INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN FLUIDS, VOL. 15, 1171–1196 (1992)

ADVECTION–DIFFUSION MODELLING USING THE MODIFIED QUICK SCHEME

YIPING CHEN AND ROGER A. FALCONER

Department of Civil Engineering, University of Bradford, Bradford BD7 1DP, U.K.

SUMMARY

In recent years the QUICK finite difference scheme has been increasingly used in solving the advection–diffusion equation, particularly for water quality modelling studies relating to coastal and estuarine flows. This scheme has the benefits of mass conservation, reasonably high accuracy and computational efficiency in comparison with many other higher-order-accurate schemes reported in the recent literature. A von Neumann stability analysis showed that the explicit QUICK scheme has a severe stability constraint which depends upon the diffusion coefficient. It can be proved that this scheme is numerically unstable for the case of pure advection. Various modified forms of the implicit QUICK scheme have been formulated and their numerical stability properties have been studied and analysed. The modified QUICK schemes considered have been tested for transient simulations for the cases of pure advection and of advection and diffusion in an idealized one-dimensional basin using three different initial boundary conditions: (a) a sharp front concentration gradient, (b) a Gaussian concentration distribution and (c) a plug source. Details of the comparisons between these modified schemes and with other typical second-order-accurate difference schemes are given, together with comparisons with the analytical solutions for each case. A two-dimensional version of the semi-time-centred QUICK scheme (ADI-QUICK), has also been applied to a two-dimensional test case using the standard ADI technique and has been shown to be attractive in comparison with other comparable second-order schemes.

KEY WORDS Advection Diffusion Finite difference schemes Numerical modelling Solute transport Stability Truncation error Computer applications

INTRODUCTION

In recent years much effort has been focused on numerically solving the advection–diffusion equation (ADE) with higher accuracy and computational efficiency for regions of high solute gradients. The transient one-dimensional source-free transport of a scalar mass or pollutant concentration $S(x, t)$ in an open channel, where the water depth varies with both location x and time t, as for the case of tidal driven flow, can be modelled using the following form of the ADE:[1]

$$\frac{\partial S}{\partial t}+\frac{\partial (uS)}{\partial x}=\frac{\partial}{\partial x}\left(D\frac{\partial S}{\partial x}\right), \tag{1}$$

where $u(x, t)$ is the advection velocity and $D(x, t)$ is the diffusion coefficient. It is now widely appreciated that whilst the first-order upwind difference scheme will not generate wiggles (or grid-scale oscillations) in regions of high solute gradients or discontinuities, the scheme will nonetheless give rise to excessive numerical diffusion and is therefore inadequate for practical applications. On the other hand, whilst the conventional second-order-accurate central difference schemes (such as the Crank–Nicolson (C–N) scheme,[2] which has no numerical dissipation, and the Lax–Wendroff (L–W) scheme,[3] which has no numerical diffusion but some higher-order

0271–2091/92/221171–26$18.00

Received November 1991
Revised May 1992

dissipation) give more accurate results with tolerable numerical diffusion for most studies, these schemes generally exhibit pronounced oscillations when applied to the ADE with relatively small diffusion coefficients. These oscillations can spread throughout the model domain and swamp the true numerical results[4] or even produce only noise.[5] This effect is particularly pronounced in model simulations where steep gradients exist and is discussed in some detail by Leendertse.[6]

Some second-order schemes such as Formm's scheme[7] and the minimax-characteristics method[8] can reduce these oscillations substantially using an explicit formulation. However, the numerical stability of these schemes requires that the Courant number ($u\Delta t/\Delta x$) must be less than unity. Moreover, the advection and diffusion processes must be computed separately, thereby requiring additional computer resources. It is also interesting to note that Fromm's scheme and the minimax-characteristics method appear to be exactly the same in form and therefore produce exactly the same results. Consequently, only the minimax-characteristics method was used for comparative purposes in the present study.

Hogarth *et al.*[9] have compared 12 different explicit and implicit finite difference schemes up to third-order accuracy and found that the theoretical order of accuracy had little effect on the results if the diffusion number (i.e. $D\Delta t/(\Delta x)^2$) was not small. However, it is worth noting that the smallest diffusion number used in their study was 0·1 which is relatively large for water quality model studies in coastal and inland waters. For example, for a grid spacing of 100 m and a flow velocity of 0·5 m s^{-1}, with a Courant number and diffusion number of 0·5 and 0·1 respectively, this would lead to a diffusion coefficient of 10 m^2 s^{-1}, which is generally an upper-bound physical value for such studies. Another higher-order-accurate scheme proposed for hydraulics simulation is the two-point fourth-order scheme by Holly and Preissmann.[10] The idea of characteristics propagation and the Hermitian cubic polynomial representation for the scalar distribution within the computational domain was used and promising results were produced. It is, however, computationally more complicated and expensive for two-dimensional flows, where additional sets of equations are required to simulate not only the scalar quantity but also its spatial derivatives for the advection and diffusion processes.

The QUICK (Quadratic Upstream Interpolation for Convective Kinematics) difference scheme, based upon assuming quadratic upstream interpolation rather than linear interpolation between the grid points,[11] is third-order-accurate in space when used for a finite volume study and second-order-accurate for a finite difference model. This scheme does not treat the advection and diffusion processes separately and has been widely used for hydraulics and water quality studies in coastal and inland waters,[12–15] many of which are multidimensional. The QUICK scheme is attractive for practical engineering applications since it is mass-conservative, reasonably accurate, economical and relatively simple to implement and exhibits much weaker oscillations than the C–N second-order central difference scheme. These factors are particularly important for many practising and consulting engineers who rely heavily upon microcomputers for their model studies. The explicit QUICK representation of the ADE, as originally proposed by Leonard, is subject to a rather restrictive time step constraint which depends upon the grid spacing, the advection velocity and the diffusion coefficient.[16] Unfortunately, as will be shown later, this version of the QUICK scheme can become unstable using the traditional von Neumann analysis for the case of pure advection. Leonard and Noye has also modified the QUICK scheme using an implicit formulation,[17] although numerical tests reported herein showed that the resulting oscillations are little better than the C–N second-order central difference scheme. Two-dimensional and three-dimensional implicit QUICK-based formulations can also be found in the literature for unsteady flow studies using complicated and iterative solution procedures.[15,18]

The QUICKEST[11] scheme, on the other hand, is third-order-accurate both in time and space and generally gives better numerical results than the QUICK scheme in one-dimensional numerical tests for a Courant number of less than unity for pure advection. However, it is interesting to note that a two-dimensional version of the QUICKEST scheme, extended directly from its one-dimensional formulation,[19] produced unstable results for the case of pure advection for two-dimensional numerical tests for a uniform flow field with a constant Courant number (0·15) in both the x- and y-directions and a rotational flow field where the angular velocity was 0·007 s^{-1}. This one-dimensional stable but two-dimensional unstable phenomenon has also been proved analytically[20] but is beyond the scope of this paper.

The objective of this current study has therefore been to formulate and analyse various representations of the modified QUICK scheme which could overcome the stability problems of the explicit form and be applicable both to pure advection and to advection and diffusion. Also, accuracy and stability properties of each scheme have been investigated with regard to the scheme representation. In all, four modified forms of the implicit QUICK scheme have been formulated, with the numerical behaviour of each scheme being considered in some detail. The various forms of the QUICK scheme considered herein include (i) the forward explicit QUICK scheme, (ii) the fully time-centred implicit QUICK scheme, (iii) the backward implicit QUICK scheme, (iv) the semi-time-centred implicit QUICK scheme and (v) the semi-backward implicit QUICK scheme. The semi-time-centred QUICK scheme can easily be extended to two-dimensional applications based upon the ADI technique and has also been compared in this study with the results obtained using the C–N central scheme and the minimax-characteristics method.

FORMULATION OF VARIOUS QUICK SCHEMES

If we express the spatial difference terms in a forward explicit ($\alpha = 0$), fully time-centred implict ($\alpha = 0{\cdot}5$) or backward implicit ($\alpha = 1$) representation with respect to time, the finite difference representations of equation (1) over a time step can be written as

$$S_j^{n+1} + \alpha(\varepsilon_{j+1/2}^{n+1} S_{j+1/2}^{n+1} - \varepsilon_{j-1/2}^{n+1} S_{j-1/2}^{n+1}) - \alpha[\gamma_{j+1/2}^{n+1}(S_{j+1}^{n+1} - S_j^{n+1}) - \gamma_{j-1/2}^{n+1}(S_j^{n+1} - S_{j-1}^{n+1})]$$
$$= S_j^n - (1-\alpha)(\varepsilon_{j+1/2}^n S_{j+1/2}^n - \varepsilon_{j-1/2}^n S_{j-1/2}^n) + (1-\alpha)[\gamma_{j+1/2}^n(S_{j+1}^n - S_j^n) - \gamma_{j-1/2}^n(S_j^n - S_{j-1}^n)], \quad (2)$$

where

$$\varepsilon_{j+1/2}^n = u_{j+1/2}^n \Delta t/\Delta x \quad \text{and} \quad \gamma_{j+1/2}^n = D_{j+1/2}^n \Delta t/\Delta x^2 \quad (3)$$

are the Courant and diffusion numbers respectively, with Δt the time step and Δx the grid size, n is the time step number and $S_{j+1/2}^n$ and $u_{j+1/2}^n$ are the concentration and velocity values respectively at grid point $j+\frac{1}{2}$ at $t = n\Delta t$, as illustrated in Figure 1. The value of $S_{j+1/2}^n$ can be obtained by quadratic upstream interpolation, giving

$$S_{j+1/2}^n = \begin{cases} \frac{1}{2}(S_{j+1}^n + S_j^n) - \frac{1}{8}\nabla^2 S_j^n & \text{if } u_{j+1/2}^n > 0, \\ \frac{1}{2}(S_{j+1}^n + S_j^n) - \frac{1}{8}\nabla^2 S_{j+1}^n & \text{if } u_{j+1/2}^n < 0 \end{cases}, \quad (4)$$

in which

$$\nabla^2 S_j^n = S_{j+1}^n - 2S_j^n + S_{j-1}^n. \quad (5)$$

The terms $\varepsilon_{j+1/2}^{n+1}$, $\gamma_{j+1/2}^{n+1}$, $S_{j+1/2}^{n+1}$ and $\nabla^2 S_j^{n+1}$ correspond to those given in equations (3)–(5) at time level $n+1$. Although equatioin (2) appears to be central in space, the resulting finite difference scheme is actually biased upwind after substituting equation (4) into equation (2). By doing so and assuming for the purpose of this analysis that $u_{j+1/2}^n > 0$ and $u_{j-1/2}^n > 0$, three different QUICK scheme representations can be obtained as follows:

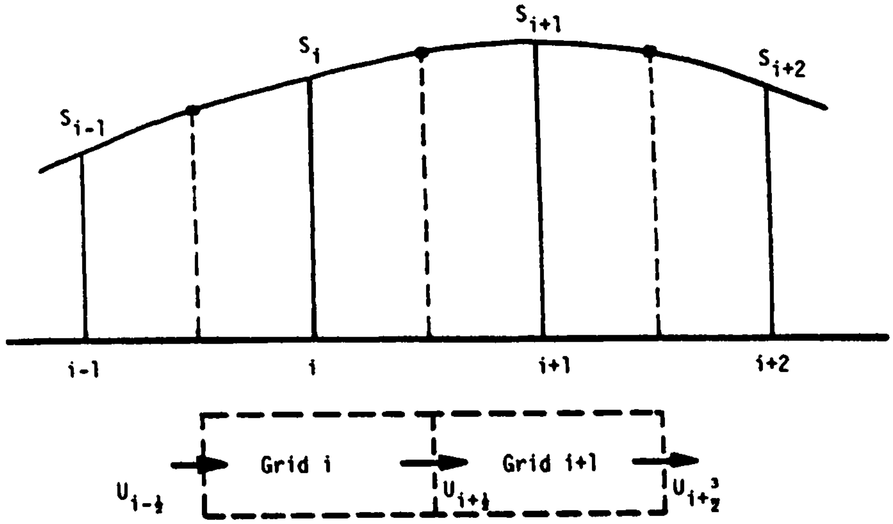


Figure 1. Sketch of grid representation for the QUICK scheme

(i) forward explicit QUICK scheme

$$S_j^{n+1} = S_j^n - \tfrac{1}{2}\left[\varepsilon^n_{j+1/2}(S^n_{j+1}+S^n_j) - \varepsilon^n_{j-1/2}(S^n_j+S^n_{j-1})\right] + \tfrac{1}{8}\left(\varepsilon^n_{j+1/2}\nabla^2 S^n_j - \varepsilon^n_{j-1/2}\nabla^2 S^n_{j-1}\right)$$
$$+\gamma^n_{j+1/2}(S^n_{j+1}-S^n_j) - \gamma^n_{j-1/2}(S^n_j - S^n_{j-1}), \tag{6}$$

(ii) fully time-centred implicit QUICK scheme

$$S_j^{n+1} + \tfrac{1}{4}\left[\varepsilon^{n+1}_{j+1/2}(S^{n+1}_{j+1}+S^{n+1}_j) - \varepsilon^{n+1}_{j-1/2}(S^{n+1}_j+S^{n+1}_{j-1})\right] - \tfrac{1}{16}\left(\varepsilon^{n+1}_{j+1/2}\nabla^2 S^{n+1}_j - \varepsilon^{n+1}_{j-1/2}\nabla^2 S^{n+1}_{j-1}\right)$$
$$-\frac{\gamma^{n+1}_{j+1/2}}{2}(S^{n+1}_{j+1}-S^{n+1}_j) + \frac{\gamma^{n+1}_{j-1/2}}{2}(S^{n+1}_j - S^{n+1}_{j-1})$$
$$= S_j^n - \tfrac{1}{4}\left[\varepsilon^n_{j+1/2}(S^n_{j+1}+S^n_j) - \varepsilon^n_{j-1/2}(S^n_j+S^n_{j-1})\right] + \tfrac{1}{16}\left(\varepsilon^n_{j+1/2}\nabla^2 S^n_j - \varepsilon^n_{j-1/2}\nabla^2 S^n_{j-1}\right)$$
$$+\frac{\gamma^n_{j+1/2}}{2}(S^n_{j+1}-S^n_j) - \frac{\gamma^n_{j-1/2}}{2}(S^n_j - S^n_{j-1}), \tag{7}$$

(iii) backward implicit QUICK scheme

$$S_j^{n+1} + \tfrac{1}{2}\left[\varepsilon^{n+1}_{j+1/2}(S^{n+1}_{j+1}+S^{n+1}_j) - \varepsilon^{n+1}_{j-1/2}(S^{n+1}_j+S^{n+1}_{j-1})\right] - \tfrac{1}{8}\left(\varepsilon^{n+1}_{j+1/2}\nabla^2 S^{n+1}_j - \varepsilon^{n+1}_{j-1/2}\nabla^2 S^{n+1}_{j-1}\right)$$
$$-\gamma^{n+1}_{j+1/2}(S^{n+1}_{j+1}-S^{n+1}_j) + \gamma^{n+1}_{j-1/2}(S^{n+1}_j - S^{n+1}_{j-1}) = S^n_j. \tag{8}$$

The value of $S^n_{j+1/2}$ obtained from equations (4) and (5) can be regarded as a combination of a linear interpolation and an upwind curvature adjustment. Including this term at the new time level $n+1$ in the above-listed schemes (ii) and (iii) has resulted in quadridiagonal matrices for unidirectional flow and pentadiagonal matrices for directional flow. Although solving a pentadiagonal matrix can be very efficient as discussed later, it requires at least 2·4 times more arithmetic operations than those needed for a tridiagonal solver and also requires more working memory space. In many practical engineering studies it is often desirable to obtain reasonably accurate results using a minimum of computational effort. For example, in flow and water quality modelling in coastal waters simulations often involves long-term predictions of many water quality parameters. Hence, since the tridiagonal solver has proved to be the most efficient method in dealing with implicit problems, it should be used whenever possible if the same magnitude of accuracy can be achieved.

Following the method first suggested by Leonard,[11] Falconer and Liu[12] represented the linear term in equation (4) at the new time level and the curvature term at the old time level when calculating the value of $S_{j+1/2}^{n+1}$. This approach is equivalent to assuming that the curvature of the concentration distribution does not change much from time level n to $n+1$, i.e. $\nabla^2 S_j^{n+1} \approx \nabla^2 S_j^n$, giving

$$S_{j+1/2}^{n+1} = \begin{cases} \frac{1}{2}(S_j^{n+1} + S_{j+1}^{n+1}) - \frac{1}{8}\nabla^2 S_j^n & \text{if } u_{j+1/2}^{n+1} > 0, \\ \frac{1}{2}(S_j^{n+1} + S_{j+1}^{n+1}) - \frac{1}{8}\nabla^2 S_{j-1}^n & \text{if } u_{j+1/2}^{n+1} < 0, \end{cases} \tag{9}$$

This representation enables two more schemes to be constructed which only result in tridiagonal matrices. These schemes include (for $u_{j+1/2}^{n+1} > 0$):

(iv) semi-time Centred Implicit QUICK Scheme

$$S_j^{n+1} + \tfrac{1}{4}[\varepsilon_{j+1/2}^{n+1}(S_{j+1}^{n+1} + S_j^{n+1}) - \varepsilon_{j-1/2}^{n+1}(S_j^{n+1} + S_{j-1}^{n+1})] - \frac{\gamma_{j+1/2}^{n+1}}{2}(S_{j+1}^{n+1} - S_j^{n+1})$$

$$+ \frac{\gamma_{j-1/2}^{n+1}}{2}(S_j^{n+1} - S_{j-1}^{n+1}) = S_j^n - \tfrac{1}{4}[\varepsilon_{j+1/2}^n(S_{j+1}^n + S_j^n) - \varepsilon_{j-1/2}^n(S_j^n + S_{j-1}^n)] + \frac{\gamma_{j+1/2}^n}{2}(S_{j+1}^n - S_j^n)$$

$$- \frac{\gamma_{j-1/2}^n}{2}(S_j^n - S_{j-1}^n) + \tfrac{1}{16}[(\varepsilon_{j+1/2}^n + \varepsilon_{j+1/2}^{n+1})\nabla^2 S_j^n - (\varepsilon_{j-1/2}^n + \varepsilon_{j-1/2}^{n+1})\nabla^2 S_{j-1}^n], \tag{10}$$

(v) semi-backward implicit QUICK scheme

$$S_j^{n+1} + \tfrac{1}{2}[\varepsilon_{j+1/2}^{n+1}(S_{j+1}^{n+1} + S_j^{n+1}) - \varepsilon_{j-1/2}^{n+1}(S_j^{n+1} + S_{j-1}^{n+1})] - \gamma_{j+1/2}^{n+1}(S_{j+1}^{n+1} - S_j^{n+1})$$

$$+ \gamma_{j-1/2}^{n+1}(S_j^{n+1} - S_{j-1}^{n+1}) = S_j^n + \tfrac{1}{8}(\varepsilon_{j+1/2}^{n+1}\nabla^2 S_j^n - \varepsilon_{j-1/2}^{n+1}\nabla^2 S_{j-1}^n). \tag{11}$$

Although other algorithms may also be formulated, such as that given by Leonard and Noye,[17] the above-listed schemes (i)–(iii) include various representative forms of the QUICK algorithm; with schemes (iv) and (v) being the simplified forms of schemes (ii) and (iii) respectively. Another alternative to schemes (ii) and (iii) in order to preserve a tridiagonal matrix is to set all values outside the tridiagonal region to the corresponding values at the previous time level. In doing so, however, a pronounced phase error was observed in all the numerical tests, giving rise to reduce accuracy. Hence this alternative formulation has not been considered further herein. In the following section the numerical stability and accuracy properties of each of the schemes listed above will be analysed in more detail.

STABILITY AND ACCURACY ANALYSIS

In analysing the numerial stability and accuracy of these various forms of the QUICK scheme, it is first convenient to assume that the flow velocity and the diffusion coefficients are constant, giving

$$\varepsilon_{j+1/2}^{n+1} = \varepsilon_{j-1/2}^{n+1} = \varepsilon_{j+1/2}^n = \varepsilon_{j-1/2}^n = \varepsilon > 0, \qquad \gamma_{j+1/2}^{n+1} = \gamma_{j-1/2}^{n+1} = \gamma_{j+1/2}^n = \gamma_{j-1/2}^n = \gamma \geqslant 0. \tag{12}$$

Stability analysis

The von Neumann method was used for the stability analysis in this study since, although the matrix method can include the boundary conditionhs on the overall stability of the scheme, previous research in comparing these two methods of stability analysis has indicated that the classical von Neumann method is generally to be preferred, regardless of the type of boundary conditions.[21] The Fourier components of $S(x, t)$ at location j and time level n can be expressed as

$$S_j^n = \xi^n \, \mathrm{e}^{\mathrm{i}kj\Delta x} \tag{13}$$

where ξ^n is the amplitude of the Fourier component at $n\Delta t$, k is the wave number and $\mathrm{i} = \sqrt{(-1)}$. Defining $\theta = k\Delta x$, the numerical stability of a scheme requires that the amplification factor over one complete time step must satisfy the following condition for all possible values of θ:[22]

$$|G(\theta)| = |\xi^{n+1}/\xi^n| \leqslant 1 \tag{14}$$

Further to this requirement and following the von Neumann stability analysis procedure outlined in Reference 22, the amplification factor can be evaluated for each scheme as follows.

For scheme (i)

$$G_1(\theta) = 1 - \varepsilon \sin^4(\theta/2) - 4\gamma \sin^2(\theta/2) - \mathrm{i}\varepsilon[1 + \tfrac{1}{2}\sin^2(\theta/2)]\sin\theta \tag{15}$$

and

$$|G_1(\theta)|^2 = 1 - \{\varepsilon[2\sin^2(\theta/2) + 3\varepsilon\sin^4(\theta/2) - 4\varepsilon - 8\gamma\sin^4(\theta/2)] + 8\gamma[1 - 2\gamma\sin^2(\theta/2)]\}\sin^2(\theta/2). \tag{16}$$

Numerical stability requires that the term in braces in equation (16) must be greater than or equal to zero, giving

$$\varepsilon \leqslant \frac{(8/P_\Delta)[1 - 2\gamma\sin^2(\theta/2)] + 2\sin^2(\theta/2)[1 - 4\gamma\sin^2(\theta/2)]}{4 - 3\sin^4(\theta/2)} \tag{17}$$

where $P_\Delta = |\varepsilon|/\gamma = |u|\Delta x/D$ is called the cell Peclet number or the cell Reynolds number. Two extreme conditions can be obtained from this equation, the first being the short-wavelength requirement when $\theta = \pi$ or $k = \pi/\Delta x$, and the second being the cut-off long-wavelength restriction when $\theta \to \theta^*$ ($= 2\pi/N$, where N is the grid number of the computational domain). The stability requirement of this scheme therefore becomes

$$\varepsilon \leqslant \min\{2 - 4\gamma,\ 2/P_\Delta + (\pi/N)^2[\tfrac{1}{2} - 4\gamma/P_\Delta - 2\gamma(\pi/N)^2]\}. \tag{18}$$

For the limiting case of $N \to \infty$, equation (18) thereby reduces to

$$\varepsilon \leqslant \min[2 - 4\gamma,\ \sqrt{(2\gamma)}]. \tag{19}$$

It can be seen from this equation that the stable region of the (ε, γ)-plane for scheme (i) depends upon the diffusion coefficient and is very small as illustrated graphically in Figure 2. It can also be noted from equation (19) that scheme (i) is numerically unstable when $N \to \infty$ for the case of pure advection, i.e. when $\gamma = 0$. For finite values of N the stability requirement for ε is much less restrictive, based upon the cut-off long-wavelength condition[23] given by equation (18). However, the stability requirement for ε is still very severe, giving, for example, $\varepsilon \leqslant 0{\cdot}00197$ and $\varepsilon \leqslant 0{\cdot}0000789$ for N-values of 50 and 250 respectively. This stability requirement is highly impractical for most flow and water quality applications in water engineering, since the number of grid cells employed in such studies is relatively large, with a typical two-dimensional model study including over 100×200 grid nodes.

For scheme (ii)

$$G_2(\theta) = \frac{1 - 2\gamma\sin^2(\theta/2) - (\varepsilon/2)\sin^4(\theta/2) - \mathrm{i}(\varepsilon/2)[1 + \tfrac{1}{2}\sin^2(\theta/2)]\sin\theta}{1 + 2\gamma\sin^2(\theta/2) + (\varepsilon/2)\sin^4(\theta/2) + \mathrm{i}(\varepsilon/2)[1 + \tfrac{1}{2}\sin^2(\theta/2)]\sin\theta} \tag{20}$$

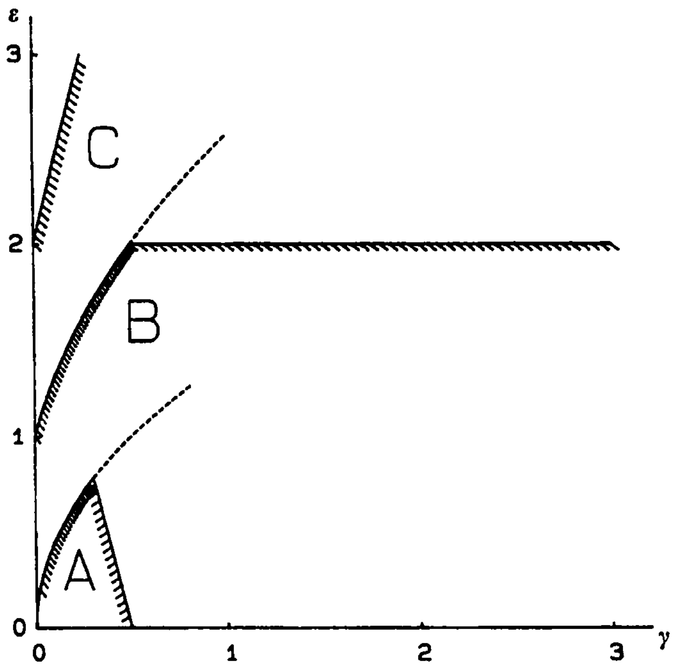


Figure 2. Stable region of (γ, ε)-plane for (A) the explicit QUICK, (B) the semi-time-centred QUICK and (C) the semi-backward QUICK schemes

and

$$|G_2(\theta)|^2 = 1 - \frac{8\gamma \sin^2(\theta/2) + 2\varepsilon \sin^4(\theta/2)}{[1 + 2\gamma \sin^2(\theta/2) + (\varepsilon/2)\sin^4(\theta/2)]^2 + (\varepsilon^2/4)[1 + \frac{1}{2}\sin^2(\theta/2)]^2 \sin^2\theta} \tag{21}$$

where $|G_2(\theta)|^2 \leqslant 1$ is always maintained for any values of θ, γ and ε (recalling that $\gamma \geqslant 0$ and $\varepsilon > 0$ for all cases), so that scheme (ii) is unconditionally stable.

For scheme (iii)

$$G_3(\theta) = \frac{1}{1 + \varepsilon \sin^4(\theta/2) + 4\gamma \sin^2(\theta/2) + \mathrm{i}\varepsilon[1 + \frac{1}{2}\sin^2(\theta/2)]\sin\theta} \tag{22}$$

and

$$|G_3(\theta)|^2 = \frac{1}{[1 + \varepsilon \sin^4(\theta/2) + 4\gamma \sin^2(\theta/2)]^2 + \varepsilon^2[1 + \frac{1}{2}\sin^2(\theta/2)]^2 \sin^2\theta}. \tag{23}$$

Again we see that $|G_3(\theta)| \leqslant 1$ is always maintained for any values of θ, γ and ε, so that scheme (iii) is also unconditionally stable.

For scheme (iv)

$$G_4(\theta) = \frac{1 - \varepsilon \sin^4(\theta/2) - 2\gamma \sin^2(\theta/2) - \mathrm{i}(\varepsilon/2)[1 + \sin^2(\theta/2)]\sin\theta}{1 + 2\gamma \sin^2(\theta/2) + \mathrm{i}(\varepsilon/2)\sin\theta}. \tag{24}$$

and

$$|G_4(\theta)|^2 = 1 - \frac{4\gamma[2-\varepsilon\sin^4(\theta/2)]\sin^2(\theta/2)+\varepsilon[2-2\varepsilon+\varepsilon\sin^2(\theta/2)]\sin^4(\theta/2)}{1+4\gamma\sin^2(\theta/2)+4\gamma^2\sin^4(\theta/2)+\varepsilon^2[1-\sin^2(\theta/2)]\sin^2(\theta/2)}. \quad (25)$$

To ensure that $|G_2(\theta)|^2 \leqslant 1$, this scheme requires that

$$4\gamma[2-\varepsilon\sin^4(\theta/2)]+\varepsilon[2-2\varepsilon+\varepsilon\sin^2(\theta/2)]\sin^2(\theta/2)\geqslant 0. \quad (26)$$

Hence the stability constraint becomes

$$\varepsilon \leqslant \begin{cases} 2 & \text{if } P_\Delta \leqslant 4, \\ 1+4/P_\Delta & \text{if } P_\Delta > 4. \end{cases} \quad (27)$$

From either $\gamma=0$ in equation (25) or $P_\Delta \to \infty$ in equation (27) we have the stability restriction for the case of pure advection that

$$\varepsilon \leqslant 1. \quad (28)$$

For scheme (v)

$$G_5(\theta) = \frac{1-\varepsilon\sin^4(\theta/2)-\mathrm{i}(\varepsilon/2)\sin\theta\sin^2(\theta/2)}{1+4\gamma\sin^2(\theta/2)+\mathrm{i}\varepsilon\sin\theta} \quad (29)$$

and

$$|G_5(\theta)|^2 = \frac{1-\varepsilon[2-\varepsilon\sin^2(\theta/2)]\sin^4(\theta/2)}{[1+4\gamma\sin^2(\theta/2)]^2+\varepsilon^2\sin^2\theta}. \quad (30)$$

The stability constraint of this scheme can be shown to be

$$\varepsilon \leqslant 2+4\gamma \quad (31)$$

for the case of advection-diffusion.

The stable regions of the (ε, γ)-plane for schemes (iv) and (v) are also shown in Figure 2, where it can be seen that the stability constraints for schemes (iv) and (v) for the case of advection and diffusion are less restrictive than those for pure advection. For the case of $\varepsilon<0$ a similar analysis has been undertaken for all schemes and similar results obtained for $|\varepsilon|$.

Truncation error

In determining the accuracy of the various representations of the QUICK scheme highlighted herein, it is first worth noting that equations (6)–(8), (10), and (11) represent the solution of the following modified transport equation for a constant advection velocity and a constant diffusion coefficient:

$$\frac{\partial S}{\partial t}+u\frac{\partial S}{\partial x}=D\frac{\partial^2 S}{\partial x^2}+TE \quad (32)$$

where TE is a truncation error term.

By carrying out a Taylor series expansion at grid point j and time level n for the five schemes listed previously, the major truncation error term for each scheme (designated by the subscripts

1–5 respectively) is given as

$$TE_1 = -\frac{\Delta t u^2}{2}\frac{\partial^2 S}{\partial x^2} - u\Delta x^2\left(\frac{1}{24}-\gamma\right)\frac{\partial^3 S}{\partial x^3} - \frac{D\Delta x^2}{2}\left(\gamma - \frac{1}{6} + \frac{P_\Delta}{8}\right)\frac{\partial^4 S}{\partial x^4} + O(\Delta t^2, \Delta x^4), \tag{33}$$

$$TE_2 = -\frac{u\Delta x^2}{24}\frac{\partial^3 S}{\partial x^3} + \frac{D\Delta x^2}{16}\left(\frac{1}{3} - P_\Delta + \frac{\varepsilon P_\Delta}{3}\right)\frac{\partial^4 S}{\partial x^4} + O(\Delta t^2, \Delta x^4), \tag{34}$$

$$TE_3 = \frac{\Delta t u^2}{2}\frac{\partial^2 S}{\partial x^2} - u\Delta x^2\left(\frac{1}{24}+\gamma\right)\frac{\partial^3 S}{\partial x^3} + \frac{D\Delta x^2}{2}\left(\gamma + \frac{1}{12} - \frac{P_\Delta}{8} + \frac{\varepsilon P_\Delta}{12}\right)\frac{\partial^4 S}{\partial x^4} + O(\Delta t^2, \Delta x^4), \tag{35}$$

$$TE_4 = -\frac{u\Delta x^2}{24}\frac{\partial^3 S}{\partial x^3} + \frac{D\Delta x^2}{4}\left(\frac{1}{12} - \frac{P_\Delta}{4} + \frac{\varepsilon P_\Delta}{3}\right)\frac{\partial^4 S}{\partial x^4} + O(\Delta t^2, \Delta x^4), \tag{36}$$

$$TE_5 = \frac{\Delta t u^2}{2}\frac{\partial^2 S}{\partial x^2} - u\Delta x^2\left(\frac{1}{24}+\gamma\right)\frac{\partial^3 S}{\partial x^3} + \frac{D\Delta x^2}{2}\left(\gamma + \frac{1}{12} - \frac{P_\Delta}{8} + \frac{\varepsilon P_\Delta}{3}\right)\frac{\partial^4 S}{\partial x^4} + O(\Delta t^2, \Delta x^4). \tag{37}$$

In comparing these schemes, it can be seen that the truncation error for schemes (iii) and (v) includes a numerical diffusion term with the numerical diffusion coefficient being $0{\cdot}5\Delta t u^2$, whereas schemes (ii) and (iv) do not exhibit numerical diffusion for the accuracy quoted. All these schemes are second-order-accurate in space for the current finite difference study, with schemes (ii) and (iv) also being second-order-accurate in time and schemes (i), (iii) and (v) only being first-order-accurate.

It is worth pointing out that third-order accuracy in space can be achieved if the above QUICK schemes are used in the finite volume approach, based upon the assumption of a local quadratic distribution. To achieve third-order spatial accuracy for advection in the finite difference model, the factor of $\frac{1}{8}$ in equations (4) and (9) needs to be replaced by $\frac{1}{6}$, thereby resulting in the third-order upwind difference scheme.[24]

The leading error effects associated with schemes (i), (iii) and (v) are amplitude-based, whereas with schemes (ii) and (iv) phase error effects are more significant. Hence schemes (ii) and (iv), which are time-centred or semi-time-centred, would therefore be expected to produce more accurate results in terms of amplitude consistency than schemes (iii) and (v). It is also worth noting that schemes (iv) and (v) have an extra truncation error term of $(u^2\Delta x^2\Delta t/16)\,\partial^4 S/\partial x^4$ and $(u^2\Delta x^2\Delta t/8)\,\partial^4 S/\partial x^4$ compared with those of schemes (ii) and (iii) respectively. These extra error terms result from the approximations of $\nabla^2 S_j^{n+1}$ by $\nabla^2 S_j^n$, which are proportional to $u\varepsilon\Delta x^3$ and do not have primary effects on the computation results when the Courant number is relatively small. The forward explicit QUICK scheme has another disadvantage as well as the severe numerical stability constraint, in that the point-to-point transfer property of the scheme when $\varepsilon = 1$ is not observed. Needless to say, this property is not obvious for implicit schemes, since linear systems must be solved simultaneously to obtain numerical results.

NUMERICAL TESTS FOR IDEALIZED ONE-DIMENSIONAL BASIN

Following the preceding analysis, the various modified forms of the implicit QUICK schemes were tested for the severest case of pure advection in an idealized one dimensional reach, of 250 grid lengths (each of length Δx), such that any disturbance at the upstream side of the test reach would take 1000 time steps to propagate out of the reach completely for a chosen value of $\varepsilon = 0{\cdot}25$, or 500 time steps for $\varepsilon = 0{\cdot}5$. Three idealized concentration gradients were considered (a) a sharp front concentration gradient with a change in concentration from zero to a maximum within a single grid length, (b) a Gaussian concentration distribution with a standard deviation of $3\Delta x$

and (c) a plug source with an initial plug width of $8\Delta x$. These initial conditions were set and centred at $x_o(=10\Delta x)$ at the commencement of simulation, with the upstream boundary condition being set to

$$S_0^{n+1}=\begin{cases} S_o & \text{for test case (a)} \\ 0 & \text{for test cases (b) and (c),} \end{cases} \tag{38}$$

and for a downstream boundary condition of

$$S_N^{n+1}=0. \tag{39}$$

Advection–diffusion simulations using these three initial boundary conditions were also undertaken for a constant Courant number and a constant diffusion coefficient. Numerical test results of the modified schemes (ii)–(v) were also compared with other second-order schemes and the exact solutions for each test case. The exact solutions of the advection-diffusion equation for test cases (a) and (c) were given by van Genuchten and Alves,[25] with the exact solution for test case (b) being obtained by solving the diffusion equation for a moving origin propagating at the advection velocity.

The standard Gauss elimination and back-substitution technique (Thomas algorithm[26]) was employed to solve the tridiagonal system for schemes (iv) and (v). However, schemes (ii) and (iii) required the solution of a quadridiagonal system for steady unidirectional flow and pentadiagonal system for unsteady directional flow. The linear equation system was expressed in matrix form as

$$\lambda\mathbf{S}=\mathbf{B}, \tag{40}$$

in which the vector $\mathbf{S}=\{S_1^{n+1}, S_2^{n+1}, \ldots, S_N^{n+1}\}^T$, $\mathbf{B}$ is a vector containing the corresponding terms associated with time level n on the right-hand side of equation (7) or (8), and the matrix λ contains only four or five non-zero diagonal elements depending upon the local flow directions. The standard LU decomposition method was used to solve equation (40) in two stages similar to that of the Thomas algorithm. The matrix λ was decomposed into two matrices $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$, with the matrix $\boldsymbol{\alpha}$ containing non-zero lower triangular elements only and the matrix $\boldsymbol{\beta}$ containing non-zero upper triangular elements only. Both matrices $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ contained no more than three non-zero diagonal lines. In solving equation (40), the method is equivalent to determining firstly the vector $\mathbf{T}$ by solving the equation $\boldsymbol{\alpha}\mathbf{T}=\mathbf{B}$ and secondly the vector $\mathbf{S}$ by solving the equation $\boldsymbol{\beta}\mathbf{S}=\mathbf{T}$, since

$$\lambda\mathbf{S}=(\boldsymbol{\alpha}\boldsymbol{\beta})\mathbf{S}=\boldsymbol{\alpha}(\boldsymbol{\beta}\mathbf{S})=\boldsymbol{\alpha}\mathbf{T}=\mathbf{B}. \tag{41}$$

This solution method has been coded up efficiently with no more than $19N-29$ arithmetic operations for a pentadiagonal system compared with $8N-7$ for the tridiagonal system if the matrix λ is of order $N\times N$.

Numerical simulation results for an advection velocity of $0{\cdot}5\ \mathrm{m\,s^{-1}}$ and a grid spacing of 100 m are shown for each modified QUICK scheme respectively in Figures 3 and 4 for pure advection, in Figures 5 and 6 for a constant diffusion coefficient of $2\ \mathrm{m^2\,s^{-1}}$ ($\gamma=0{\cdot}008$) and in Figures 7 and 8 for a diffusion coefficient of $8\ \mathrm{m^2\,s^{-1}}$ ($\gamma=0{\cdot}032$), with a Courant number of 0·20 for all cases.

From the results it can be seen that schemes (iii) and (v) exhibited no wiggles but resulted in a relatively strong numerical diffusion effect, with the numerical diffusion coefficient being equal to $\Delta t u^2/2$ as compared to zero for schemes (ii) and (iv). The numerical diffusion effects associated with schemes (iii) and (v) would commonly be larger than the physical diffusion for water quality model studies, especially when the physical diffusion is relatively small and the Courant number large. For instance, under our test conditions the numerical diffusion coefficient was $5\ \mathrm{m^2\,s^{-1}}$

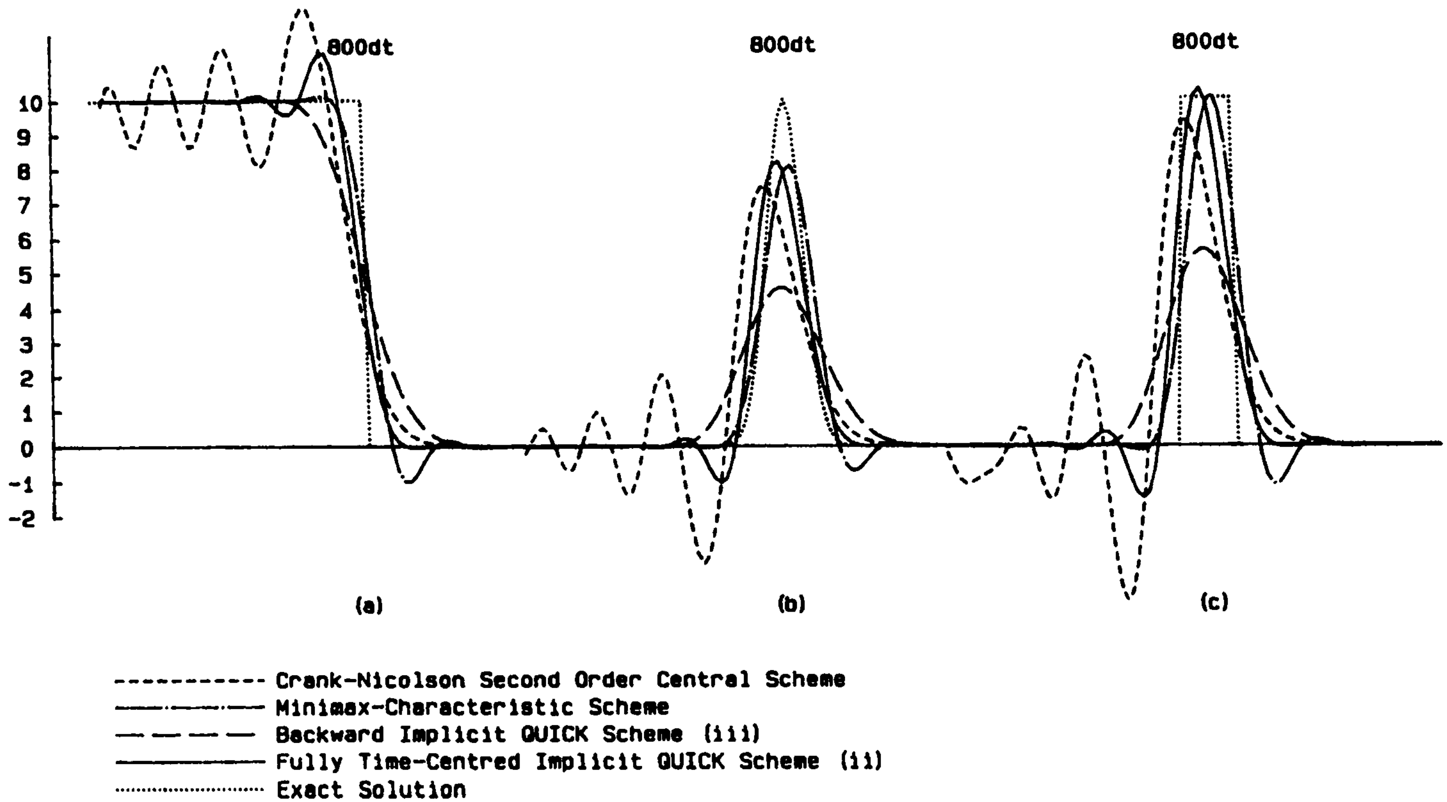


Figure 3. Advection of (a) a sharp front, (b) a Gaussian distribution and (c) a plug source for $\varepsilon=0{\cdot}20$ and $\gamma=0$

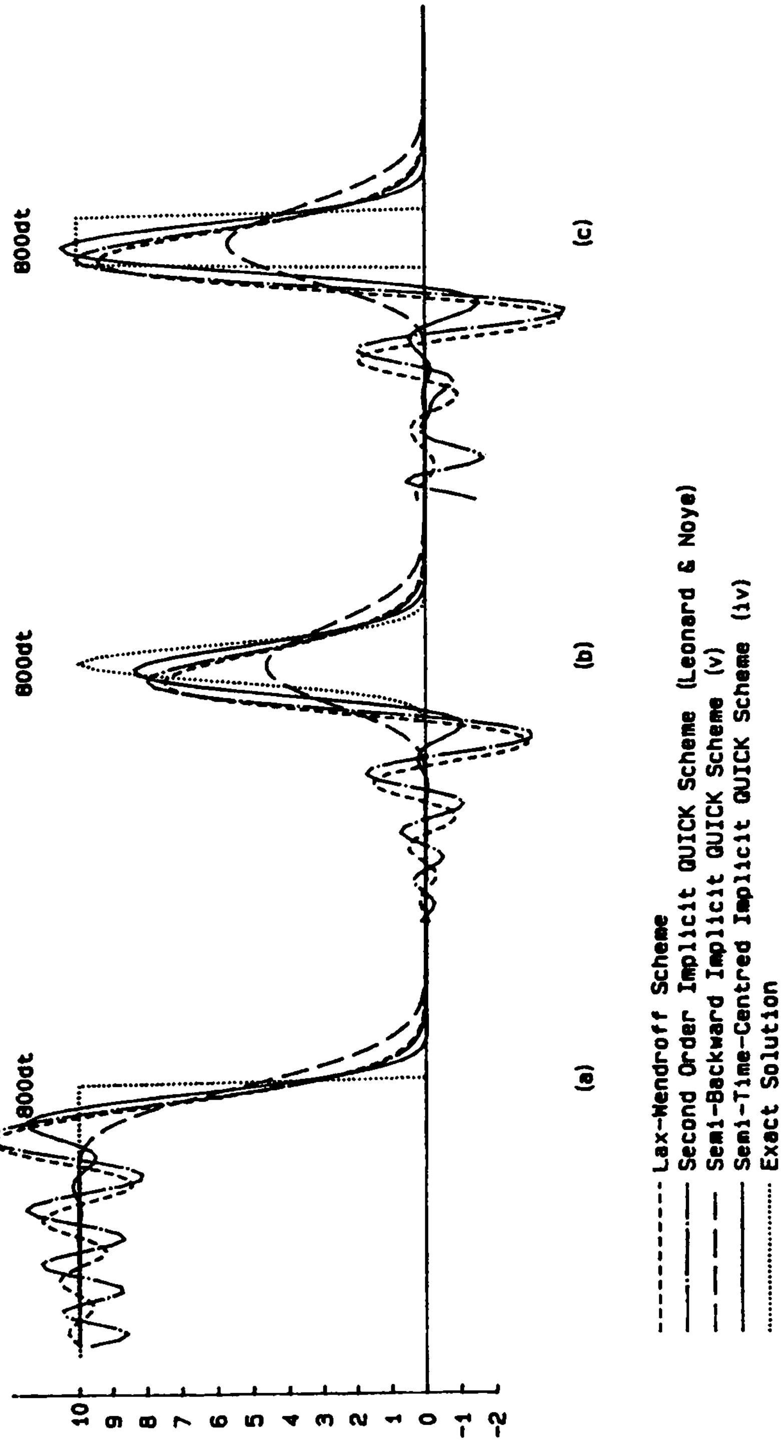


Figure 4. Advection of (a) a sharp front, (b) a Gaussian distribution and (c) a plug source for $\varepsilon = 0{\cdot}20$ and $\gamma = 0$

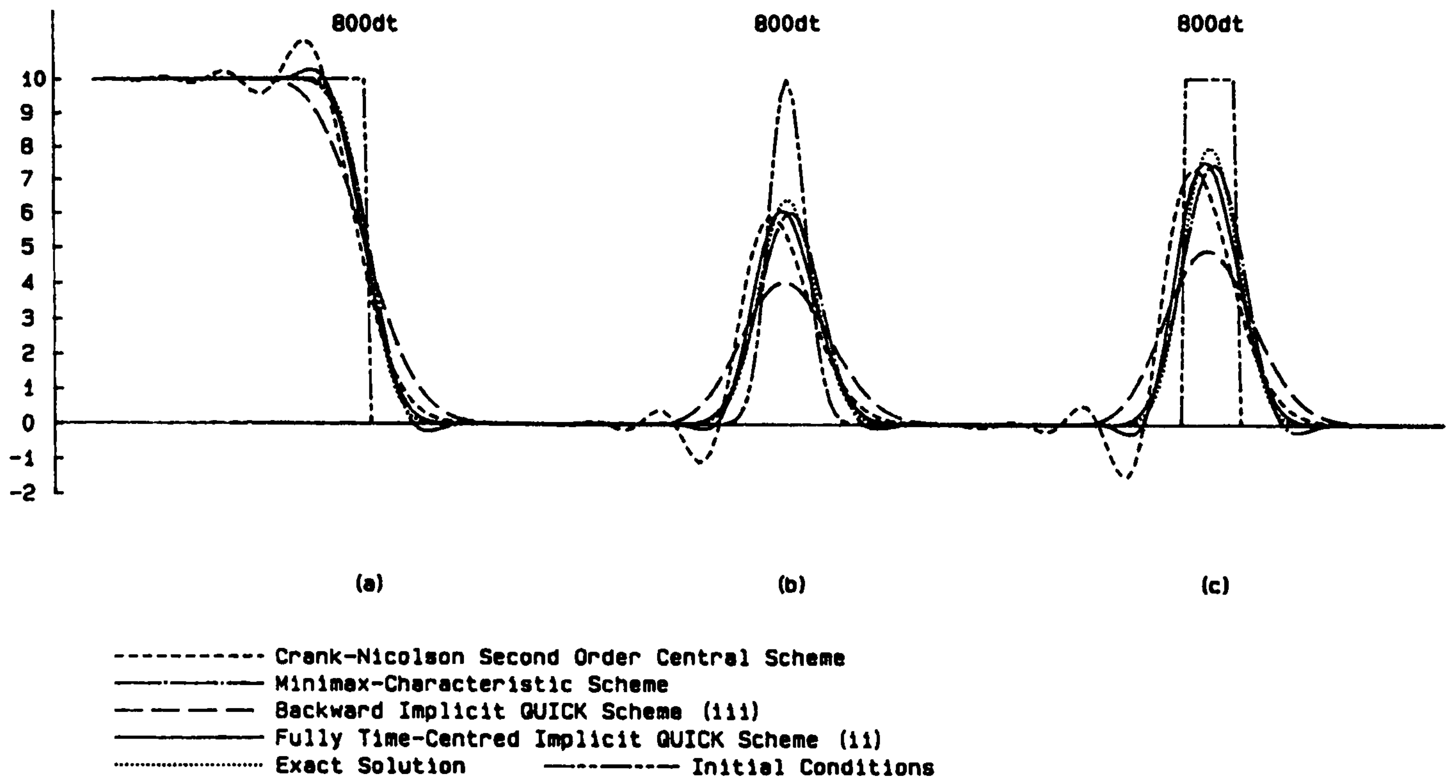


Figure 5. Advection–diffusion of (a) a sharp front, (b) a Gaussian distribution and (c) a plug source for $\varepsilon = 0{\cdot}20$ and $D = 2\ \mathrm{m^2\,s^{-1}}$ ($\gamma = 0{\cdot}008$)

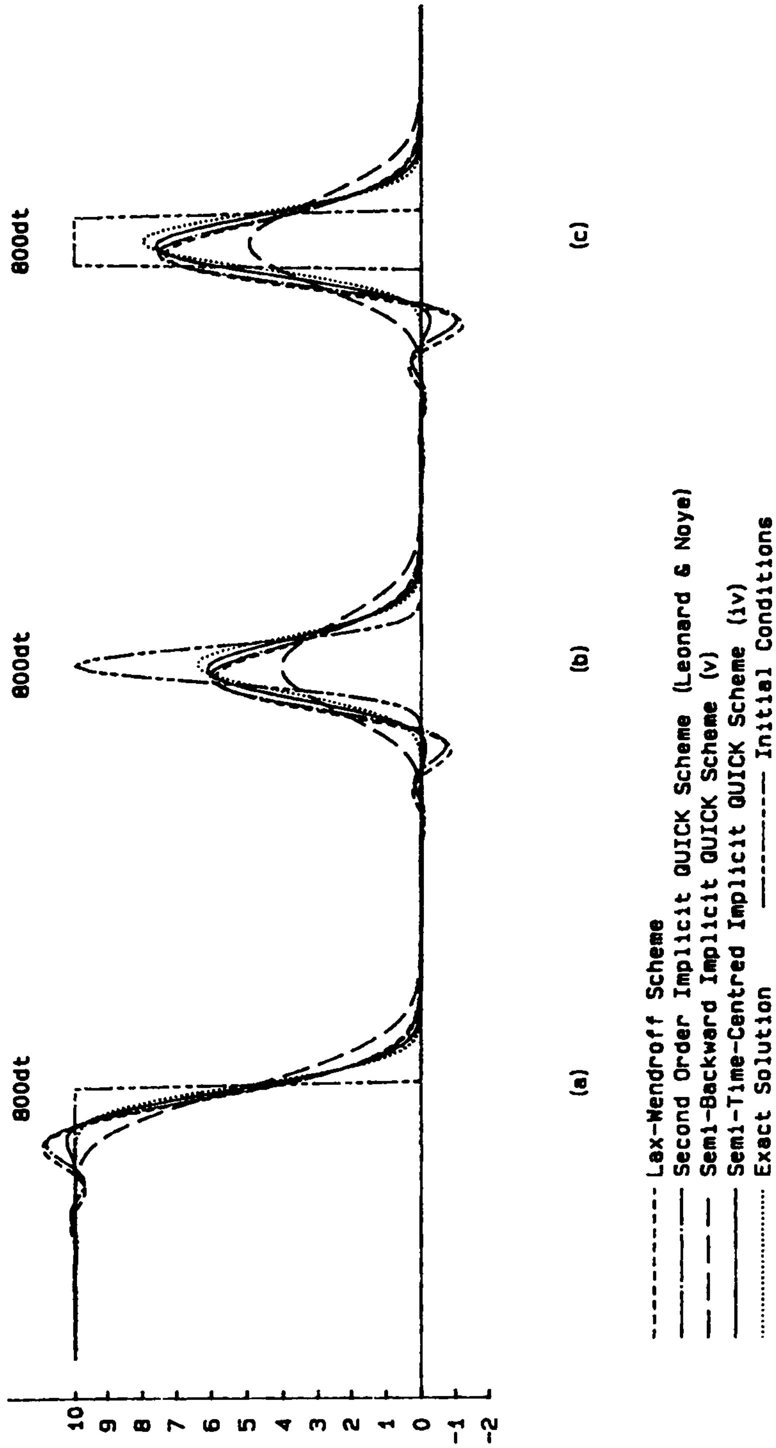


Figure 6. Advection–diffusion of (a) a sharp front, (b) a Gaussian distribution and (c) a plug source for $\varepsilon = 0{\cdot}20$ and $D = 2\ \mathrm{m}^2\,\mathrm{s}^{-1}$ ($\gamma = 0{\cdot}008$)

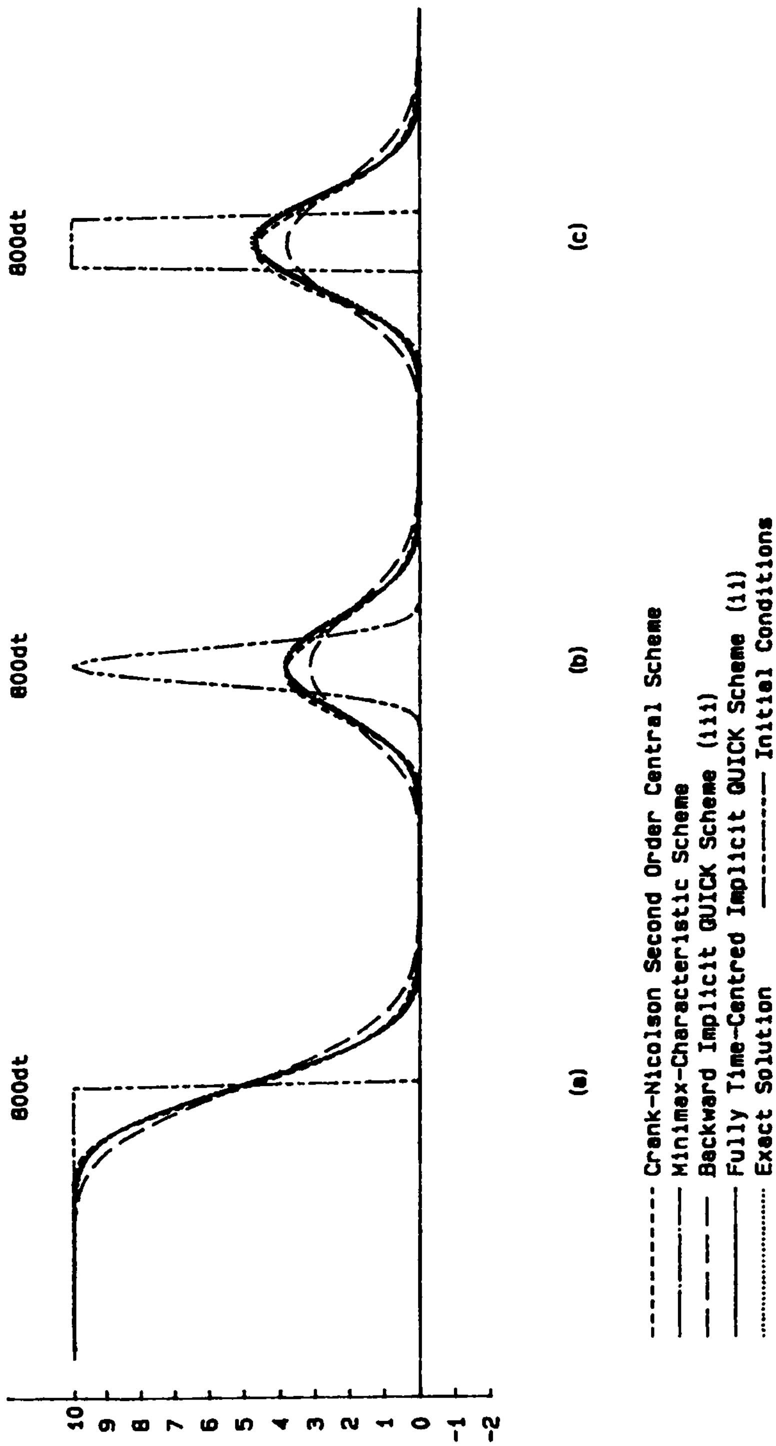


Figure 7. Advection–diffusion of (a) a sharp front, (b) a Gaussian distribution and (c) a plug source for $\varepsilon=0{\cdot}20$ and $D=8\ \mathrm{m^2\,s^{-1}}$ ($\gamma=0{\cdot}032$)

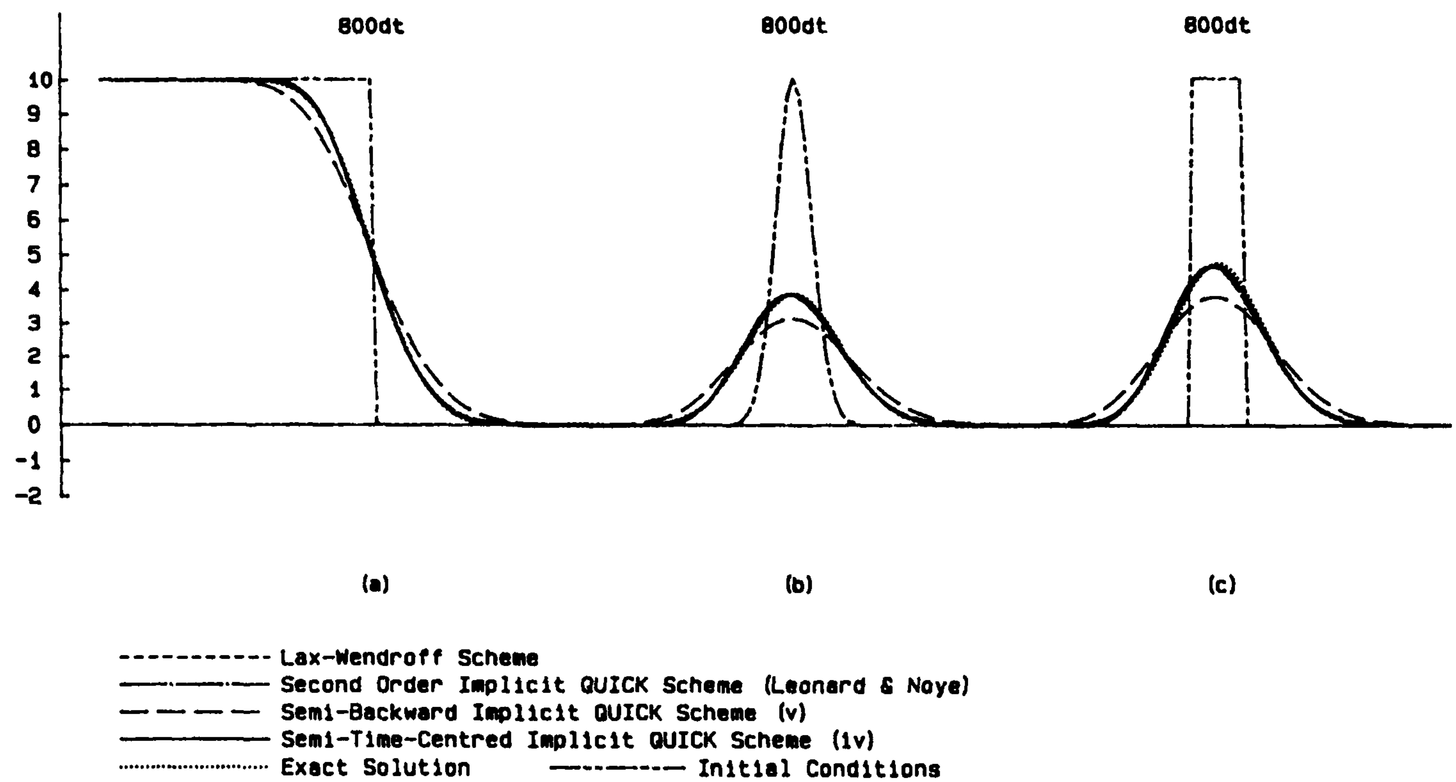


Figure 8. Advection–diffusion of (a) a sharp front, (b) a Gaussian distribution and (c) a plug source for $\varepsilon = 0{\cdot}20$ and $D = 8\ \mathrm{m^2\,s^{-1}}$ ($\gamma = 0{\cdot}032$)

when $\varepsilon = 0{\cdot}20$, and 70·31 or 18·75 $m^2 s^{-1}$ when $\varepsilon = 0{\cdot}75$ for an increase in the advection velocity or time step number respectively. Although these two backward schemes are considerably better than the first-order upwind scheme, they are still considered to be inadequate for practical modelling applications. Schemes (ii) and (iv), on the other hand, gave rise to more accurate results than the other two schemes—as to be expected from the previous analysis—but suffered from exhibiting some degree of grid-scale oscillations. The results showed that the amplitude of the undershoot and overshoot and the degree of the phase error associated with schemes (ii) and (iv) were about the same as those for the minimax-characteristics scheme and Fromm's method, both of which require separate computations for advection and diffusion. The undershoot and overshoot associated with schemes (ii) and (iv) appeared behind the advancing wave, in contrast to the minimax-characteristics scheme where the undershoot and overshoot were ahead of the wave. However, in general, schemes (ii) and (iv) are a considerable improvement, both in terms of the phase error and the amplitude of the grid-scale oscillations, over the second-order central difference representations (i.e. C–N and L–W) and the second-order implicit QUICK scheme,[17] which behaves in a similar manner to a second-order central difference scheme as shown in Figures 3–6. Also, it can be seen that the grid-scale oscillations obtained using schemes (ii) and (iv) were considerably weaker for the advection and diffusion case for a relatively small diffusion number (0·008), as shown in Figures 5–8, when compared with the predictions for pure advection only, as shown in Figures 3 and 4. Therefore the presence of physical diffusion not only enlarges the stability region for the implicit schemes but also reduces the grid-scale oscillations. Furthermore, as the physical diffusion is increased, the grid-scale oscillations are reduced further and disappear completely for a diffusion coefficient of about 8 $m^2 s^{-1}$ (the diffusion number being 0·032), as can be seen in Figures 7 and 8. In this case schemes (ii) and (iv) produce very accurate results which are almost identical to the exact solution.

The difference in the predicted results between schemes (iii) and (v) was found to be negligible for both simulations with pure advection and with advection and diffusion and for all Courant numbers considered. On the other hand, although there was only a small difference between the predicted results for schemes (ii) and (iv) for the case of pure advection with a Courant number ε of 0·20, this difference was more pronounced when the Courant number was increased to 0·75, as can be seen in Figure 9, with scheme (iv) showing slightly stronger oscillations than scheme (ii). The magnitude of these oscillations and the phase error were also increased for this severe test. Hence, from the point of view of accuracy, a smaller Courant number is always preferable for pure advection, although stable results will be obtained for larger Courant numbers for both the above-mentioned modified QUICK schemes. However, the difference between schemes (ii) and (iv) was unnoticeable when the Courant number was 0·75 and the diffusion coefficient was 2 $m^2 s^{-1}$, as shown in Figure 10, where the oscillations can be seen to have been greatly reduced. With stronger physical diffusion of 5 $m^2 s^{-1}$, these oscillations vanished completely. In Figure 11 the test results are shown for the application of these two modified schemes to the advection and diffusion case with $\varepsilon = 1{\cdot}5$ and $\gamma = 0{\cdot}195$. The results are still reasonably accurate except for some degree of phase error, with the results obtained for the case of advection and diffusion being better than those obtained for pure advection only.

NUMERICAL TEST FOR TWO DIMENSIONS

On the basis of previous analyses it has been found that in general the pure advection case poses the most severe numerical test for any finite difference representation of the ADE. Thus, in testing the modified QUICK scheme for two dimensions, the analysis will be restricted to pure advection for a constant depth domain. The simplified governing two-dimensional advection equation can

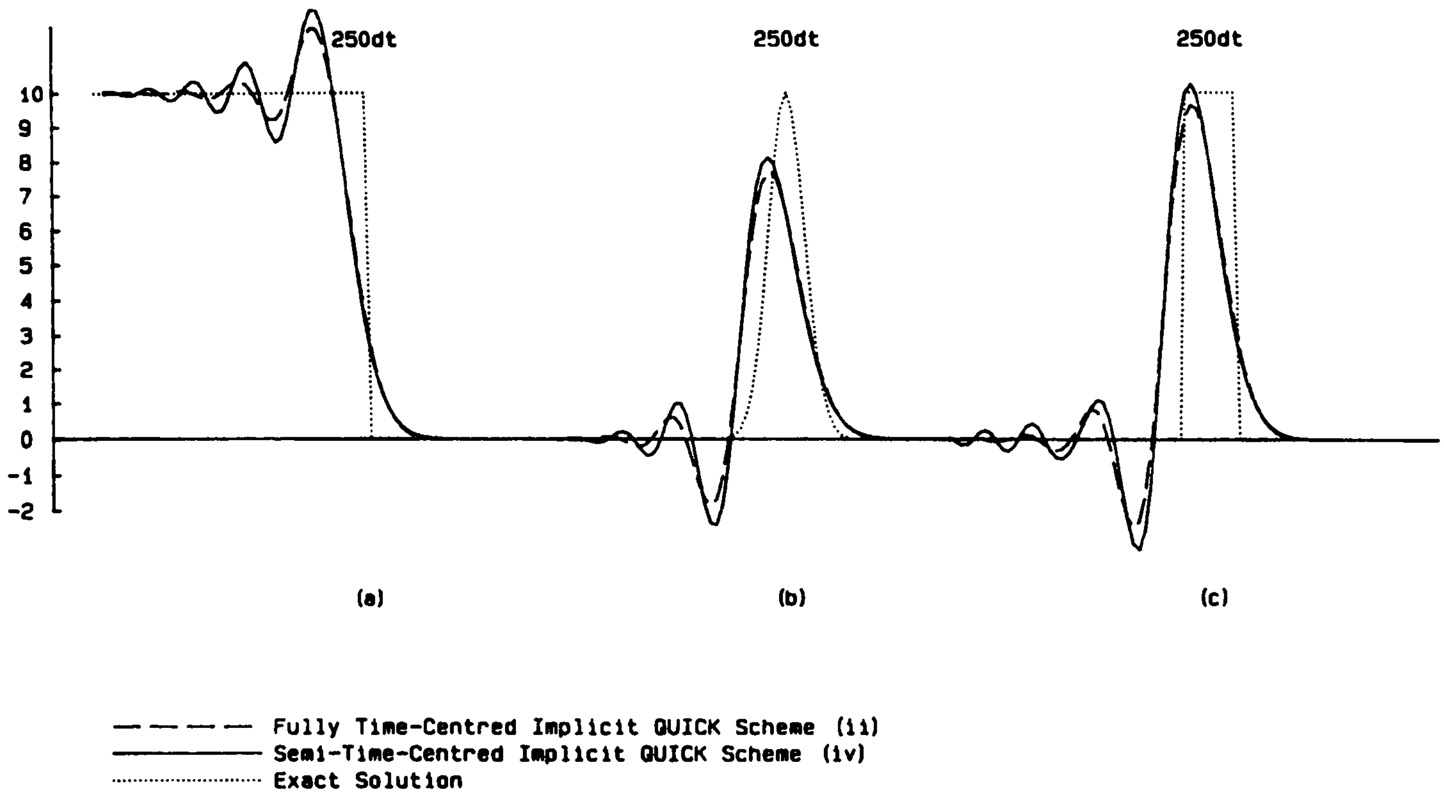


Figure 9. Advection–diffusion of (a) a sharp front, (b) a Gaussian distribution and (c) a plug source for $\varepsilon=0{\cdot}75$ and $\gamma=0$ by increasing Δt

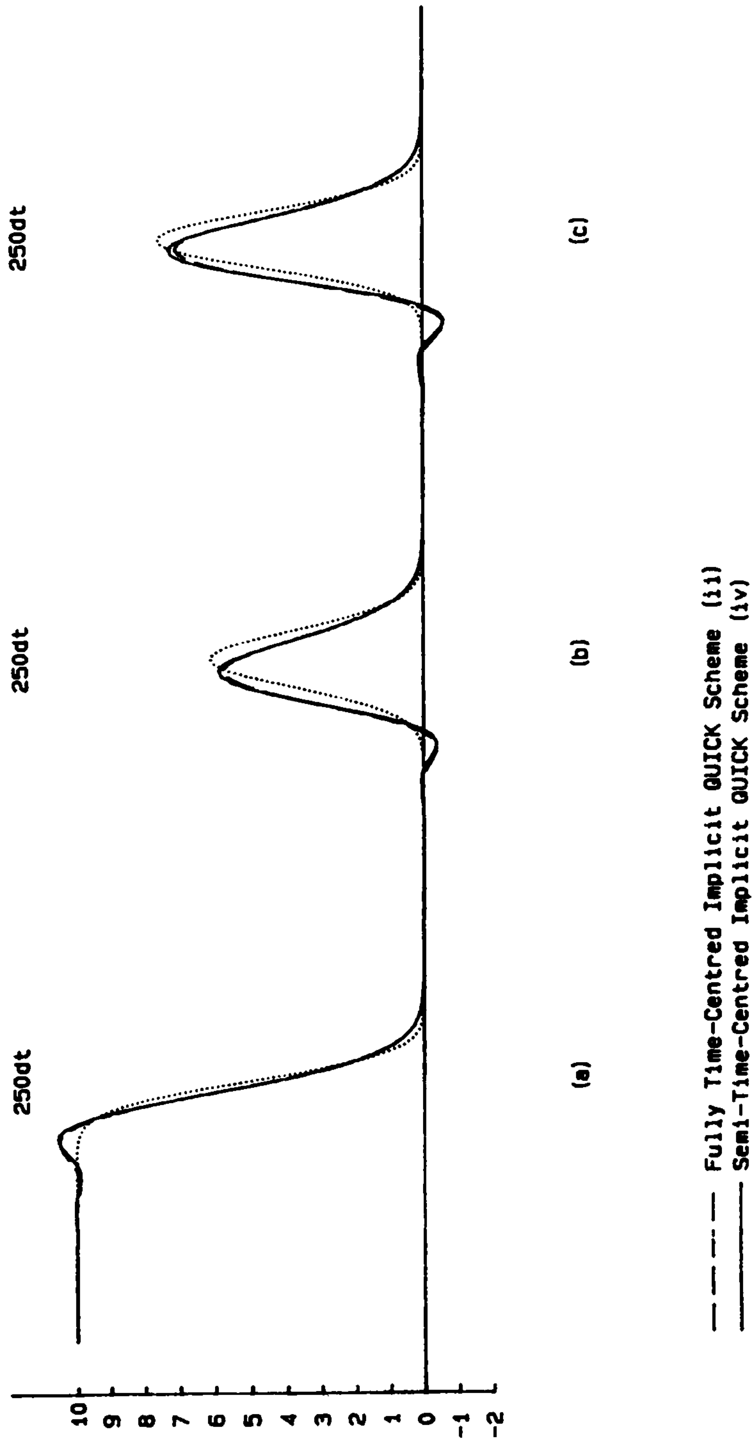


Figure 10. Advection–diffusion of (a) a sharp front, (b) a Gaussian distribution and (c) a plug source for $\varepsilon = 0{\cdot}75$ and $D = 2\ \mathrm{m^2\,s^{-1}}$ ($\gamma = 0{\cdot}06$)

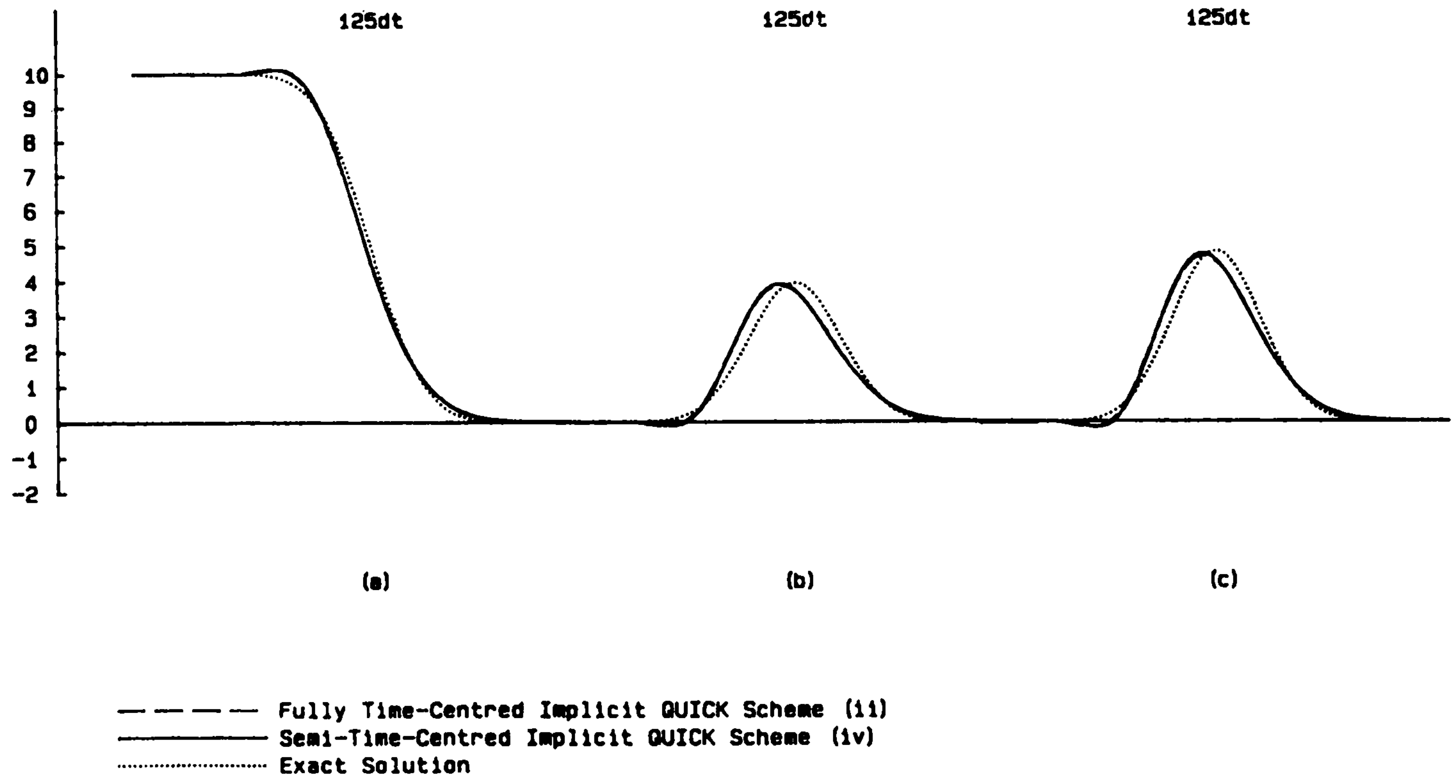


Figure 11. Advection–diffusion of (a) a sharp front, (b) a Gaussian distribution and (c) a plug source for $\varepsilon=1{\cdot}5$ and $D=6{\cdot}5\ \mathrm{m^2\,s^{-1}}$ ($\gamma=0{\cdot}195$)

be written as

$$\frac{\partial S}{\partial t}+\frac{\partial (uS)}{\partial x}+\frac{\partial (vS)}{\partial y}=0, \tag{42}$$

where $u(x, y, t)$ and $v(x, y, t)$ are the advection velocities in the x- and y-directions respectively.

As an example to illustrate the numerical properties of the QUICK scheme in two dimensions, a semi-time-centred ADI-QUICK formulation has been constructed based upon the ADI technique. The finite difference equation for this scheme, for the first half-time-step from $t=n\Delta t$ to $t=(n+\frac{1}{2})\Delta t$, can be written as

$$\begin{aligned}
&S_{i,j}^{n+1/2}+\tfrac{1}{4}\left[\xi_{i+1/2,j}^{n+1/2}\left(S_{i+1,j}^{n+1/2}+S_{i,j}^{n+1/2}\right)-\xi_{i-1/2,j}^{n+1/2}\left(S_{i,j}^{n+1/2}+S_{i-1,j}^{n+1/2}\right)\right]\\
&\quad=S_{i,j}^{n}-\tfrac{1}{4}\left[\eta_{i,j+1/2}^{n}\left(S_{i,j+1}^{n}+S_{i,j}^{n}\right)-\eta_{i,j-1/2}^{n}\left(S_{i,j}^{n}+S_{i,j-1}^{n}\right)\right]\\
&\qquad+\tfrac{1}{16}\left(\xi_{i+1/2,j}^{n+1/2}\nabla_x^2 S_{i,j}^{n}-\xi_{i-1/2,j}^{n+1/2}\nabla_x^2 S_{i-1,j}^{n}+\eta_{i,j+1/2}^{n}\nabla_y^2 S_{i,j}^{n}-\eta_{i,j-1/2}^{n}\nabla_y^2 S_{i,j-1}^{n}\right),
\end{aligned} \tag{43}$$

where i and j are grid square locations in the x- and y-directions respectively, ξ and η are the Courant numbers in the x- and y- directions respectively and

$$\nabla_x^2 S_{i,j}^{n}=\begin{cases} S_{i+1,j}^{n}-2S_{i,j}^{n}+S_{i-1,j}^{n} & \text{if } u_{i+1/2,j}>0,\\ S_{i+2,j}^{n}-2S_{i+1,j}^{n}+S_{i,j}^{n} & \text{if } u_{i+1/2,j}<0,\end{cases} \tag{44}$$

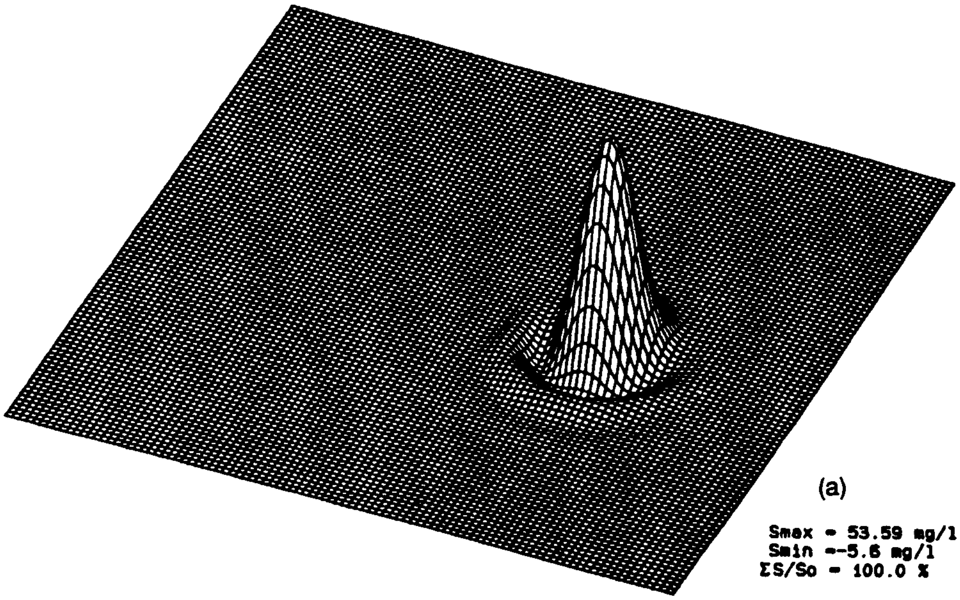
$$\nabla_y^2 S_{i,j}^{n}=\begin{cases} S_{i,j+1}^{n}-2S_{i,j}^{n}+S_{i,j-1}^{n} & \text{if } v_{i,j+1/2}>0,\\ S_{i,j+2}^{n}-2S_{i,j+1}^{n}+S_{i,j}^{n} & \text{if } v_{i,j+1/2}<0.\end{cases} \tag{45}$$

The stability requirement for this scheme, assuming a constant velocity with $u=u_{i+1/2,j}=u_{i-1/2,j}>0$ and $v=v_{i,j+1/2}=v_{i,j-1/2}>0$, can be given as

$$\xi+\eta\leqslant 2. \tag{46}$$

The test domain consisted of 100×100 grid cells (with $\Delta x=\Delta y$), with the velocity field being similar to that for an anticlockwise rigid-body rotation about the domain centre at an angular speed of 2π radians in 1256 time steps. The co-ordinate system was taken as being a right-handed Cartesian system, with the bottom left and top right corners having coordinates of $(-50, -50)$ and $(50, 50)$ respectively. Two initial conditions were considered with the same peak concentrations of 50 mg L^{-1}: (a) a circular column source with a diameter of $9\Delta x$ and (b) a Gaussian distribution of $\sigma_x=\sigma_y=3{\cdot}25\Delta x$. The column diameter is chosen to be narrow, since practical studies for sea outfall contaminant distribution usually cover less than a few hundred meters of disposal area. However, it can be expected that a wider column would give better results, thus requiring a smaller grid size and more computation time. The initial non-zero concentration distribution was located at the centre of the cell $(-20, 0)$ at time $t=0$, with the upstream boundary concentration being set to zero and the downstream boundary concentration being obtained by assuming zero derivatives.

The results obtained after one and a half revolutions (i.e. $t=1884\Delta t$) using the above scheme, the C–N second-order central scheme and the minimax-characteristics or Fromm's scheme for these two initial conditions are shown in Figures 12–14 respectively. Biquadratic profiles were used for both the ADI-QUICK scheme and the minimax-characteristics method. It is worth noting that the minimax-characteristics method needs 16 points (4×4) for two-dimensional interpolations, compared with seven points for unidirectional flow or nine points for directional flow for the ADI-QUICK scheme. It can be seen by comparing the results that the ADI-QUICK scheme produced tolerable levels of undershoot and overshoot, with the results being similar to those predicted for the one-dimensional test results. Similarly, the minimax-characteristics



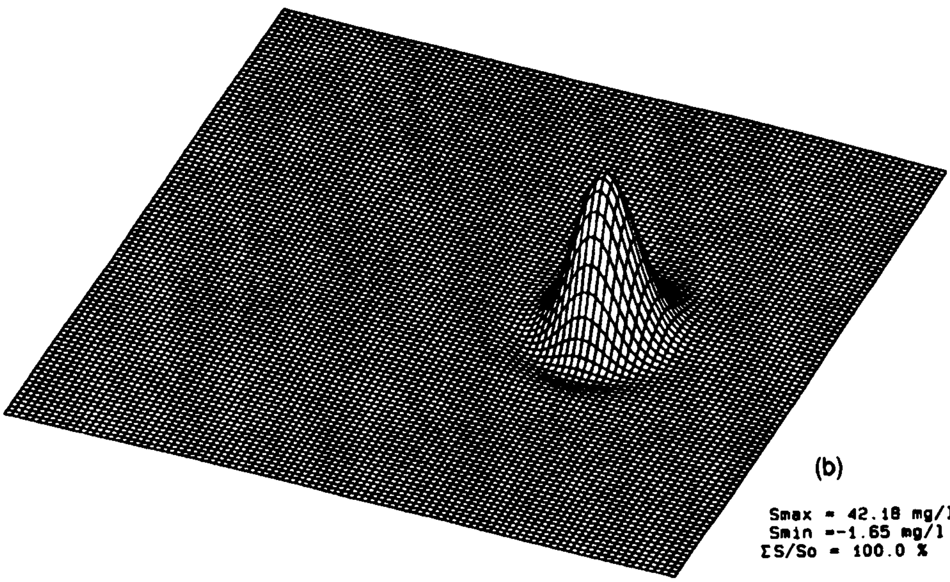


Figure 12. Advection of (a) a column source and (b) a Gaussian distribution using the ADI-QUICK scheme in two dimensions

scheme also produced overshoot and undershoot and the central scheme produced very severe oscillations which rapidly spread over the whole modelling domain. The degree of undershoot and overshoot for each scheme can be obtained by comparing the values of S_{max} and S_{min} with the original peak and zero values for each scheme respectively for each figure. The quantity $\Sigma S/S_0$

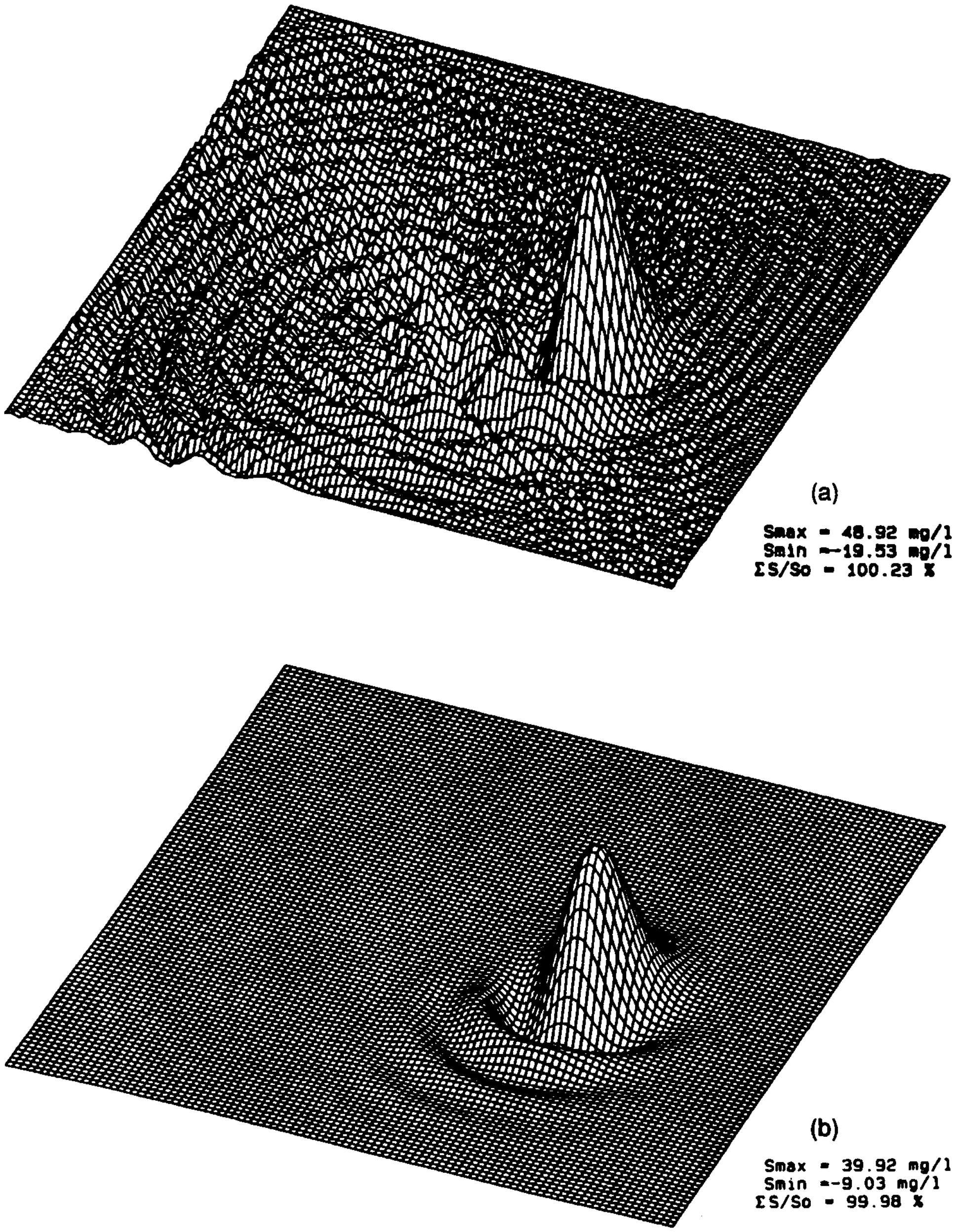


Figure 13. Advection of (a) a column source and (b) a Gaussian distribution using the C–N second-order central scheme in two dimensions

gives the mass balance percentage, which is the percentage ratio of the total mass at the specified time step to the initial total mass. As can be seen from the results, the minimax-characteristics scheme performed poorly in terms of mass conservation when compared with the other schemes tested. Similar results were also obtained for a two-dimensioinal uniform flow field with constant velocities in both the x- and y-directions.

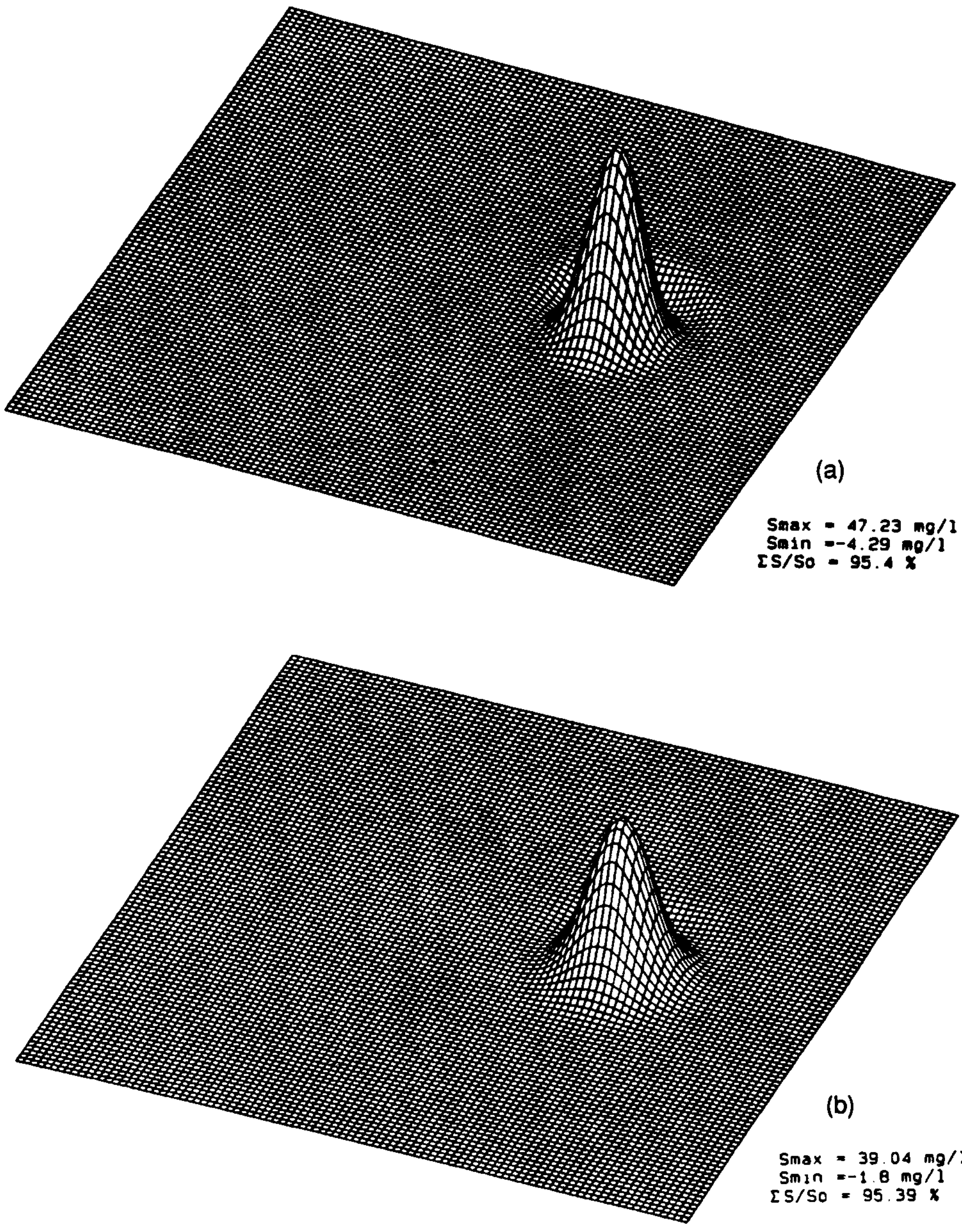


Figure 14. Advection of (a) a column source and (b) a Gaussian distribution using the minimax-characteristics scheme in two dimensions

CONCLUSIONS

The QUICK scheme can be written in a number of different finite difference forms when applied to slowly time-varying problems, with the various formulations having different numerical properties and computational efficiencies. The main findings of the analysis of five different representations of the QUICK scheme can be summarized as follows.

(i) The explicit forward difference QUICK scheme was shown to have a severe stability constraint for the ADE and became numerically unstable when applied to the pure advection transport equation. The backward and fully time-centred implicit QUICK schemes were unconditionally stable, although they were also computationally inefficient compared with other formulations. The semi-backward and semi-time-centred implicit QUICK schemes had a stability constraint as given by equations (31) and (27) respectively.

(ii) The backward and semi-backward implicit QUICK schemes were comparatively more diffusive than the fully time-centred or semi-time-centred QUICK schemes and were therefore considered to be inadequate for practical use, although they were still considerably more accurate than the first-order upwind difference scheme.

(iii) The fully time-centred and semi-time-centred implicit QUICK schemes exhibited some degree of gird-scale oscillations in advection-dominant transport problems. However, these oscillations were found to be of a similar magnitude to those obtained for the minimax -characteristics and Fromm's schemes for the test cases considered. These oscillations were found to be considerably improved compared with those obtained using the second-order central difference schemes and the second-order implicit QUICK scheme modified by Leonard and Noye,[17] with both versions of the time-centred QUICK scheme presented in this study being more accurate.

(iv) Two dimensioinal numerical tests for pure advection showed that the ADI-QUICK scheme was mass-conservative after a long-time simulation whereas the minimax-characteristics scheme was not. The ADI-QUICK scheme performed considerably better than the second-order central difference scheme and marginally better than the minimax-characteristics scheme in two dimensions.

(v) The difference between the fully time-centred and semi-time-centred implicit QUICK schemes was negligible when the Courant number was relatively small or there was a minimum amount of physical diffusion. For such conditions the semi-time-centred implicit QUICK scheme was therefore preferable owing to its computational efficiency.

(vi) Numerical tests also confirmed that physical diffusion improved the stability properties of all the finite difference schemes tested and also reduced the amplitude of grid-scale oscillations.

ACKNOWLEDGEMENTS

This research study was undertaken in the Department of Civil Engineering, University of Bradford and was funded by the Science and Engineering Research Council (SERC). The authors would like to express their appreciation to the SERC for their support and to IBM U.K. Ltd. for providing extensive computing facilities under an IBM study grant.

REFERENCES

1. D. R. F. Harleman, 'Diffusion processes in stratified flow, in A. T. Ippen (ed.), *Estuarine and Coastal Hydrodynamics*, McGraw-Hill, New York, 1966, Chap. 12.
2. J. Crank and P. Nicolson, 'A practical method for numerical evaluation of solutions of partial differential equations of the heat conduction type', *Proc. Camb. Phil. Soc.*, **43**, 50–67 (1947).
3. P. D. Lax and B. Wendroff, 'Difference methods with high order of accuracy for solving hyperbolic equations', *Commun. Pure Appl. Math.*, **17**, 381–398 (1964).
4. E. S. Oran and J. P. Boris, *Numerical Simulation of Reactive Flow*, Elsevier, New York, 1987.
5. M. B. Abbott and D. R. Basco, *Computational Fluid Dynamics*, Longman, Scientific & Technical, Harlow, Essex, 1989.
6. J. J. Leendertse, 'A water quality simulation model for well-mixed estuaries and coastal seas: Volume 1, Principles of computation', *Rand Corporation Report RM*-6230-*RC*, 1970, pp. 1–71.
7. J. E. Fromm, 'A method for reducing dispersion in convective difference schemes', *J. Comput. Phys.*, **3**, 176–189 (1968).
8. C. W. Li, 'Advection simulation by minimax-characteristics method', *J. Hydraul. Eng., ASCE*, **116**, 1138–1144 (1990).

9. W. L. Hogarth, B. J. Noye, J. Stagnitti, J. Y. Parlange and G. Bolt, 'A comparative study of finite difference methods for solving the one-dimensional transport equation with an initial-boundary value discontinuity', *Comput. Math. Appl.*, **20**, 67–82 (1990).
10. F. M. Holly, Jr. and A. Preissmann, 'Accurate calculation of transport in two dimensions', *Proc. ASCE, J. Hydraul. Div.*, **103**, 1259–1277 (1977).
11. B. P. Leonard, 'A stable and accurate convective modelling procedure based on quadratic upstream interpolation', *Comput. methods appl. mech. eng.*, **19**, 59–98 (1979).
12. R. A. Falconer and S. Q. Liu, 'Modeling solute transport using QUICK scheme', *J. Environ. Eng. ASCE*, **114**, 3–20 (1988).
13. A. O. Demuren and W. Rodi, 'Calculation of flow and pollutant dispersion in meandering channels', *J. Fluid Mech.*, **172**, 63–92 (1986).
14. Y. Takemoto and Y. Nakamura, 'Numerical simulation of 2-D and 3-D channel flows using a 3rd-ordered accurate generalized QUICK scheme', *Proc. Third Int. Symp. on Refined Flow Modelling and Turbulence Measurements*, Tokyo, 1988 (Eds. Y. Iwasa, N. Tamai and A. Wada). IAHR, Delft, 1988, pp. 53–60.
15. C. J. Freitas, R. L. Street, A. N. Findikakis and J. R. Koseff, 'Numerical simulation of three-dimensional flow in a cavity', *Int. j. numer. methods fluids*, **5**, 561–575 (1985).
16. B. P. Leonard, 'Elliptic systems: finite-difference method IV', in W. J. Minkowicz *et al.* (eds), *Hand Book of Numerical Heat Transfer*, Wiley, New York, 1988, Chap. 9.
17. B. P. Leonard and B. J. Noye, 'Second and third order two level implicit FDM's for unsteady one-dimensional convection–diffusion', *Computational Techniques and Applications: CTAC-89*, Hemisphere, New York, 1990, pp. 311–317.
18. C. Y. Perng and R. L. Street, 'Three-dimensional unsteady flow simulations: alternative strategies for a volume-averaged calculation', *Int. j. numer. methods fluids*, **9**, 341–362 (1989).
19. R. W. Davis and E. F. Moore 'A numericl study of vortex shedding from rectangles', *J. Fluid Mech.*, **116**, 475–506 (1982).
20. Y. Chen, 'Solute transport modelling using higher order finite difference schemes', *Ph. D Thesis*, University of Bradford, 1992.
21. A. C. Hindmarsh and P. M. Gresho, 'The stability of explicit Euler time-integration for certain finite difference approximations of the multi-dimensional advection–diffusion equation', *Int. j. numer. methods fluids*, **4**, 853–897 (1984).
22. R. D. Richtmyer and K. W. Morton, *Difference Methods for Initial-value Problems*, Interscience, New York, 1967.
23. S. Paolucci and D. R. Chenoweth, 'Note on the stability of the explicit finite differenced Transport equation', *J. Comput. Phys.*, **47**, 489–496 (1982).
24. B. P. Leonard, 'A survey of finite differences with upwinding for numerical modelling of the incompressible convective diffusion equation', in C. Taylor and K. Morgan (eds), *Computational Techniques in Transient and Turbulent Flow*, Vol. 2, Pineridge, Swansea, 1981, Chap. 1, pp. 1–35.
25. M. Th. van Genuchten and W. J. Alves, 'Analytical solutions of the one-dimensional convective–dispersive solute transport equation', *U.S. Department of Agriculture, Technical Bulletin* 1661, 1982.
26. L. H. Thomas, *Elliptic Problems in Linear Difference Equations over a Network*, Waston Scientific Computing Laboratory, Columbia, NY, 1949.