2} - \omega \right) \left(\frac{\partial^2 c}{\partial x^2} \right)_{im} + \left(\tau - \frac{1}{2} \right) \Delta t \left(\frac{\partial^2 c}{\partial t^2} \right)_{im} + O(\Delta x^2) + O(\Delta t^2) \quad (12)$$

On differentiating Eq. (5) w.r.t. t and x , respectively

$$\frac{\partial^2 c}{\partial t^2} = -v \frac{\partial^2 c}{\partial t \partial x} = -v \frac{\partial^2 c}{\partial x \partial t} \quad \text{and} \quad \frac{\partial^2 c}{\partial x \partial t} = -v \frac{\partial^2 c}{\partial x^2}$$

$$\text{Therefore} \quad \frac{\partial^2 c}{\partial t^2} = v^2 \frac{\partial^2 c}{\partial x^2} \quad (13)$$

Substituting Eq. (13) into Eq. (12), the truncation error emerges as

$$\delta = v \Delta x \left[\left(\omega - \frac{1}{2} \right) + \alpha \left(\tau - \frac{1}{2} \right) \right] \left(\frac{\partial^2 c}{\partial x^2} \right)_{im} + O(\Delta x^2) + O(\Delta t^2) \quad (14)$$

where $\alpha = v \Delta t / \Delta x$.

Rearranging Eq. (4)

$$c_d = c_p + \delta = -v \frac{\partial c}{\partial x} - \frac{\partial c}{\partial t} + \delta \quad (15)$$

Substituting Eq. (14) in Eq. (15)

$$c_d = -v \frac{\partial c}{\partial x} - \frac{\partial c}{\partial t} + D_n \frac{\partial^2 c}{\partial x^2} + O(\Delta x^2) + O(\Delta t^2) \quad (16)$$

where
$$D_n = v\Delta x \left[\left(\omega - \frac{1}{2} \right) + \alpha \left(\tau - \frac{1}{2} \right) \right] \quad (17)$$

Thus, we find that on solving the finite difference approximation of the pure advection problem represented by Eq.(5), we arrive at a solution for the following 1-D ADE:

$$\frac{\partial c}{\partial t} = D_n \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} \quad (18)$$

Eq.(18) is similar to Eq. (1) except the higher order terms. The artificial dispersion D_n term arising from the truncation error, associated with the use of difference equations, is therefore termed as numerical dispersion. It is clear from Eq. (17) that D_n can be reduced by using small values of Δx and Δt .

Table 1 lists the values of D_n for different schemes of FD. In every case, positive D_n is associated with stability, while negative D_n is associated with instability. For two cases namely, forward-in-time, backward-in-distance (with $\alpha = 1$) and centered-in-time, centered-in-distance, D_n is 0. Thus, as evident from Table 1, a close connection exists between stability and numerical dispersion.

Table 1. Special cases of first-order difference equation (Peaceman,1977).

	Backward-in-distance $\omega = 1$	Centered-in-distance $\omega = 1/2$	Forward-in-distance $\omega = 0$
Backward-in-time $\tau = 1$	Always stable $D_n = v\Delta x(\alpha+1)/2$	Always stable $D_n = v\Delta x(\alpha)/2$	Stable if $\alpha \geq 1$ $D_n = v\Delta x(\alpha-1)/2$
Centered-in-time $\tau = 1/2$	Always stable $D_n = v\Delta x/2$	Neutrally stable $D_n = 0$	Always unstable $D_n = -v\Delta x/2$
Forward-in-time $\tau = 0$	Stable if $\alpha \leq 1$ $D_n = v\Delta x(1-\alpha)/2$	Always unstable $D_n = -v\Delta x(\alpha)/2$	Always unstable $D_n = -v\Delta x(\alpha+1)/2$

NUMERICAL EXAMPLES

Consider a 1-D solute transport problem in a saturated porous medium (described by Eq. (1)) with constant seepage velocity and the following initial and boundary conditions:

$$c(x,0) = 0, \quad x > 0; \quad c(x_0,t) = c_o, \quad t > 0; \quad \text{and} \quad \partial c(x_L,t) / \partial x = 0, \quad t > 0$$

where x_0 and x_L = positions of the inlet and outlet, respectively, and c_o = concentration at inlet.

Analytical Solution: For the initial condition $c(x,0) = 0, x > 0$ and boundary conditions $c(0,t) = 1, c(\infty,t) = 0, t > 0$, the solution of Eq. (1) is (Ogata and Banks, 1961)

$$c(x,t) = \frac{c_0}{2} \operatorname{erfc}\left\{\frac{x-vt}{2\sqrt{Dt}}\right\} + \frac{1}{2} \exp\left(\frac{vx}{D}\right) \operatorname{erfc}\left\{\frac{x+vt}{2\sqrt{Dt}}\right\} \quad (19)$$

where $c(x,t)$ = concentration at distance x and time t , and $\operatorname{erfc}\{*\}$ = complementary error function = $1 - \operatorname{erf}\{*\}$.

Numerical Solution: Applying the weighting factors ω and τ to the advective term, the centered-in-space and centered-in-time finite difference approximation of the 1-D ADE (Eq. (1)) for an interior node in the FD grid is written as

$$\frac{c_{ik+1} - c_{ik}}{\Delta t} = \frac{D\Delta t}{2\Delta x^2} (c_{i+1k+1} - 2c_{ik+1} + c_{i-1k+1} + c_{i+1k} - 2c_{ik} + c_{i-1k}) - \frac{v}{\Delta x} \left[\tau \{ (1-\omega)c_{i+1k+1} + (2\omega-1)c_{ik+1} - \omega c_{i-1k+1} \} + (1-\tau) \{ (1-\omega)c_{i+1k} + (2\omega-1)c_{ik} - \omega c_{i-1k} \} \right] \quad (20)$$

At each time step, the solution of the system of equations represented by Eq. (20) and the corresponding initial and boundary conditions are solved using the Thomas algorithm (Remson et al., 1978).

With $x_0 = 0$ and $x_L = 40$ cm, the following parameter values were used over a uniform grid: $c_0 = 1$ g/l, $\Delta x = 1$ cm, $\Delta t = 0.5$ hr, $v = 1$ cm/hr with $\alpha = 0.5$. Initially two values of dispersion coefficients viz., $D = 1$ cm²/hr and 0.1 cm²/hr, which correspond to grid Peclet number values of $Pe = 1$ and 10 , respectively, were used.

The exact and simulated results at time 15.0 hr, for both values of Pe , are shown in Fig. 1. In Fig. 1(A), which corresponds to a lower value of Pe , the match between analytical and numerical solution is very good. However, in Fig. 1(B), which corresponds to larger value of Pe implying advection-dominated transport, a considerable difference is visible between the two solutions. This difference is due to the problem of numerical dispersion. Therefore, in order to illustrate the numerical dispersion associated with different FD schemes, subsequent runs were taken with $Pe = 10$ for varying values of ω , τ and α .

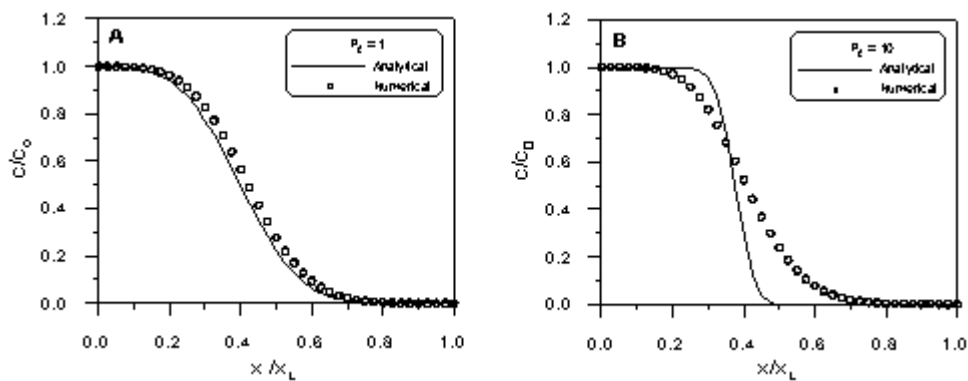


Figure 1. Analytical and numerical solutions for $P_0=1$ and 10.

In all, six cases were considered. Table 2 gives the values of ω , τ and α for each case, along with corresponding numerical values of D_n computed using Eq. (17) and the total dispersion coefficient $D_t = D + D_n$.

Table 2. Computed values of D_n and D_t .

	FD Scheme	Physical Dispersion (D)	Numerical Dispersion (D_n)	Total Dispersion ($D_t = D + D_n$)
1	$\omega = 1.0, \tau = 0.0, \alpha = 0.5$	0.1	0.25	0.35
2	$\omega = 1.0, \tau = 0.5, \alpha = 0.5$	0.1	0.5	0.6
3	$\omega = 1.0, \tau = 1.0, \alpha = 0.5$	0.1	0.75	0.85
4	$\omega = 1.0, \tau = 1.0, \alpha = 1.0$	0.1	1.0	1.1
5	$\omega = 0.5, \tau = 1.0, \alpha = 0.5$	0.1	0.25	0.35
6	$\omega = 0.5, \tau = 0.5, \alpha = 0.5$	0.1	0.5	0.6

Fig. 2 illustrates the analytical solution (shown as solid curve) and the corresponding numerical solution for each case. The analytical solution was also obtained using the total dispersion coefficient D_t (shown as dashed curve). It is clear from Fig. 2 that as the value of D_n increases, the deviation between the analytical and numerical solution increases. It is largest for the backward-in-distance, backward-in-time (i.e., $\omega = 1, \tau = 1$) scheme with $\alpha = 1$ (refer Fig. 2 (D)). The match between numerical solution and the analytical solution using D_t varies from satisfactory to good. For the centered-in-distance, centered-in-time scheme $D_n = 0$. Compared to others, the numerical solution (refer Fig. 2(F)) using this scheme is closest to the analytical solution. However, the solution shows some oscillation in the form of overshoot. Thus, it is evident from above that when numerical dispersion tends to zero, the problem of numerical oscillation becomes dominant. In this context, it would be useful to briefly discuss the various alternative techniques proposed by researchers over the years to minimize/eliminate these problems.

TECHNIQUES TO REDUCE NUMERICAL DISPERSION

Most of the numerical methods usually employed to solve ADE can be broadly classified into three major categories: Eulerian, Lagrangian and mixed Eulerian-Lagrangian approaches (Neuman, 1984). In the Eulerian approach the equation is discretized by a FD/FE grid system fixed in space. In the Lagrangian approach, either a deforming grid or a fixed grid in deforming coordinates can be used. In the mixed Lagrangian-Eulerian approach, a fixed grid is used but with two steps of computations: the first step is to compute the Lagrangian concentration with particle tracking methods, and the second step is to compute the final concentration with either FD, FE, or some other variant numerical method.

In the Eulerian approach, as mentioned previously, numerical dispersion can be reduced by using a fine grid and correspondingly a smaller time step size to keep grid Courant number less than 1. However, for most realistic 2- and 3-D problems, using both fine grid

and small time step is not practical. Numerical dispersion can be reduced by using higher-order approximations in space, time, or both (Holly and Preissman, 1977; Van Genuchten and Gray, 1978). But the use of higher-order approximations may introduce oscillations (Neuman, 1983). Hence higher order approximations have not proven capable of entirely eliminating both numerical dispersion and oscillation. Upstream methods (Chaudhari 1971; Leventhal, 1980; Lapidus and Pinder, 1982) can eliminate oscillations for grid Peclet numbers ranging from 0 to ∞ with grid Courant number smaller than 1, but upstream methods introduce a large numerical dispersion.

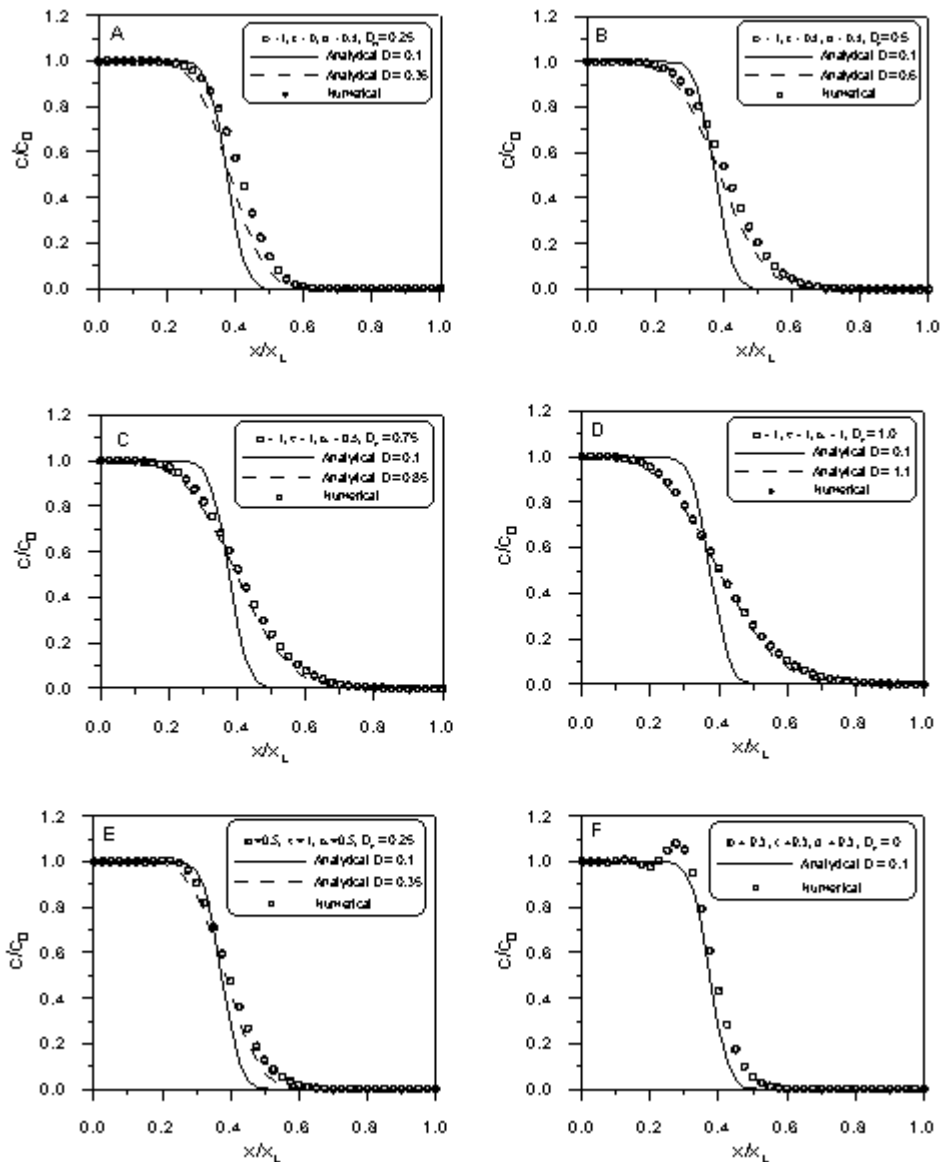


Figure 2. Non-dimensional plot of analytical and numerical solutions of 1-D ADE.

The Lagrangian method has also been used to circumvent the problem of oscillations (O'Neill, 1981; Botha et al., 1982, Thomson et al., 1984) however, it has several drawbacks related to mesh deformation (Yeh and Chou, 1981).

The mixed Lagrangian-Eulerian approach adopts a Lagrangian viewpoint when dealing with advection terms and an Eulerian viewpoint when dealing with rest of the terms in the transport equations. In the Lagrangian step, either continuous forward particle tracking CFPT (Konikow and Bredehoeft, 1978), single-step reverse particle tracking SRPT (Neuman and Sorek, 1982) or a combination of both (Neuman, 1984) is used. SRPT can introduce a significant amount of numerical dispersion near sharp concentration fronts (Neuman, 1984). This can be reduced by using a smaller grid size, which, nevertheless is impractical for a large region. Zhang et al., (1993) presented a modified single step reverse particle tracking (MSRPT) method to deal with advection-dominated problems. This technique, separately, controls the movement of particles in the upstream and downstream regions of the concentration front. MSRPT maintains the advantages of traditional SRPT, but eliminates the associated numerical dispersion. The method is currently limited to grid Courant numbers less than or equal to 1. Yeh (1990) noted that since numerical dispersion is important only in regions where a steep gradient of concentration occurs, there is no need to reduce numerical dispersion in the region where the gradient of concentration is very small. Therefore a Lagrangian-Eulerian method with a zoomable hidden fine-mesh approach (LEZOOM) was proposed to solve the ADE. This technique entirely eliminates numerical oscillation and efficiently reduces numerical dispersion. However, the process of zooming and refining the element at each time step is complicated in terms of its practical implementation.

Zheng (1993) modified the method of characteristics (MOC) which utilizes CFPT, to make it more efficient and accurate by including a dynamic particle allocation procedure and higher order particle tracking technique. Liu and Dane (1996) proposed an interpolation-corrected modified method of characteristics (ICMMOC) for solving the ADE, which is an improved version of the modified method of characteristics utilizing SRPT. It uses a high order interpolation scheme to reduce numerical dispersion and an interpolation correction procedure to eliminate numerical clipping. The simulated results showed that ICMMOC can eliminate numerical oscillation and reduce numerical dispersion to a small level for a large range of grid Peclet number.

CONCLUSIONS

Numerical solution of ADE by finite difference approximation poses a computational difficulty which originates due to an additional term *numerical dispersion* introduced from the truncation of Taylor's series of mixed derivatives (time and space).

The analysis of pure advection problem ($D = 0$), could delineate the numerical dispersion associated with different schemes of the finite difference method. Numerical dispersion is found to be dependable on space and time discretization size. Numerical simulations

illustrate that for zero value of numerical dispersion obtained in centered-in-distance, centered-in-time difference equation, the numerical solution tends to oscillate. The mixed Lagrangian-Eulerian techniques are an attractive alternative to the traditional FD/FE methods to minimize the problem of numerical dispersion.

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