# ANALYSIS OF SOME DISPERSION CORRECTED NUMERICAL SCHEMES FOR SOLUTION OF THE TRANSPORT EQUATION

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## SUMMARY

In the last decade or so finite element techniques have been applied with increased frequency to contaminant transport problems. Whereas most of the attention has focused on finite element approximations of spatial derivatives, standard finite difference techniques are generally used for approximation of the time derivative. Such an approach yields a scheme which is at best second order correct in time. In this study several higher order approximations of the time derivative are developed and analyzed using a finite difference approximation, and Galerkin-type finite element approximations in conjunction with several sets of basis functions. Results obtained with the different schemes exhibit significant improvements in the numerical solution of the convective-dispersive equation.

## INTRODUCTION

Considerable effort has been directed in recent years towards the development of improved numerical schemes for solution of the convective-dispersive equation which describes contaminant transport in porous media. Oscillations are often computed in the region of a sharp concentration front when convection is much greater than dispersion (Peaceman and Rachford[1]; Price et al[2]). These oscillations can often be damped out at the expense of a smeared front by using standard finite difference or finite element techniques. Chaudhari[3] in 1971 used an explicit, backwards in space, finite difference scheme and showed that by adding a term to the dispersion coefficient, the smearing of the front could be reduced without generating oscillatory numerical solutions. Several other schemes have since been proposed (Bresler,[4] Chaudhari,[5] van Genuchten and Wierenga,[6] Lantz[7]) to minimize the effects of numerical dispersion through the use of dispersion coefficient corrections in the transport equation. In the present paper, correction factors are derived which are applicable to several higher order finite difference and finite element schemes for solution of the convective-dispersive equation. The stability of the corrected schemes is analyzed and some computed results for finite differences and for linear, quadratic and Hermitian finite elements are presented.

## THEORY

The equation to be considered in this analysis is the one-dimensional convective-dispersive equation given by

$$\frac{\partial c}{\partial \tau} + U \frac{\partial c}{\partial \xi} - D \frac{\partial^2 c}{\partial \xi^2} = 0 \tag{1}$$

where

    $c$ is the solute concentration $(ML^{-3})$,

    $U$ is the velocity, assumed to be constant $(LT^{-1})$,

    $D$ is the dispersion coefficient, assumed to be constant $(L^2T^{-1})$,

    $\tau$ is the time dimension $(T)$, and

    $\xi$ is the space dimension $(L)$.

This equation can be made dimensionless with respect to the uniform time and space increments, $\Delta\tau$ and $\Delta\xi$ respectively, which will be used in the finite element and finite difference calculations. For this purpose the following dimensionless variables are defined

$$t = \tau/\Delta\tau \tag{2a}$$

$$x = \xi/\Delta\xi \tag{2b}$$

such that $\Delta t$ and $\Delta x$, the dimensionless time and space increments, respectively, equal unity. Equation (1) then becomes

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} - \mathcal{D}\frac{\partial^2 c}{\partial x^2} = 0 \tag{3}$$

where

$$u = \frac{U\Delta\tau}{\Delta\xi} \qquad \mathcal{D} = \frac{D\Delta\tau}{(\Delta\xi)^2}$$

Consider now the following difference approximation to (3)

$$\frac{\Delta c}{\Delta t} = \left[-a_1 u\frac{\Delta c}{\Delta x} + a_2\mathcal{D}\frac{\Delta^2 c}{\Delta x^2}\right]^{t+\Delta t} + \left[-b_1 u\frac{\Delta c}{\Delta x} + b_2\mathcal{D}\frac{\Delta^2 c}{\Delta x^2}\right]^{t} \tag{4}$$

where $\Delta c/\Delta t$ is given by

$$\frac{\Delta c}{\Delta t} = \frac{c^{t+\Delta t} - c^t}{\Delta t} \tag{5}$$

and where the spatial difference quotients are as yet unspecified, since they depend on the particular finite difference or finite element scheme adopted. The coefficients $a_i$ and $b_i$ ($i = 1, 2$) in this difference equation will be determined such that (4) becomes a higher order accurate approximation to differential equation (3).

*Time corrections only*

When higher order basis functions are used in the finite element formulation, the truncation errors associated with the spatial derivatives can be assumed small compared to the time differencing errors. Thus, equation (4) may be written as

$$\frac{\Delta c}{\Delta t} = \left[-a_1 u\frac{\partial c}{\partial x} + a_2\mathcal{D}\frac{\partial^2 c}{\partial x^2}\right]^{t+\Delta t} + \left[-b_1 u\frac{\partial c}{\partial x} + b_2\mathcal{D}\frac{\partial^2 c}{\partial x^2}\right]^{t} \tag{6}$$

The basic technique upon which the derivation of the correction factors depends, is the replacement of the spatial derivatives $\partial c/\partial x$ and $\partial^2 c/\partial x^2$ by appropriate time derivatives. To obtain an expression for $\partial c/\partial x$ in terms of the time derivatives, constraint equation (3) may be rewritten in the following form

$$u\frac{\partial c}{\partial x} = -\frac{\partial c}{\partial t} + \mathcal{D}\frac{\partial^2 c}{\partial x^2} \tag{7}$$

Multiplication of this equation by $u$ and rearrangement yields

$$u^2 \frac{\partial c}{\partial x} = -u \frac{\partial c}{\partial t} + \mathscr{D} \frac{\partial}{\partial x}\left(u \frac{\partial c}{\partial x}\right) \tag{8}$$

Equation (7) may now be substituted into the last term of (8) to obtain

$$u^2 \frac{\partial c}{\partial x} = -u \frac{\partial c}{\partial t} - \mathscr{D} \frac{\partial}{\partial x}\left(\frac{\partial c}{\partial t}\right) + \mathscr{D}^2 \frac{\partial^3 c}{\partial x^3} \tag{9}$$

This equation may be multiplied also by $u$ and rearranged to the form

$$u^3 \frac{\partial c}{\partial x} = -u^2 \frac{\partial c}{\partial t} - \mathscr{D} \frac{\partial}{\partial t}\left(u \frac{\partial c}{\partial x}\right) + \mathscr{D}^2 \frac{\partial^2}{\partial x^2}\left(u \frac{\partial c}{\partial x}\right) \tag{10}$$

Again (7) may be substituted into the last terms of equation (10). Repeating this successive substitution until all spatial derivatives up to the fourth order are converted to time derivatives, one obtains

$$u \frac{\partial c}{\partial x} = -\frac{\partial c}{\partial t} + \frac{\mathscr{D}}{u^2} \frac{\partial^2 c}{\partial t^2} - \frac{2\mathscr{D}}{u^4} \frac{\partial^3 c}{\partial t^3} + \frac{5\mathscr{D}^3}{u^6} \frac{\partial^4 c}{\partial t^4} + \cdots \tag{11a}$$

A similar expression may be obtained for the second derivative by differentiating (11a) with respect to $x$ and using (7) to again convert the spatial derivatives to time derivatives. The following expression results

$$u^2 \frac{\partial^2 c}{\partial x^2} = \frac{\partial^2 c}{\partial t^2} - \frac{2\mathscr{D}}{u^2} \frac{\partial^3 c}{\partial t^3} + \frac{5\mathscr{D}^2}{u^4} \frac{\partial^4 c}{\partial t^4} + \cdots \tag{11b}$$

Proceeding in an analogous manner, one may also obtain expressions for the third and fourth spatial derivatives

$$u^3 \frac{\partial^3 c}{\partial x^3} = -\frac{\partial^3 c}{\partial t^3} + \frac{3\mathscr{D}}{u^2} \frac{\partial^4 c}{\partial t^4} + \cdots \tag{11c}$$

$$u^4 \frac{\partial^4 c}{\partial x^4} = \frac{\partial^4 c}{\partial t^4} + \cdots \tag{11d}$$

Equations (11), which were derived subject to the constraint imposed by the convective-dispersive equation (3), may now be substituted into (6), to obtain

$$\frac{\Delta c}{\Delta t} = \left[ a_1 \frac{\partial c}{\partial t} + (a_2 - a_1) \frac{\mathscr{D}}{u^2} \frac{\partial^2 c}{\partial t^2} + 2 \frac{\mathscr{D}^2}{u^4}(a_1 - a_2) \frac{\partial^3 c}{\partial t^3} + 5 \frac{\mathscr{D}^3}{u^6}(a_2 - a_1) \frac{\partial^4 c}{\partial t^4} \right]^{t+\Delta t}$$
$$+ \left[ b_1 \frac{\partial c}{\partial t} + (b_2 - b_1) \frac{\mathscr{D}}{u^2} \frac{\partial^2 c}{\partial t^2} + 2 \frac{\mathscr{D}^2}{u^4}(b_1 - b_2) \frac{\partial^3 c}{\partial t^3} + 5 \frac{\mathscr{D}^3}{u^6}(b_2 - b_1) \frac{\partial^4 c}{\partial t^4} \right]^{t} \tag{12}$$

By making use of equation (12) optimal values of the coefficients $a_i$ and $b_i$ for second or higher order accurate difference schemes may now be developed.

*Implicit schemes.* The first case to be considered is the implicit scheme. In such a scheme the terms on the right hand side of (12) at the known time level $t$ are not considered. Thus $b_1$ and $b_2$ are zero. Because only two independent parameters, $a_1$ and $a_2$, are left to be determined, the implicit scheme can generally be made only second order accurate in time. Optimal values for $a_1$ and $a_2$ may be selected by requiring that equation (12) be exact for $c = t^2$. Substitution of this

relation into (12) and recalling that $\Delta t = 1$, one obtains (with $b_1 = b_2 = 0$)

$$(t+1)^2 - t^2 = 2a_1(t+1) + 2(a_2 - a_1)\frac{\mathscr{D}}{u^2} \tag{13}$$

Because this equation holds for all values of $t$, the coefficients of like powers of $t$ on both sides of the equation must be equal. Hence

$$2 = 2a_1 \tag{14a}$$

$$1 = 2a_1 + 2(a_2 - a_1)\frac{\mathscr{D}}{u^2} \tag{14b}$$

Simultaneous solution of equations (14a) and (14b) yields

$$a_1 = 1 \tag{15a}$$

$$a_2 = 1 - \frac{u^2}{2\mathscr{D}} \tag{15b}$$

After substitution of (15) into (4), the following implicit, second order, time corrected representation of the convective-dispersion equation is obtained

$$\frac{\Delta c}{\Delta t} = \left[ -u\frac{\Delta c}{\Delta x} + \left( \mathscr{D} - \frac{u^2}{2} \right)\frac{\Delta^2 c}{\Delta x^2} \right]^{t+\Delta t} \tag{16}$$

*Explicit schemes.* For an explicit scheme the parameters $a_1$ and $a_2$ in (12) will be zero. Again only two parameters are left to be determined, and thus the explicit scheme can also be only second order correct in time. Substitution of $c = t^2$ into equation (12) with $a_1 = a_2 = 0$ yields

$$(t+1)^2 - t^2 = 2b_1 t + 2(b_2 - b_1)\frac{\mathscr{D}}{u^2} \tag{17}$$

Equating the coefficients of like powers of $t$ on both sides of this equation and solving for $b_1$ and $b_2$, one obtains

$$b_1 = 1 \tag{18a}$$

$$b_2 = 1 + \frac{u^2}{2\mathscr{D}} \tag{18b}$$

Therefore, an explicit scheme which is second order correct in time, is given by

$$\frac{\Delta c}{\Delta t} = \left[ -u\frac{\Delta c}{\Delta x} + \left( \mathscr{D} + \frac{u^2}{2} \right)\frac{\Delta^2 c}{\Delta x^2} \right]^{t} \tag{19}$$

It should be noted that equations (16) and (19) have been derived also with the use of Taylor series expansions for the time derivative (Chaudhari,[3] van Genuchten and Wierenga[6]). The method of analysis followed here, however, appears to be more easily extended to the derivation of third and fourth order correct numerical schemes. This will be shown next.

*Third order correct schemes.* Third order correct schemes may be obtained by requiring that (12) be satisfied when $c$ is a cubic polynomial in time. With the constraint that $c = t^3$, equation

(12) becomes

$$3t^2+3t+1 = \left[3a_1(t+1)^2+6(a_2-a_1)\frac{\mathscr{D}}{u^2}(t+1)+12(a_1-a_2)\frac{\mathscr{D}^2}{u^4}\right]$$
$$+\left[3b_1t^2+6(b_2-b_1)\frac{\mathscr{D}t}{u^2}+12(b_1-b_2)\frac{\mathscr{D}^2}{u^4}\right] \tag{20}$$

For this equation to be exact for all $t$, the coefficients of the same powers of $t$ on both sides of the equal sign must be the same. Hence

$$3 = 3a_1+3b_1 \tag{21a}$$

$$3 = 6a_1+6(a_2-a_1+b_2-b_1)\frac{\mathscr{D}}{u^2} \tag{21b}$$

$$1 = 3a_1+6(a_2-a_1)\frac{\mathscr{D}}{u^2}+12(a_1-a_2+b_1-b_2)\frac{\mathscr{D}^2}{u^4} \tag{21c}$$

Hence three equations in four unknowns are obtained. The parameter $a_1$ will not be solved for, but instead will be left to take an arbitrary value $\theta$. Solution for the remaining unknowns yields then

$$a_2 = 1-\theta+\frac{(1-3\theta)u^2}{6\mathscr{D}} \tag{22a}$$

$$b_1 = 1-\theta \tag{22b}$$

$$b_2 = \theta+\frac{(2-3\theta)u^2}{6\mathscr{D}} \tag{22c}$$

Using this relation in (4), one obtains

$$\frac{\Delta c}{\Delta t} = \theta\left[-u\frac{\Delta c}{\Delta x}+\left\{\mathscr{D}\left(\frac{1-\theta}{\theta}\right)+\frac{(1-3\theta)}{6\theta}u^2\right\}\frac{\Delta^2 c}{\Delta x^2}\right]^{t+\Delta t}$$
$$+(1-\theta)\left[-u\frac{\Delta c}{\Delta x}+\left\{\mathscr{D}\left(\frac{\theta}{1-\theta}\right)+\frac{(2-3\theta)}{6(1-\theta)}u^2\right\}\frac{\Delta^2 c}{\Delta x^2}\right]^t \tag{23}$$

In the present study, this equation will be used only when $\theta=\frac{1}{2}$, and (23) thus reduces to

$$\frac{\Delta c}{\Delta t} = \frac{1}{2}\left[-u\frac{\Delta c}{\Delta x}+\left(\mathscr{D}-\frac{1}{6}u^2\right)\frac{\Delta^2 c}{\Delta x^2}\right]^{t+\Delta t}+\frac{1}{2}\left[-u\frac{\Delta c}{\Delta x}+\left(\mathscr{D}+\frac{1}{6}u^2\right)\frac{\Delta^2 c}{\Delta x^2}\right]^t \tag{24}$$

This equation represents essentially a Crank–Nicolson scheme with correction factors applied to the dispersion coefficient, the value of the correction factor being dependent upon the time level at which the dispersion term is evaluated.

*Fourth order correct scheme.* To obtain a scheme which is fourth order correct in time, equation (12) is required to be exact when $c$ is a fourth degree polynomial in $t$. Analogously to the previous derivations, the requirement that $c=t^4$ be exactly represented by (12) yields now

$$a_1 = \frac{1}{2}+\frac{2\mathscr{D}u^2}{12\mathscr{D}^2+u^4} \tag{25a}$$

$$\frac{a_2}{a_1} = 1 - \frac{1}{6}\left[\frac{60\mathscr{D}^2 + 12u^2\mathscr{D} + u^4}{12\mathscr{D}^2 + 4u^2\mathscr{D} + u^4}\right]\frac{u^2}{\mathscr{D}} \qquad (25\text{b})$$

$$b_1 = \frac{1}{2} - \frac{2\mathscr{D}u^2}{12\mathscr{D}^2 + u^4} \qquad (25\text{c})$$

$$\frac{b_2}{b_1} = 1 + \frac{1}{6}\left[\frac{60\mathscr{D}^2 - 12u^2\mathscr{D} + u^4}{12\mathscr{D}^2 - 4u^2\mathscr{D} + u^4}\right]\frac{u^2}{\mathscr{D}} \qquad (25\text{d})$$

Thus the special case of equation (4) which is found to be fourth order correct in time is

$$\frac{\Delta c}{\Delta t} = \left[\frac{1}{2} + \frac{2\mathscr{D}u^2}{12\mathscr{D}^2 + u^4}\right]\left[-u\frac{\Delta c}{\Delta x} + \left\{\mathscr{D} - \frac{1}{6}\left(\frac{60\mathscr{D}^2 + 12u^2\mathscr{D} + u^4}{12\mathscr{D}^2 + 4u^2\mathscr{D} + u^4}\right)u^2\right\}\frac{\Delta^2 c}{\Delta x^2}\right]^{t+\Delta t}$$

$$+ \left[\frac{1}{2} - \frac{2\mathscr{D}u^2}{12\mathscr{D}^2 + u^4}\right]\left[-u\frac{\Delta c}{\Delta x} + \left\{\mathscr{D} + \frac{1}{6}\left(\frac{60\mathscr{D}^2 - 12u^2\mathscr{D} + u^4}{12\mathscr{D}^2 - 4u^2\mathscr{D} + u^4}\right)u^2\right\}\frac{\Delta^2 c}{\Delta x^2}\right]^{t} \qquad (26)$$

Note that if $\theta$ in equation (23) is chosen to be

$$\theta = \frac{1}{2} + \frac{2\mathscr{D}u^2}{12\mathscr{D}^2 + u^4}$$

equation (23) becomes identical to (26). Furthermore for the special case when $\mathscr{D} = 0$, equations (23) and (26) reduce to the same form.

## Space–time corrections

So far only truncation errors associated with the time derivative have been considered, while those associated with the spatial derivatives were assumed to be negligible. This assumption may be correct for those finite element schemes where higher order basis functions are used (e.g. cubic or first order continuous Hermitian basis functions). For simple finite differences and linear finite element schemes, however, it is reasonable to include also the truncation errors associated with the spatial derivatives in the analysis.

The following difference operators are first introduced

$$\frac{\delta c_i}{\delta t} = \frac{1}{6}\left[\frac{\Delta c_{i+1}}{\Delta t} + 4\frac{\Delta c_i}{\Delta t} + \frac{\Delta c_{i-1}}{\Delta t}\right] \qquad (27)$$

$$\frac{\Delta c_i}{\Delta x} = \frac{c_{i+1} - c_{i-1}}{2\Delta x} \qquad (28)$$

$$\frac{\Delta^2 c_i}{\Delta x^2} = \frac{c_{i+1} - 2c_i + c_{i-1}}{\Delta x^2} \qquad (29)$$

The time discretization defined by equation (27) results when the time derivative is integrated over the element, using linear basis functions (Gray and Pinder[8]). The approximations of the spatial derivatives as defined by (28) and (29) apply both for finite difference and linear finite element schemes.

Estimates of the truncation errors associated with the spatial derivative approximations are obtained directly from Taylor series expansions as

$$\frac{\Delta c}{\Delta x} = \frac{\partial c}{\partial x} + \frac{1}{6}\frac{\partial^3 c}{\partial x^3} + \ldots \qquad (30)$$

and

$$\frac{\Delta^2 c}{\Delta x^2} = \frac{\partial^2 c}{\partial x^2} + \frac{1}{12} \frac{\partial^4 c}{\partial x^4} + \cdots \qquad (31)$$

*Finite differences.* Substitution of (30) and (31) into (4) yields the following general difference scheme

$$\frac{\Delta c}{\Delta t} = \left[ -a_1 u \frac{\partial c}{\partial x} + a_2 \mathscr{D} \frac{\partial^2 c}{\partial x^2} - \frac{a_1 u}{6} \frac{\partial^3 c}{\partial x^3} + \frac{a_2 \mathscr{D}}{12} \frac{\partial^4 c}{\partial x^4} \right]^{t+\Delta t} + \left[ -b_1 u \frac{\partial c}{\partial x} + b_2 \mathscr{D} \frac{\partial^2 c}{\partial x^2} - \frac{b_1 u}{6} \frac{\partial^3 c}{\partial x^3} + \frac{b_2 \mathscr{D}}{12} \frac{\partial^4 c}{\partial x^4} \right]^t \qquad (32)$$

The analysis now proceeds in exactly the same fashion as before. The constraint imposed by equation (3) is again satisfied by substitution of equations (11a)-(11d) into (32), resulting in

$$\frac{\Delta c}{\Delta t} = \left[ a_1 \frac{\partial c}{\partial t} + \frac{\mathscr{D}}{u^2}(a_2 - a_1)\frac{\partial^2 c}{\partial t^2} + \left\{ \frac{2\mathscr{D}^2}{u^4}(a_1 - a_2) + \frac{a_1}{6u^2} \right\} \frac{\partial^3 c}{\partial t^3} \right.$$
$$+ \left\{ \frac{5\mathscr{D}^3}{u^6}(a_2 - a_1) + \frac{\mathscr{D}}{2u^4}\left( \frac{a_2}{6} - a_1 \right) \right\} \frac{\partial^4 c}{\partial t^4} \right]^{t+\Delta t}$$
$$+ \left[ b_1 \frac{\partial c}{\partial t} + \frac{\mathscr{D}}{u^2}(b_2 - b_1)\frac{\partial^2 c}{\partial t^2} + \left\{ \frac{2\mathscr{D}^2}{u^4}(b_1 - b_2) + \frac{b_1}{6u^2} \right\} \frac{\partial^3 c}{\partial t^3} \right.$$
$$+ \left\{ \frac{5\mathscr{D}^3}{u^6}(b_2 - b_1) + \frac{\mathscr{D}}{2u^4}\left( \frac{b_2}{6} - b_1 \right) \right\} \frac{\partial^4 c}{\partial t^4} \right]^t \qquad (33)$$

Because four parameters are left to be determined, this equation can be made fourth order correct by requiring it to be exact for all fourth degree polynomials in time. Substitution of $c = t^4$ into (33) and solution for the four correction parameters yields

$$a_1 = \frac{1}{2} + \frac{\mathscr{D}(2u^2 - 1)}{u^4 + 12\mathscr{D}^2 - u^2} \qquad (34a)$$

$$\mathscr{D}\frac{a_2}{a_1} = \mathscr{D} - \left[ \frac{60\mathscr{D}^2 - 6\mathscr{D} + 12\mathscr{D}u^2 - 2 + u^2 + u^4}{12\mathscr{D}^2 - 2\mathscr{D} + 4\mathscr{D}u^2 - u^2 + u^4} \right]\frac{u^2}{6} \qquad (34b)$$

$$b_1 = \frac{1}{2} - \frac{\mathscr{D}(2u^2 - 1)}{u^4 + 12\mathscr{D}^2 - u^2} \qquad (34c)$$

$$\mathscr{D}\frac{b_2}{b_1} = \mathscr{D} + \left[ \frac{60\mathscr{D}^2 + 6\mathscr{D} - 12\mathscr{D}u^2 - 2 + u^2 + u^4}{12\mathscr{D}^2 + 2\mathscr{D} - 4\mathscr{D}u^2 - u^2 + u^4} \right]\frac{u^2}{6} \qquad (34d)$$

The following fourth order correct finite difference scheme is then obtained from (4):

$$\frac{\Delta c}{\Delta t} = \theta \left[ -u \frac{\Delta c}{\Delta x} + \left( \mathscr{D} - \frac{\gamma_1 u^2}{6} \right)\frac{\Delta^2 c}{\Delta x^2} \right]^{t+\Delta t} + (1-\theta)\left[ -u \frac{\Delta c}{\Delta x} + \left( \mathscr{D} + \frac{\gamma_2 u^2}{6} \right)\frac{\Delta^2 c}{\Delta x^2} \right]^t \qquad (35)$$

where

$$\theta = a_1 = \frac{1}{2} + \frac{\mathscr{D}(2u^2 - 1)}{u^4 + 12\mathscr{D} - u^2} \qquad (36a)$$

$$\gamma_1 = \frac{60\mathscr{D}^2 - 6\mathscr{D} + 12\mathscr{D}u^2 - 2 + u^2 + u^4}{12\mathscr{D}^2 - 2\mathscr{D} + 4\mathscr{D}u^2 - u^2 + u^4} \qquad (36b)$$

$$\gamma_2 = \frac{60\mathscr{D}^2 + 6\mathscr{D} - 12\mathscr{D}u^2 - 2 + u^2 + u^4}{12\mathscr{D}^2 + 2\mathscr{D} - 4\mathscr{D}u^2 - u^2 + u^4} \qquad (36c)$$

*Linear finite elements*. When linear finite elements instead of finite differences are used, $\Delta c/\Delta t$ in equation (4) is replaced by $\delta c/\delta t$ as defined in (27). Rewriting (6) for this case gives

$$\frac{\delta c}{\delta t} = \left[ -a_1 u \frac{\Delta c}{\Delta x} + a_2 \mathscr{D} \frac{\Delta^2 c}{\Delta x^2} \right]^{t+\Delta t} + \left[ -b_1 u \frac{\Delta c}{\Delta x} + b_2 \mathscr{D} \frac{\Delta^2 c}{\Delta x^2} \right]^t \tag{37}$$

The left hand side of (37) is easily expressed in terms of $\Delta c/\Delta t$ as

$$\frac{\delta c_i}{\delta t} = \frac{\Delta c_i}{\Delta t} + \frac{1}{6}\left[ \frac{\Delta c_{i+1}}{\Delta t} - \frac{2\Delta c_i}{\Delta t} + \frac{\Delta c_{i-1}}{\Delta t} \right]$$

$$= \frac{\Delta c_i}{\Delta t} + \frac{\Delta x^2}{6\Delta t}\left[ \frac{\Delta^2 c}{\Delta x^2} \right]^{t+\Delta t} - \frac{\Delta x^2}{6\Delta t}\left[ \frac{\Delta^2 c}{\Delta x^2} \right]^t \tag{38}$$

Because of the way the time and space domains were made dimensionless, $\Delta x$ and $\Delta t$ are both equal to unity. Combination of equations (37) and (38) and solution for $\Delta c/\Delta t$ yields

$$\frac{\Delta c}{\Delta t} = \left[ -a_1 u \frac{\Delta c}{\Delta x} + \left(a_2 \mathscr{D} - \frac{1}{6}\right) \frac{\Delta^2 c}{\Delta x^2} \right]^{t+\Delta t} + \left[ -b_1 u \frac{\Delta c}{\Delta x} + \left(b_2 \mathscr{D} + \frac{1}{6}\right) \frac{\Delta^2 c}{\Delta x^2} \right]^t \tag{39}$$

One technique to obtain optimal values for the parameters $a_i$ and $b_i$ in this equation is to again convert the spatial derivatives to time derivatives and requiring the resulting equation to be fourth order correct in time. Alternatively, the required corrected scheme may be obtained directly by substituting equation (38) into (35) and rearranging to show that

$$\frac{\delta c}{\delta t} = \theta \left[ -u \frac{\Delta c}{\Delta x} + \left\{ \mathscr{D} - \frac{\gamma_1 u^2}{6} + \frac{1}{6\theta} \right\} \frac{\Delta^2 c}{\Delta x^2} \right]^{t+\Delta t} + (1-\theta)\left[ -u \frac{\Delta c}{\Delta x} + \left\{ \mathscr{D} + \frac{\gamma_1 u^2}{6} - \frac{1}{6(1-\theta)} \right\} \frac{\Delta^2 c}{\Delta x^2} \right]^t \tag{40}$$

where $\theta$, $\gamma_1$ and $\gamma_2$ are as defined in equation (36). Thus the fourth order correct finite difference and linear finite element schemes with their appropriate correction factors are identical.

## RESULTS AND CONCLUSIONS

Numerical results obtained with the various finite difference and finite element schemes derived in the theoretical part of this study will be presented now. The results were obtained with equation (3) subject to the conditions

$$c(0, t) = 1 \qquad t \geq 0 \tag{41a}$$

$$c(x, 0) = 0 \qquad x > 0 \tag{41b}$$

The concentration distribution *versus* distance hence can be closely approximated by the analytical solution of Lapidus and Amundson[9] as

$$c = \tfrac{1}{2} \operatorname{erfc}[(x - ut)/(4\mathscr{D}t)^{1/2}] + \tfrac{1}{2} \exp (ux/\mathscr{D}) \operatorname{erfc}[(x + ut)/(4\mathscr{D}t)^{1/2}] \tag{42}$$

To further assess the accuracy of the numerical results, a Fourier analysis was used to determine the ability of the schemes to accurately propagate a sharp concentration front. The details of the procedure have been previously given in Gray and Pinder[8] and will not be repeated here. The basic idea of the procedure is to express the concentration front as a series of sine and cosine waves. The error with which each wave is computed is then determined by comparing the phase and amplitude of the numerical wave with the corresponding properties of the analytical wave. The comparison is made at the time for which the analytical wave will have propagated one wavelength. A wave which is not propagated at all will thus lag the analytical wave by a full 360

degrees. Gray and Pinder[8] have shown that when the amplitude of the numerical wave is significantly damped in comparison with the analytical wave, the concentration front will be smeared or spread out more than it should be. Furthermore a phase lag of the numerical wave is responsible for the overshoot–undershoot phenomena commonly observed at the upstream side of the concentration front. A phase lead on the other hand will lead to oscillations at the downstream side of the front.

In the present study values chosen for $u$ and $\mathscr{D}$ are 0·369 and 0·00689, respectively, and results will be presented after 65 time steps ($\Delta t = 1$). The Fourier series analysis indicated that all second order corrected, implicit schemes with $\theta = 1$ are unstable. Thus these schemes will not be considered in further discussions. Figure 1 gives the concentration profiles for a few computational schemes calculated when no correction factors are used. The schemes are time-centred, Crank–Nicolson type approximations of the convective–dispersive equation. Note the poor performance of the finite difference scheme as compared to the other schemes. None of the schemes are able to remove the oscillations upstream of the concentration front. Also the scheme which uses $c^1$ Hermitian basis functions in space generates oscillations, roughly equal in amplitude to those obtained with $c^0$ quadratic functions. Because it is not the purpose of this study to discuss the relative merits of the different basis functions used in the finite element
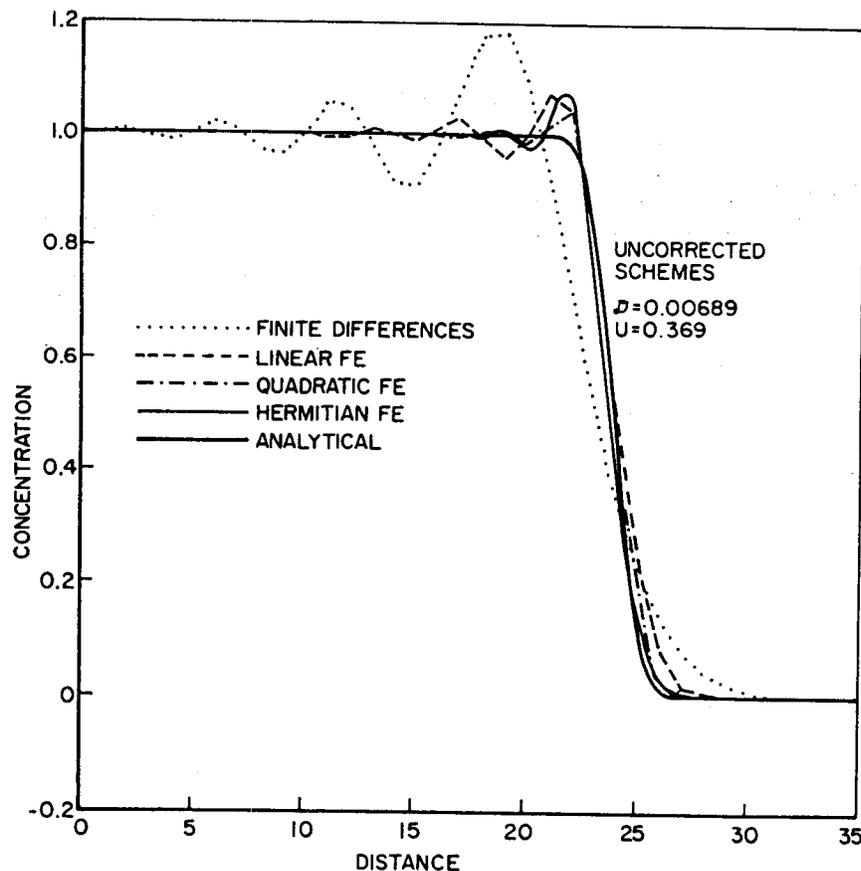


Figure 1. Concentration profiles obtained with various uncorrected finite difference and finite element schemes
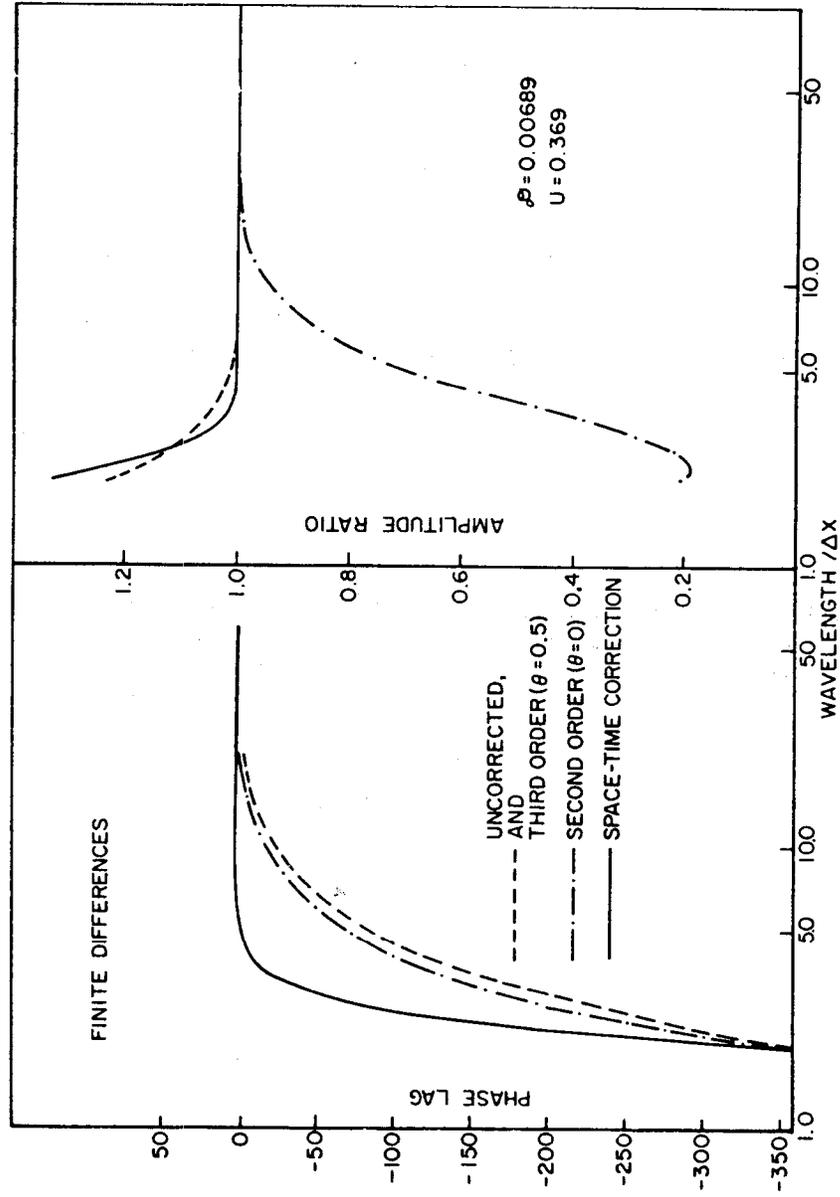
Figure 2. Phase lag and amplitude ratio obtained with several dispersion corrected finite difference schemes

formulation, we will now proceed with a discussion of each numerical method employed, showing the effects of the different dispersion corrections on the numerical results.

Results for standard finite differences using the various dispersion corrections are presented in Figures 2 and 3. Figure 2 gives a plot of the phase lag and amplitude ratio for each scheme, while Figure 3 compares the numerical solutions with the analytical results. The two figures indicate that the uncorrected and the third order correct schemes generate the same results. The fourth order correct scheme, although not shown, generated results which roughly duplicated those obtained with the uncorrected scheme. The fact that the small wavelengths are damped more and propagated somewhat better by the explicit scheme in comparison to the uncorrected, time centred scheme, leads to a marginally better description of the concentration profile. The space-time correction, when included in the difference scheme, markedly decreases the phase lag and, in general, improves the amplitude modification ratio. Figure 3 confirms that the space-time corrected scheme provides results which are better than those obtained with the other finite difference schemes considered here.

The phase lag and amplitude modification plots for the linear finite element schemes are given in Figure 4. It is apparent that the phase errors are reduced in comparison to the finite difference schemes. Errors in the amplitudes are, however, only slightly less in comparison to finite
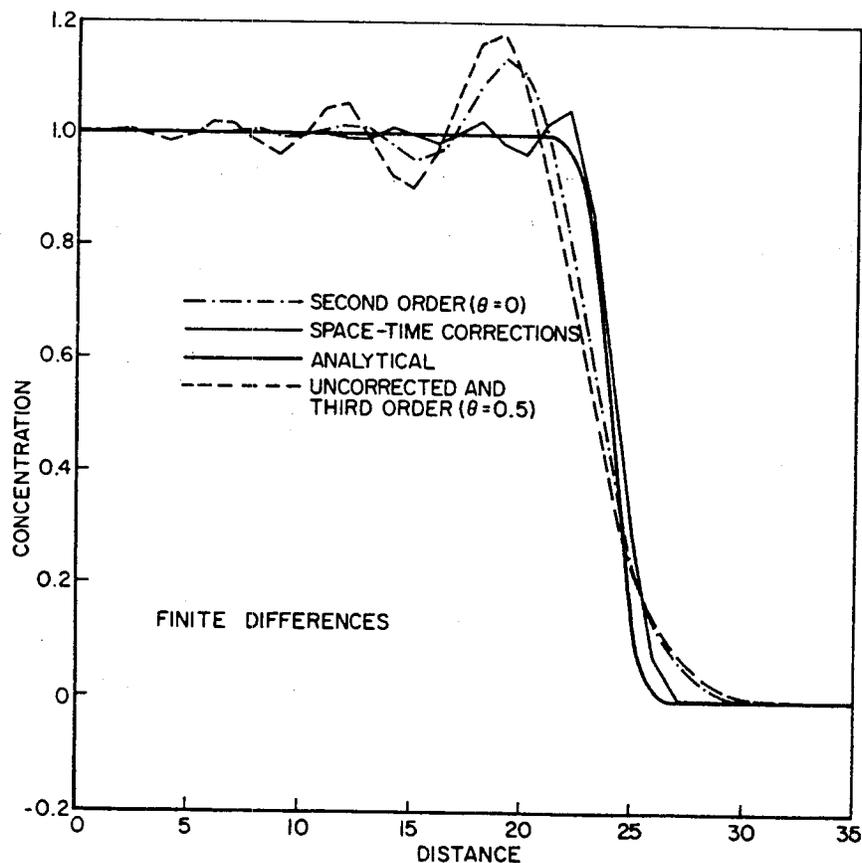


Figure 3. Concentration profiles obtained with several dispersion corrected finite difference schemes
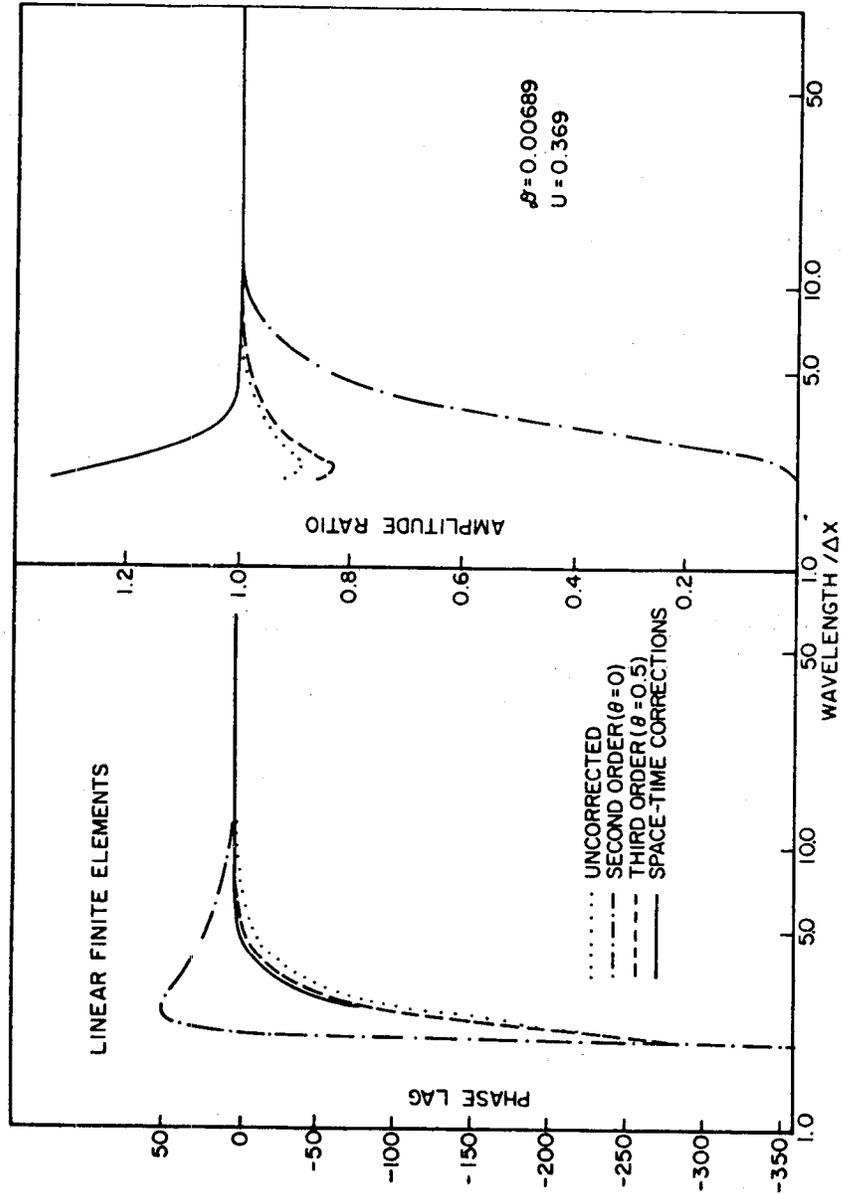
Figure 4. Phase lag and amplitude ratio obtained with several dispersion corrected linear finite element schemes

differences. Thus the oscillations near the concentration front should be reduced by the finite element schemes, but the steepness of the concentration front will be roughly the same as with finite differences, except for the uncorrected scheme. This is evidenced by the results plotted in Figure 5. Note that the space–time corrections and the third order time corrections lead now to approximately the same results. Perhaps the most interesting curves in Figures 4 and 5 are those for the second-order (explicit) scheme. The tremendous amount of damping observed with this scheme will smear the concentration front, while the phase lead for most wavelengths will cause oscillations to occur on the downstream side of the front. Thus this scheme produces a solution inferior to the other finite element schemes.

The curves in Figures 6 and 7 indicate that the third order correct in time scheme provides a slight improvement over the uncorrected scheme when quadratic elements are used. The phase lag plots of both schemes indicate that these two techniques are superior in accurately propagating the concentration fronts to all other schemes thus far considered. The third order in time correction reduces the oscillations in comparison to the uncorrected scheme by distributing the oscillations between the upstream and downstream sides of the concentration front. This is also evidenced by the fact that the corrected scheme shows a phase lag at the lower wavelengths and a phase lead at the higher wavelengths. The second order (explicit) scheme is very
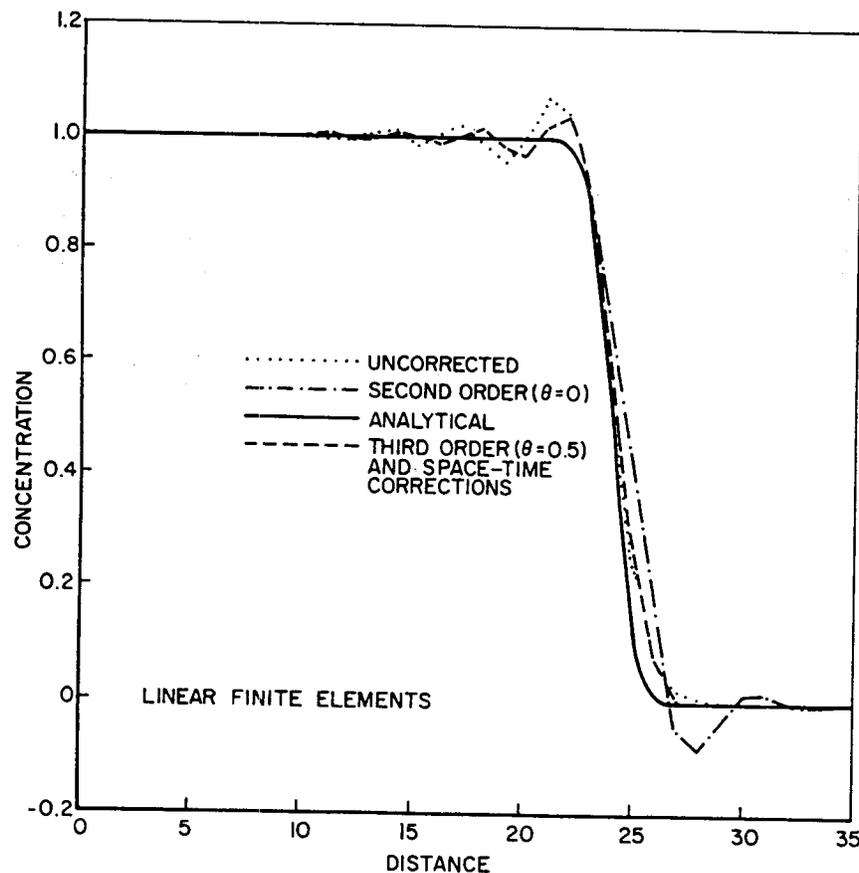


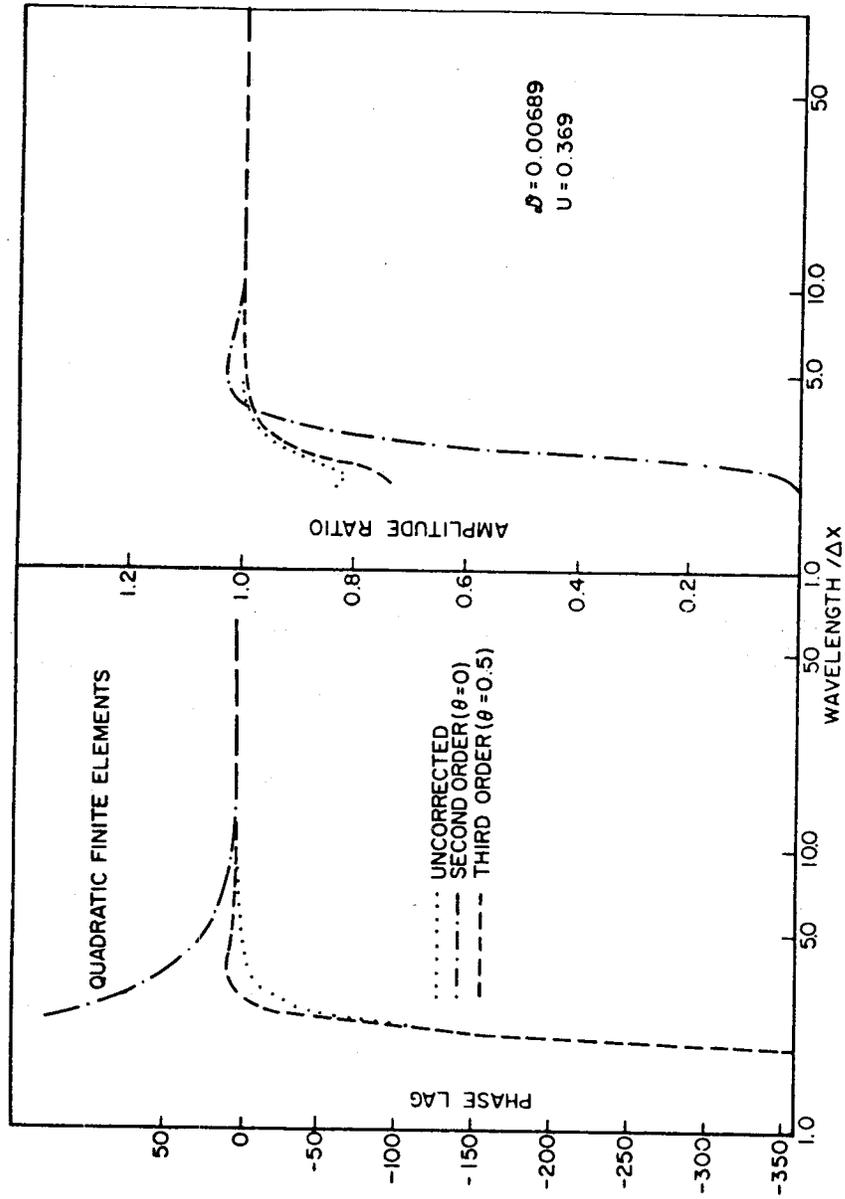Figure 5. Concentration profiles obtained with several dispersion corrected linear finite element schemes

Figure 6. Phase lag and amplitude ratio obtained with several dispersion corrected quadratic finite element schemes

disappointing in that it causes a large phase lead for small wavelengths. Thus the oscillations appear almost exclusively on the downstream side of the front (Figure 7). The severe damping of the amplitude modification at the same time causes the front to be smeared in comparison to the analytical solution.

The plots of the phase lag and amplitude ratio for the Hermitian scheme (Figure 8) indicate a tremendous improvement over the linear and quadratic finite element schemes. The very small wavelengths in particular are propagated much more accurately than by the previously analyzed methods, even for the uncorrected scheme. The phase lag for the third and fourth order in time corrected schemes is never more than half a degree, while the amplitude modification ratio for the fourth order corrected scheme is accurate to within half a per cent. The accuracy of the two corrected schemes is further evidenced by the numerical results plotted in Figure 9. The nodal values of the concentrations obtained with the two schemes nearly duplicate the analytical solution. Note the relatively severe overshoot upstream of the front obtained with the uncorrected scheme.

It should be mentioned that the Hermitian schemes have two possible stability eigenvalues. One corresponds to the physical problem being considered and the other corresponds to the computational mode. For the parameter values investigated here, the physical modes were
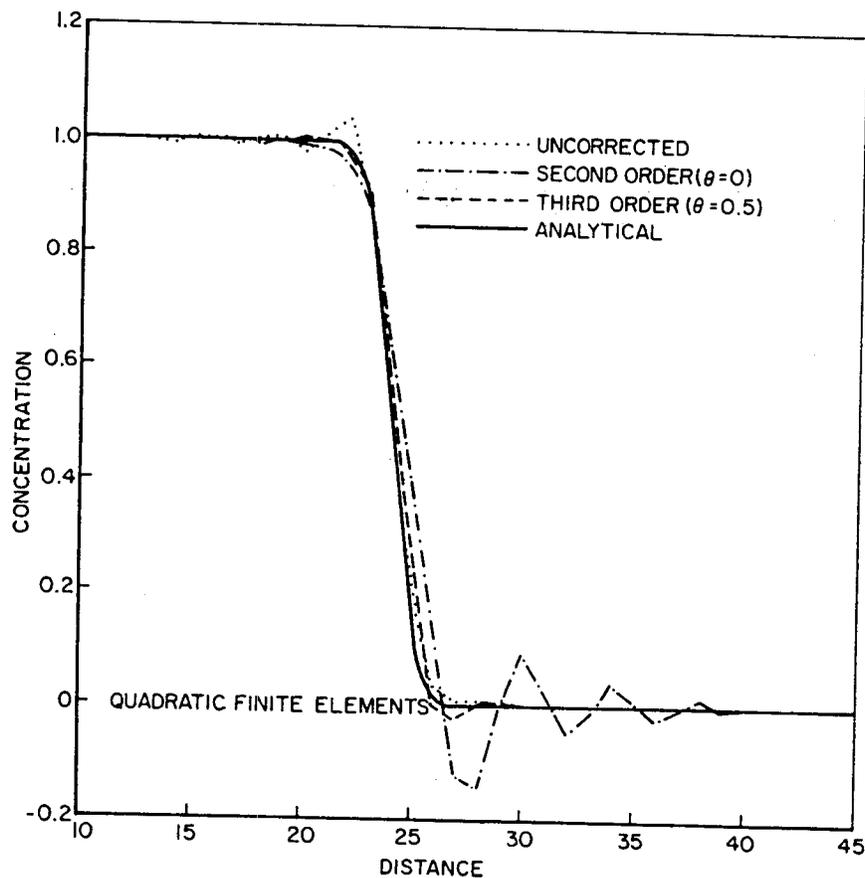


Figure 7. Concentration profiles obtained with several dispersion corrected quadratic finite element schemes
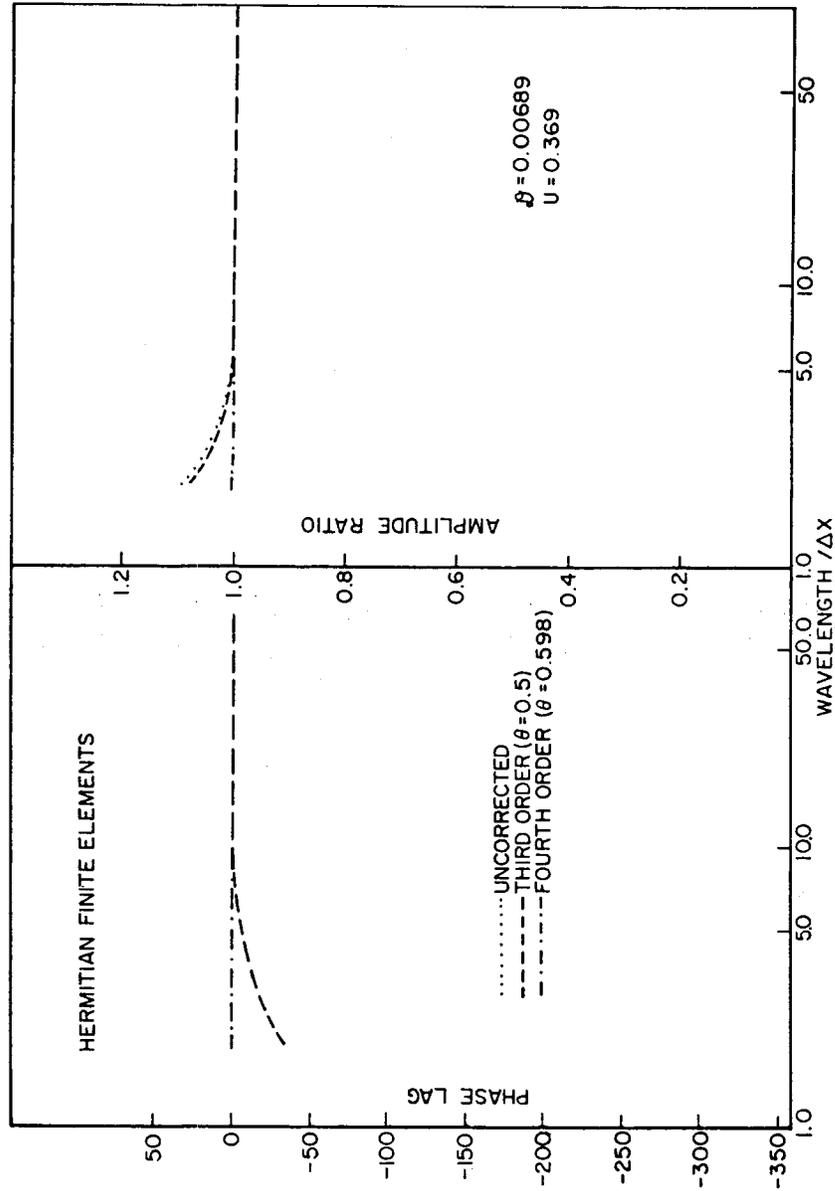
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Figure 8. Phase lag and amplitude ratio obtained with several dispersion corrected Hermitian finite element schemes

HERMITIAN FINITE ELEMENTS

.......... UNCORRECTED
————— ANALYTICAL
o o o o o o NODAL VALUES OF
THIRD ORDER($\theta$=0.5) AND
FOURTH ORDER($\theta$=0.598)
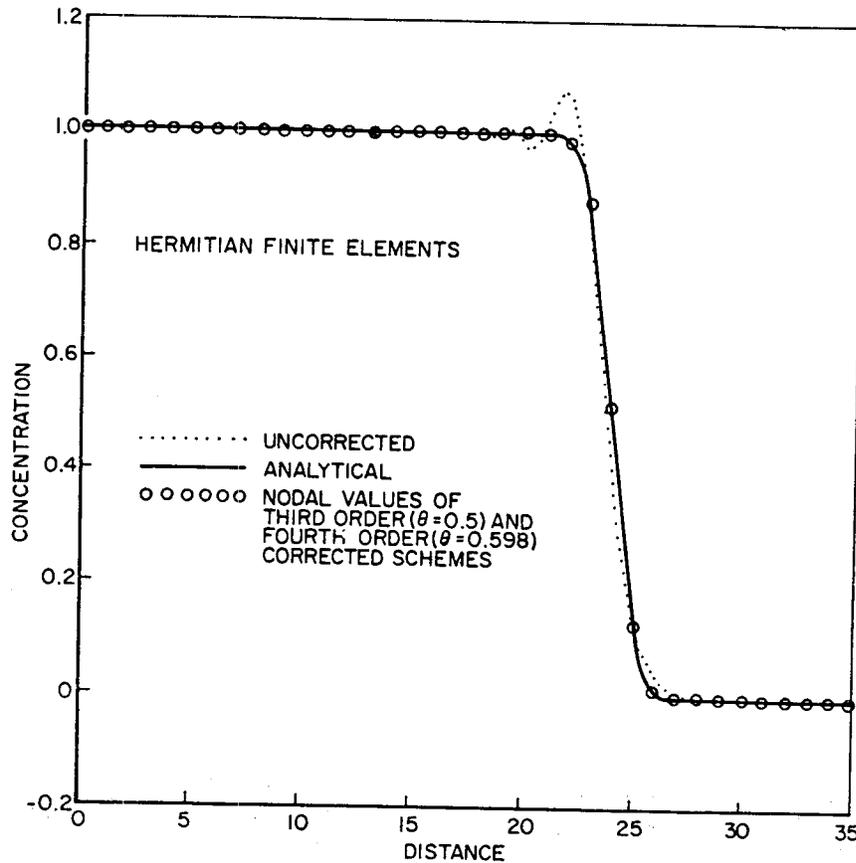CORRECTED SCHEMES

CONCENTRATION

DISTANCE

Figure 9. Concentration profiles obtained with several dispersion corrected Hermitian finite element schemes

found to be stable for the three schemes considered. The numerical mode for the uncorrected and the third order corrected schemes was also stable. A very slightly unstable numerical mode was detected, however, for the fourth order corrected scheme. This indicates that if this mode is introduced, possibly by numerical roundoff errors, it will grow and eventually swamp the physical solution. This difficulty was not encountered during the numerical calculations performed here, but it may cause some problems if the computations are carried out over a very long simulation time.

## CONCLUSIONS

Several higher order accurate finite difference and finite element computational schemes have been presented for solution of the convective–dispersive equation. The various schemes were made higher order accurate in time through the introduction of appropriate dispersion corrections in the numerical formulations. The most accurate standard finite difference and linear finite element schemes were obtained when fourth order space–time corrections were applied to each of the two schemes, in which case the two methods become identical. The quadratic finite element schemes which provided the best results were based on third and fourth order correct difference equations in time. Superior results were obtained with the dispersion corrected

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Hermitian schemes. A Fourier analysis showed that the phase lag for the corrected Hermitian schemes never exceeded half a degree, while the amplitude modification ratio for the fourth order corrected scheme was accurate to within half a per cent.

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