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MOSQUITO: AN EFFICIENT FINITE DIFFERENCE SCHEME FOR NUMERICAL SIMULATION OF 2D ADVECTION

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SUMMARY

An explicit finite difference method for the treatment of the advective terms in the 2D equation of unsteady scalar transport is presented. The scheme is a conditionally stable extension to two dimensions of the popular QUICKEST scheme. It is deduced imposing the vanishing of selected components of the truncation error for the case of steady uniform flow. The method is then extended to solve the conservative form of the depth-averaged transport equation. Details of the accuracy and stability analysis of the numerical scheme with test case results are given, together with a comparison with other existing schemes suitable for the long-term computations needed in environmental modelling. Although with a truncation error of formal order $0(\Delta x \Delta t, \Delta y \Delta t, \Delta t^2)$, the present scheme is shown actually to be of an accuracy comparable with schemes of third-order in space, while requiring a smaller computational effort and/or having better stability properties. In principle, the method can be easily extended to the 3D case.

KEY WORDS: advection modelling; finite difference; solute transport; upwind; truncation error; stability

1. INTRODUCTION

Numerical simulation of advection in advection-dominated transport processes is a common problem in practical applications of computational hydraulics and fluid dynamics. Although a great deal of research has been carried out on the subject [1–6], a method of general applicability that conjugates the properties of stability, accuracy, positivity and conservation of the tracer with the important practical requirement of running fast enough in a computer implementation for the present variety of possible applications is still to be devised. In different scientific and engineering fields some of the above conditions are, therefore, relaxed in order to achieve the most important properties in view of the specific problem to be solved. Computational speed is a factor of particular relevance in environmental studies, in which long-term simulations of advection-dominated hydrodynamics and scalar transport are typically required, possibly on quite large computational domains and with fine spatial detail [7], or involving a number of chemically reactive species [8].

As a consequence, besides the investigation of highly accurate, positive-defined computational schemes suitable for the simulation of sharp gradients [1,9–15], a substantial research

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effort is still being oriented to methods by which a reasonable compromise between accuracy and computational speed can be achieved. Basically, methods of this kind are required to avoid both the computational noise generated by heavy wave dispersion and the unphysical smoothing related to large numerical diffusion, which can be revealed by Fourier analysis.

Earlier attempts in this direction led to hybrid formulations using the second-order central difference scheme or the first-order upwind scheme, depending on local flow conditions [16,17]. Since then, a number of high-order schemes based on the upwind concept have been proposed, with some of them being still very popular today [4]. However, schemes that were proposed for the 1D case often cannot be easily extended to the 2D or 3D case without losing the simplicity of the original formulation [18].

It is to be noted that, particularly in shallow water problems of subcritical flow, the presence of numerical diffusion—here specifically related to second-order spatial derivatives—is particularly awkward in scalar transport models. In fact, although in hydrodynamic models advection is non-linear, in practice the artificial dissipation introduced by numerical algorithms can often be acceptable when compared with the physical dissipation effect related to bottom friction [19]. For the above reasons this study deals with numerical simulation of advection in linear advection-dominated scalar transport models.

A finite difference scheme for 2D advection will be described, which is efficient and reasonably accurate for the range of practical applications mentioned above. The present scheme can be referred to as an extension of the well-known QUICKEST scheme [4], which is recovered in the 1D case. However, the derivation of the method is somehow different from that by the original author. Moreover, its extension to the 3D case is straightforward in principle.

A recent, thorough review and comparison of popular finite difference schemes well-suited for long-term and large-scale simulation of 2D advection–diffusion in the sense stated above, has been carried out by Chen and Falconer [20]. The study was primarily concerned with a generalized formulation of the so-called third-order convection second-order diffusion scheme, originally proposed by Bradley *et al.* [21]. After theoretical accuracy and stability analysis for the 1D formulation, the so-called semi-time-centred (TCS) and fully-time-centred (TCF) implicit versions have proved suitable for practical applications, with the former being preferred for overall efficiency reasons (this point will be reconsidered in the following).

Chen and Falconer then compare a 2D ADI formulation of TCS with the following models: the semi-time-centred ADI-QUICK scheme [18], the Crank–Nicolson central scheme [22], a direct 2D implementation of the explicit QUICKEST scheme [4], a modified QUICKEST scheme [23], and the two-point fourth-order scheme [3,24]. On a global balance as to accuracy, stability and mass conservation, TCS proved more efficient than the other methods.

Further to Chen and Falconer's comprehensive analysis, a new valuable numerical scheme has been proposed by Webb *et al.* [7], based on a modification of the popular QUICK scheme [4]. It represents a conservative formulation of the Bradley *et al.* method [21]. The scheme (modified split QUICK, MSQ) is split into an advective term and a higher-order dissipation term. Each term is then time stepped so as to achieve stability, namely by the leapfrog and the Euler-forward schemes respectively, as outlined further in this paper.

Besides TCS, TCF and MSQ, the present method is compared with the QUICK scheme with Matsuno time stepping [5] (QMA), mentioned in [7] as a suitable way to stabilize the 2D explicit QUICK scheme.

2. RATIONALE OF THE METHOD

The 2D depth-averaged advection–diffusion equation in conservation form can be written as

$$\frac{\partial(hc)}{\partial t}+\frac{\partial(huc)}{\partial x}+\frac{\partial(hvc)}{\partial y}-\frac{\partial}{\partial x}\left(D_x h\frac{\partial c}{\partial x}\right)-\frac{\partial}{\partial y}\left(D_y h\frac{\partial c}{\partial y}\right)=0, \tag{1}$$

where c is the depth-averaged concentration of the modelled species, x and y the Cartesian co-ordinates, t the time, h the water depth, u and v the depth-averaged x and y velocity components respectively, D_x and D_y the diffusion coefficients. Though the final aim of this work is to devise a conservative scheme for 2D advection, in order to outline the derivation of the method we first resort to the pure 2D advection equation in non-conservation form in a field of uniform and constant velocity of components u and v:

$$\frac{\partial c}{\partial t}+u\frac{\partial c}{\partial x}+v\frac{\partial c}{\partial y}=0. \tag{2}$$

Consider the following explicit, biased upwind discretization of Equation (2) on the regular grid shown in Figure 1 for the case of positive u and v:

$$\begin{aligned} c_i^{n+1} = {} & c_i^n-\frac{u\Delta t}{\Delta x}\left(\alpha c_{i+1,j}^n+\beta c_{i,j}^n+\gamma c_{i-1,j}^n+\delta c_{i-2,j}^n\right) \\ & -\frac{v\Delta t}{\Delta y}\left(\alpha' c_{i,j+1}^n+\beta' c_{i,j}^n+\gamma' c_{i,j-1}^n+\delta' c_{i,j-2}^n\right)+\epsilon c_{i-1,j-1}^n, \end{aligned} \tag{3}$$

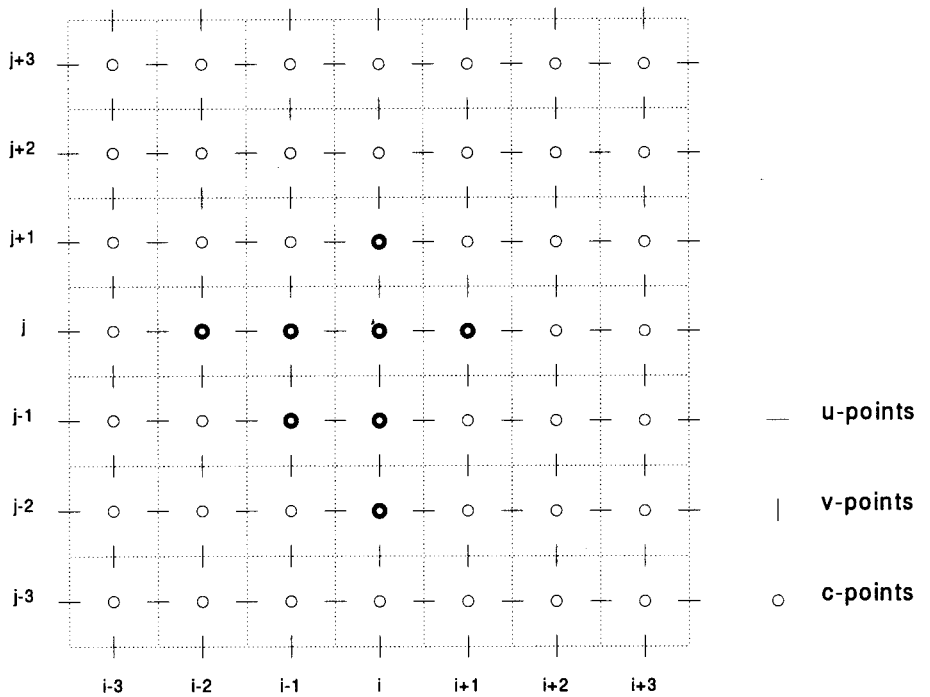

Figure 1. Computational stencil for positive velocity components u, v.

where i and j are the space indices, n is the time index, and the coefficients α, β, γ, δ, α', β', γ', δ' and ϵ, are presently to be determined. Developing Equation (3) by Taylor series, and making use of the relations between higher-order time and space derivatives of the concentration c, leads to the following expression:

$$\frac{\partial c}{\partial t}+\left[u\frac{\alpha+\beta+\gamma+\delta}{\Delta x}+v\frac{\alpha'+\beta'+\gamma'+\delta'}{\Delta y}-\frac{\epsilon}{\Delta t}\right]c+\left[-u(-\alpha+\gamma+2\delta)+\epsilon\frac{\Delta x}{\Delta t}\right]\frac{\partial c}{\partial x}$$
$$+\left[-v(-\alpha'+\gamma'+2\delta')+\epsilon\frac{\Delta y}{\Delta t}\right]\frac{\partial c}{\partial y}+\left[u\left(\frac{\alpha}{2}+\frac{\gamma}{2}+2\delta\right)\Delta x-\frac{\epsilon}{2}\frac{\Delta x^2}{\Delta t}+\frac{u^2}{2}\Delta t\right]\frac{\partial^2 c}{\partial x^2}$$
$$+\left[v\left(\frac{\alpha'}{2}+\frac{\gamma'}{2}+2\delta'\right)\Delta y-\frac{\epsilon}{2}\frac{\Delta y^2}{\Delta t}+\frac{v^2}{2}\Delta t\right]\frac{\partial^2 c}{\partial y^2}+\left[-\epsilon\frac{\Delta x\Delta y}{\Delta t}+uv\Delta t\right]\frac{\partial^2 c}{\partial x\,\partial y}$$
$$+\left[\frac{\epsilon}{2}\frac{\Delta x\Delta y^2}{\Delta t}-\frac{uv^2}{2}\Delta t^2\right]\frac{\partial^3 c}{\partial x\,\partial y^2}+\left[\frac{\epsilon}{2}\frac{\Delta x^2\Delta y}{\Delta t}-\frac{u^2 v}{2}\Delta t^2\right]\frac{\partial^3 c}{\partial x^2\,\partial y}$$
$$-\left[u\left(-\frac{\alpha}{6}+\frac{\gamma}{6}+\frac{4}{3}\delta\right)\Delta x^2-\frac{\epsilon}{6}\frac{\Delta x^3}{\Delta t}+\frac{u^3}{6}\Delta t^2\right]\frac{\partial^3 c}{\partial x^3}$$
$$-\left[v\left(-\frac{\alpha'}{6}+\frac{\gamma'}{6}+\frac{4}{3}\delta'\right)\Delta y^2-\frac{\epsilon}{6}\frac{\Delta y^3}{\Delta t}+\frac{v^3}{6}\Delta t^2\right]\frac{\partial^3 c}{\partial y^3}=\mathrm{HOT}, \tag{4}$$

where HOT stands for higher-order terms. The nine unknown coefficients can now be set so as to ensure that the finite difference scheme is consistent with the transport equation and that some selected truncation error terms vanish. Consistency is achieved by imposing the vanishing of the term multiplied by the concentration c in the second term on the left-hand-side and that the terms multiplied by the first-order space derivatives, $\partial c/\partial x$ and $\partial c/\partial y$, be equal to u and v respectively.

As far as regards the remainder of the truncation error, the vanishing of the factors of the three second-order space derivatives related to numerical diffusion and of the third-order derivatives with respect to the same variable (i.e. $\partial^3 c/\partial x^3$, $\partial^3 c/\partial y^3$) is imposed. The ϵ coefficient can be easily determined explicitly, while the remaining eight unknown coefficients depend on seven relations only. The extra degree of freedom is used to impose separately $u(\alpha+\beta+\gamma+\delta)/\Delta x-\epsilon/2\Delta t=0$ and $v(\alpha'+\beta'+\gamma'+\delta')/\Delta y-\epsilon/2\Delta t=0$ in the factor of the concentration c in Equation (4). Solving the resultant linear system leads eventually to the expressions of the unknown coefficients:

$$\alpha=\frac{1}{6}(2-3C_x+C_x^2),\quad \alpha'=\frac{1}{6}(2-3C_y+C_y^2),$$
$$\beta=\frac{1}{2}(1+2C_x-C_x^2-C_y),\quad \beta'=\frac{1}{2}(1+2C_y-C_y^2-C_x),$$
$$\gamma=\frac{1}{2}(-2-C_x+C_x^2+2C_y),\quad \gamma'=\frac{1}{2}(-2-C_y+C_y^2+2C_x),$$
$$\delta=\frac{1}{6}(1-C_x^2),\quad \delta'=\frac{1}{6}(1-C_y^2),$$
$$\epsilon=C_xC_y, \tag{5}$$

where $C_x=u\Delta t/\Delta x$ and $C_y=v\Delta t/\Delta y$ are the Courant numbers relating to the x- and y-directions respectively. By substituting these coefficients back into Equation (4), the trunca-

tion error can be shown to be $0(\Delta x\Delta t, \Delta y\Delta t, \Delta t^2)$ (see Equation (11)). The scheme can be said to be of second-order, in a loose sense, if it is assumed that space and time increments tend to zero for fixed values of the Courant numbers, C_x and C_y.

It should be noted that for the special case of 1D flow, which is achieved by dropping the primed and the ϵ coefficients in Equation (3), all the truncation error terms up to second-order both in space and time would vanish, yielding precisely Leonard's QUICKEST scheme [4]. The present scheme can thus be regarded as a MOdified Second-order QUIckest scheme for Two-dimensional advectiOn and will be referred to in the following as MOSQUITO (MOS).

Indeed, the direct 2D extension of the QUICKEST scheme on a grid not including the diagonal cell, i.e. dropping the ϵ coefficient alone in Equation (4), would result in a numerical diffusion term of first-order in time in the truncation error, related to the mixed second space derivative, with diffusion coefficient $D_n = -uv$. This diffusive term would lead to instability when $uv > 0$, or to relatively high dissipation when $uv < 0$.

The scheme can be easily recast in conservation form expressing it in terms of fluxes through the sides of the cell control volume. Further extending it to solve the 2D depth-averaged equation (1), with variable u and v, and considering all four possible combinations of their signs and a variable depth h, leads eventually to the following conservative scheme:

$$h_{i,j}^{n+1}c_{i,j}^{n+1} = h_{i,j}^{n}c_{i,j}^{n} - \frac{u_{i+1/2,j}^{n}h_{i+1/2,j}^{n}\bar{c}_{i+1/2,j}^{n} - u_{i-1/2,j}^{n}h_{i-1/2,j}^{n}\bar{c}_{i-1/2,j}^{n}}{\Delta x}\Delta t - \frac{v_{i,j+1/2}^{n}h_{i,j+1/2}^{n}\bar{c}_{i,j+1/2}^{n} - v_{i,j-1/2}^{n}h_{i,j-1/2}^{n}\bar{c}_{i,j-1/2}^{n}}{\Delta y}\Delta t, \tag{6}$$

where

$$\bar{c}_{i+1/2,j}^{n} = \begin{cases} pc_{i+1,j}^{n} + qc_{i,j}^{n} + rc_{i-1,j}^{n} + sc_{i,j-1}^{n} & u > 0,\ \bar{v} > 0 \\ pc_{i,j}^{n} + qc_{i+1,j}^{n} + rc_{i+2,j}^{n} + sc_{i+1,j-1}^{n} & u < 0,\ \bar{v} > 0 \\ pc_{i,j}^{n} + qc_{i+1,j}^{n} + rc_{i+2,j}^{n} + sc_{i+1,j+1}^{n} & u < 0,\ \bar{v} < 0 \\ pc_{i+1,j}^{n} + qc_{i,j}^{n} + rc_{i-1,j}^{n} + sc_{i,j+1}^{n} & u > 0,\ \bar{v} < 0 \end{cases}, \tag{7}$$

with

$$\begin{cases} p = \dfrac{1}{6}(2 - 3|C_{x_{i+1/2,j}}| + C_{x_{i+1/2,j}}^2) \\ q = \dfrac{1}{6}(5 + 3|C_{x_{i+1/2,j}}| - 2C_{x_{i+1/2,j}}^2 - 3|\bar{C}_{y_{i+1/2,j}}|) \\ r = \dfrac{1}{6}(C_{x_{i+1/2,j}}^2 - 1) \\ s = \dfrac{1}{2}|\bar{C}_{y_{i+1/2,j}}| \end{cases} \tag{8}$$

and

$$C_{x_{i+1/2,j}} = \frac{u_{i+1/2,j}\Delta t}{\Delta x}, \qquad \bar{C}_{y_{i+1/2,j}} = \frac{\bar{v}_{i+1/2,j}\Delta t}{\Delta y},$$

$$\bar{v}_{i+1/2,j} = \frac{1}{4}(v^n_{i,j+1/2} + v^n_{i,j-1/2} + v^n_{i+1,j+1/2} + v^n_{i+1,j-1/2}), \tag{9}$$

with C_x, $\overline{C_y}$ being Courant numbers. Similar expressions hold for the y-flux terms.

3. ACCURACY AND STABILITY ANALYSIS

The MOSQUITO scheme has been compared for accuracy, stability and performance with four 2D schemes, namely TCS [20], TCF [20], MSQ [7] and QMA [7], with the last one being included as an example of unsatisfying stabilization of the explicit QUICK scheme. In the above quoted paper, the MSQ properties have been shown for the semi-discretized transport equation, i.e. regardless of time discretization. Here, that scheme will be considered in conjunction with the mixed leapfrog Euler-forward time stepping actually needed for stability in an explicit formulation:

$$\begin{aligned} c^{n+1}_{i,j} = c^{n-1}_{i,j} &- 2\frac{u\Delta t}{\Delta x}\left(\frac{-c^n_{i+2,j} + 8c^n_{i+1,j} - 8c^n_{i-1,j} + c^n_{i-2,j}}{12}\right. \\ &\left. + \frac{c^{n-1}_{i+2,j} - 4c^{n-1}_{i+1,j} + 6c^{n-1}_{i,j} - 4c^{n-1}_{i-1,j} + c^{n-1}_{i-2,j}}{16}\right) \\ &- 2\frac{v\Delta t}{\Delta y}\left(\frac{-c^n_{i,j+2} + 8c^n_{i,j+1} - 8c^n_{i,j-1} + c^n_{i,j-2}}{12}\right. \\ &\left. + \frac{c^{n-1}_{i,j+2} - 4c^{n-1}_{i,j+1} + 6c^{n-1}_{i,j} - 4c^{n-1}_{i,j-1} + c^{n-1}_{i,j-2}}{16}\right). \end{aligned} \tag{10}$$

Resorting to the usual hypotheses of steady uniform flow (u, $v = \text{constant}$), the truncation errors of the finite difference schemes, TE, can be evaluated by a Taylor series expansion:

$$\mathrm{TE}_{\mathrm{MOS}} = -\frac{uv}{2}\frac{\partial^3 c}{\partial x^2\,\partial y}\Delta t\Delta x - \frac{uv}{2}\frac{\partial^3 c}{\partial x\,\partial y^2}\Delta t\Delta y + \left(\frac{u^2 v}{2}\frac{\partial^3 c}{\partial x^2\,\partial y} + \frac{uv^2}{2}\frac{\partial^3 c}{\partial x\,\partial y^2}\right)\Delta t^2 + \mathrm{HOT}, \tag{11}$$

$$\begin{aligned} \mathrm{TE}_{\mathrm{TCS}} = &-\frac{1}{4}\left(\frac{u^3}{3}\frac{\partial^3 c}{\partial x^3} + \frac{v^3}{3}\frac{\partial^3 c}{\partial y^3} - u^2 v\frac{\partial^3 c}{\partial x^2\,\partial y} - uv^2\frac{\partial^3 c}{\partial x\,\partial y^2}\right)\Delta t^2 \\ &+ \left(\frac{u^2}{12}\frac{\partial^4 c}{\partial x^4} + \frac{uv}{12}\frac{\partial^4 c}{\partial x^3\,\partial y}\right)\Delta x^2\Delta t + \left(\frac{v^2}{12}\frac{\partial^4 c}{\partial y^4} + \frac{uv}{12}\frac{\partial^4 c}{\partial x\,\partial y^3}\right)\Delta y^2\Delta t - \frac{u}{12}\frac{\partial^4 c}{\partial x^4}\Delta x^3 \\ &- \frac{v}{12}\frac{\partial^4 c}{\partial y^4}\Delta y^3 + \mathrm{HOT}, \end{aligned} \tag{12}$$

$$\mathrm{TE}_{\mathrm{TCF}} = -\frac{1}{4}\left(\frac{u^3}{3}\frac{\partial^3 c}{\partial x^3} + \frac{v^3}{3}\frac{\partial^3 c}{\partial y^3}\right)\Delta t^2 - \frac{u}{12}\frac{\partial^4}{\partial x^4}\Delta x^3 - \frac{v}{12}\frac{\partial^4 c}{\partial y^4}\Delta y^3 + \mathrm{HOT}, \tag{13}$$

$$\begin{aligned} \mathrm{TE}_{\mathrm{QMA}} = &\left[\frac{u^2}{2}\left(1 - \frac{1}{8}\frac{C_y}{C_x}\right)\frac{\partial^2 c}{\partial x^2} + \frac{v^2}{2}\left(1 - \frac{1}{8}\frac{C_x}{C_y}\right)\frac{\partial^2 c}{\partial y^2} + uv\frac{\partial^2 c}{\partial x\,\partial y}\right]\Delta t - \frac{u}{24}\frac{\partial^3 c}{\partial x^3}\Delta x^2 \\ &- \frac{v}{24}\frac{\partial^3 c}{\partial y^3}\Delta y^2 + \mathrm{HOT} \end{aligned} \tag{14}$$

$$\mathrm{TE}_{\mathrm{MSQ}} = \frac{1}{6}\left(\frac{u^3}{3}\frac{\partial^3 c}{\partial x^3} + \frac{v^3}{3}\frac{\partial^3 c}{\partial y^3} + 3u^2 v\frac{\partial^3 c}{\partial x^2\,\partial y} + uv^2\frac{\partial^3 c}{\partial x\,\partial y^2}\right)\Delta t^2 - \frac{u}{16}\frac{\partial^4 c}{\partial x^4}\Delta x^3 - \frac{v}{16}\frac{\partial^4 c}{\partial y^4}\Delta y^3 + \mathrm{HOT}. \tag{15}$$

From Equation (14) it can be seen that QMA is affected by a numerical diffusion error component that is first-order in time. This would also occur with the fully explicit QUICK scheme [18]. However, in that case a negative defined numerical diffusion coefficient would result in unconditional instability of the scheme. The effect of the Matsuno time stepping is that of stabilizing the scheme by making it dissipative. All other schemes are free from numerical diffusion. Note that TCS can be said to be actually third-order-accurate in the same sense as MOS can be said to be second-order-accurate. It should also be noted that the effect of leapfrog time stepping used in MSQ is that of introducing a computational mode besides the physical mode in the numerical solution [5].

This can be shown by Fourier analysis for the case of steady uniform flow, substituting into the finite difference schemes the harmonic component in complex form:

$$c(x_i, y_j, t^n) = \mathrm{Re}(\hat{c}(t^n)\exp[I(k_x i\Delta x + k_y j\Delta y)]), \tag{16}$$

where Re stands for real part of a complex number, $I = \sqrt{-1}$, k_x and k_y are the wave numbers in the x- and y-directions respectively, and $\hat{c}(t^n)$ is the wave amplitude. A thorough 2D analysis consisting of the evaluation of the attenuation characteristics of the single wave components (whose behaviour, however, converges rather quickly to the long wave conditions), leads to the following stability conditions:

$$\text{MOS} \qquad \max\{C_x, C_y\} \le 1, \tag{17}$$

$$\text{TCS} \qquad C_x + C_y \le 2, \tag{18}$$

$$\text{QMA} \qquad C_x + C_y \le 1, \tag{19}$$

$$\text{MSQ (physical mode)} \qquad C_x + C_y \le 1, \tag{20}$$

$$\text{MSQ (computational mode)} \qquad C_x + C_y \le 0.5, \tag{21}$$

while TCF is unconditionally stable. Equation (18) has been already given in [20]. For brevity, the amplification factor, $|\lambda|$—defined as $\lambda = \hat{c}^{n+1}/\hat{c}^n$ [5]—and the numerical over exact celerity ratio of the 2D wave as a function of the Courant number and the normalized wave number, $\vartheta = k\Delta s/\pi$, $\Delta s = \Delta x = \Delta y$, are shown in graphic form in Figures 2 and 3 respectively, for $C_x = C_y = Cr$ and $k_x = k_y = k$.

4. TEST CASES

The numerical schemes have been verified for solution accuracy and CPU time performance with several classical test cases, either for advection alone or for advection–diffusion. Diffusion was included through a standard second-order Euler forward scheme [6]. For the case of advection alone, actual computations were carried out including the diffusion terms with zero diffusion coefficients. Moreover, although the computational domain of the test cases is quite simple, the schemes have been implemented in the kernel routine with all the options for a realistic simulation, i.e. including controls for possible closed or open boundaries. Thus, the timings reported in the following for the kernel routine are representative of realistic advection–diffusion simulations.

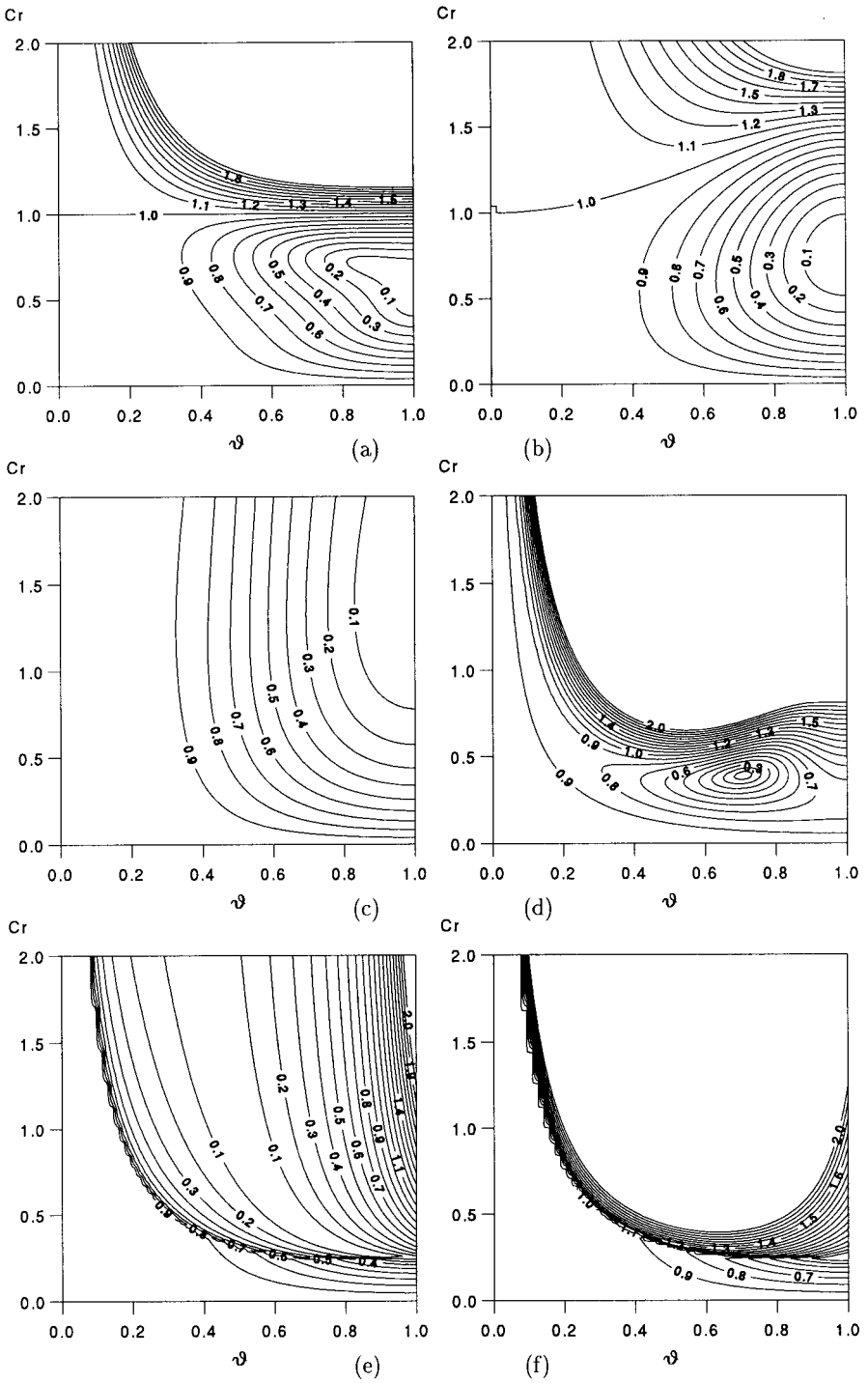

Figure 2. Amplification factor of 2D schemes (a) MOS, (b) TCS, (c) TCF, (d) QMA, (e) MSQ-physical mode, and (f) MSQ-computational mode, as a function of the normalized wave number, $\vartheta = k\Delta s/\pi$, and the Courant number, Cr, for $k_x = k_y = k$ and $C_x = C_y = Cr$.

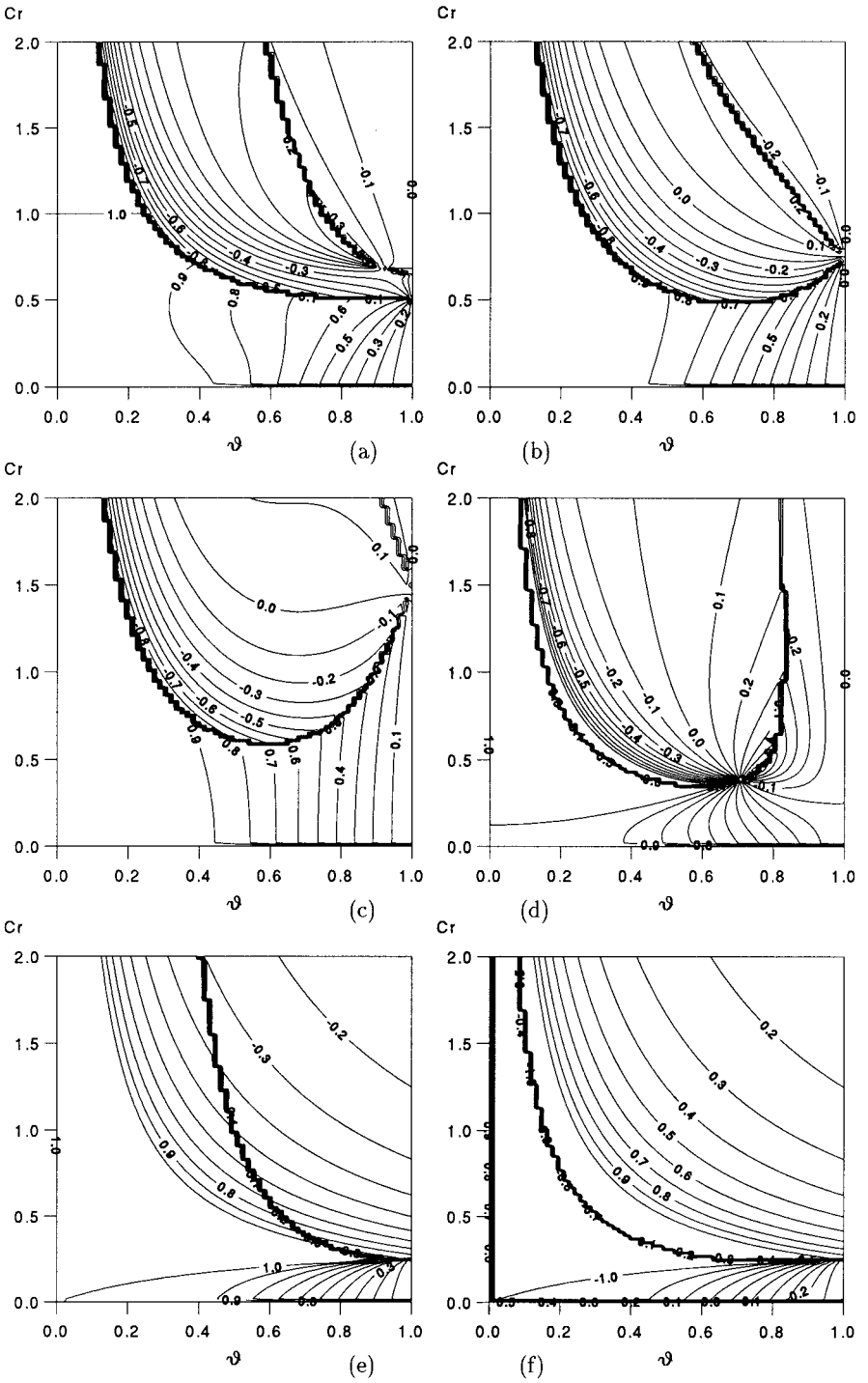

Figure 3. Numerical over exact phase celerity ratio of the 2D schemes (a) MOS, (b) TCS, (c) TCF, (d) QMA, (e) MSQ-physical mode, and (f) MSQ-computational mode, as a function of the normalized wave number, $\vartheta = k\Delta s/\pi$, and the Courant number, Cr, for $k_x = k_y = k$ and $C_x = C_y = Cr$.

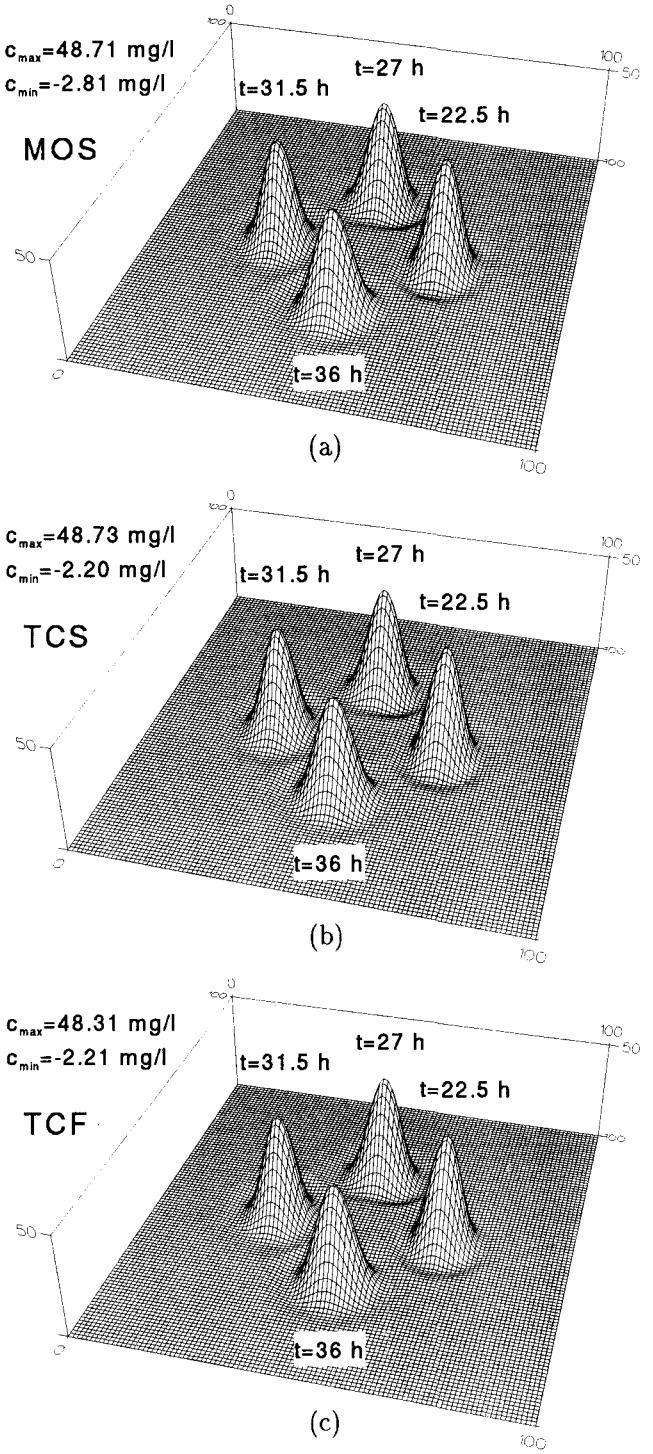

Figure 4. 2D advection of a circular column source in a rotational flow using (a) MOS, (b) TCS, and (c) TCF schemes.

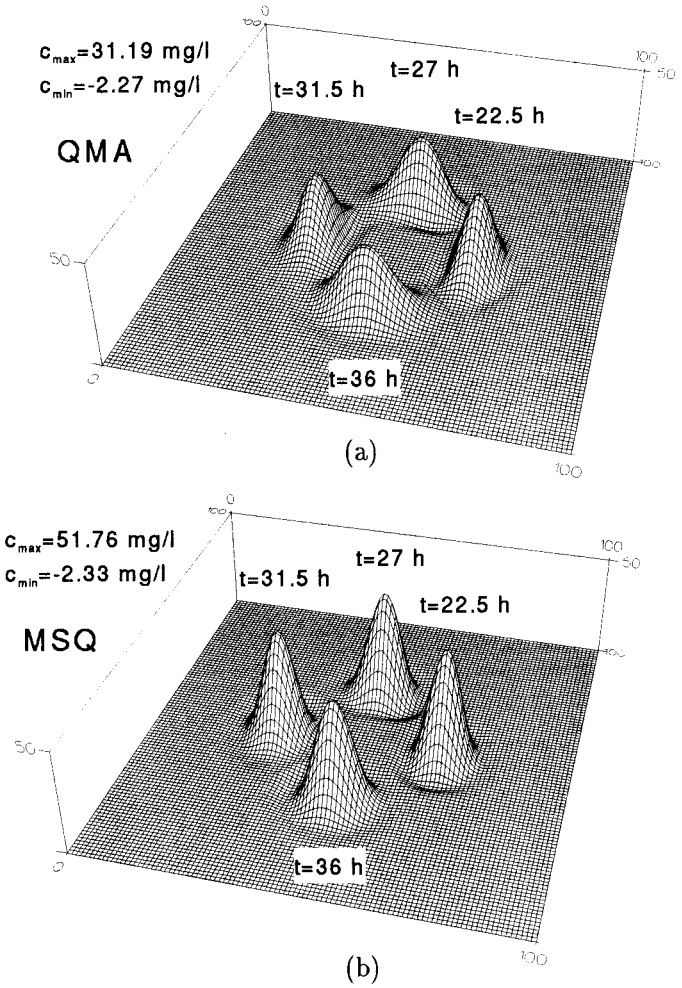

Figure 5. 2D advection of a circular column source in a rotational flow using (a) QMA and (b) MSQ schemes.

The first test case refers to pure advection of a circular column concentration distribution of peak value $c_{\max} = 50$ mg L^{-1} in a rotational flow [20]. The domain is an ideal one of size 101×101, $\Delta x = \Delta y = 100$ m, and constant depth. The centre of the concentration column of radius $R = 9\Delta x$ is located at time $t = 0$ in the cell (51, 31). The rotation period is $T = 18$ h. Zero concentrations were imposed at inflow boundaries and zero normal derivatives at outflow boundaries. The test was run with the time steps $\Delta t = 50$, 100, 200 and 400 s. In Figures 4 and 5, the results obtained for $\Delta t = 50$ are presented. This was the only value of Δt for which all five methods were stable. The figures show a snapshot of four positions of the concentration distributions during the second rotation. The maximum and minimum concentration values over the whole domain refer to the final situation, after 36 h from the start.

In all the tests with the three-time-level scheme, MSQ, the first time step was computed by the most accurate of the two-time-level schemes, namely TCF. All methods showed relative mass variations compared with the initial value of order $\pm 10^{-6} \div 10^{-4}$. As can be seen, the quality of the solution is slightly different among MOS, TCS, TCF and MSQ, while QMA,

showing a significant attenuation as a result of the $0(\Delta t)$ numerical diffusivity introduced with the Matsuno time stepping, is by far the least accurate of the five schemes. MSQ was unstable for $\Delta t = 100$ s, QMA for $\Delta t = 200$ s, and MOS for $\Delta t = 400$ s. It is to be noted, however, that TCS becomes actually unstable for values of Δt slightly greater than 400 s, and MOS for $\Delta t > 300$ s.

CPU times for the above test case run with $\Delta t = 50$ s on a Pentium 200 PC with a Linux operating system and a GNU FORTRAN compiler are shown in Table I.

MSQ is clearly the most efficient of the five schemes for the same time step; however, as already noticed, it has a rather severe stability condition, since it is no longer stable, not even from values of $\Delta t = 100$ s. QMA suffers because of the predictor–corrector algorithm, which, more or less, doubles the computational effort. Surprisingly, despite requiring $8N - 7$ and $19N - 29$ arithmetical operations for each ADI sweep to invert the three- and five-diagonal matrices respectively with the Thomas algorithm for a mesh of N cells [18], TCS and TCF take only slightly different CPU times. Therefore, the above results suggest that whenever large values of the Courant number are expected, TCF would be more attractive than TCS because of its unconditional stability.

MOS seems to be a good compromise between accuracy and stability properties compared with MSQ. However, being a two-time-level scheme, it is not affected by computational modes. Note that the effect of spurious roots on MSQ accuracy could be more pronounced in less simple cases than the above test case.

The second test case deals with pure advection of the same circular column concentration distribution in the same domain as in the case of rotational flow. However, in this case uniform flow at 45° with respect the Cartesian axes with $u = v = 0.3$ m s^{-1} takes place. The centre of the concentration column is located in the cell (11, 11) at time $t = 0$. The test was run with the time steps $\Delta t = 50$, 100, 200, and 400 s. In Figures 6 and 7 the results obtained for $\Delta t = 50$ s in four instants from start to about 6.7 h later are presented. Again, this was the only value of Δt for which all five methods were stable.

As in the previous test, the quality of the solution is slightly different among MOS, TCS, TCF and MSQ, while QMA shows remarkable damping. Instabilities occurred for the various methods with the same time steps as in the previous test case.

Addition of physical diffusion further reduces the differences between the performances of the methods. Figure 8 shows the longitudinal and transverse sections of the concentration distributions yielded by the various methods after release of a Gaussian source in the same rotational flow as in the first test, at the end of each rotation. The Gaussian source has a peak value $C_{\max} = 50$ mg L^{-1} and standard deviations $\sigma_x = \sigma_y = 350$ m, while the diffusion coefficients were constant and representative of typical conditions in practical applications of environmental hydraulics, $D_x = D_y = 0.5$ m^2 s^{-1}. The numerical results compare favourably with the exact solution, except for QMA, which again undergoes excessive numerical damping, while negative values are kept at a reduced magnitude.

Table I. CPU times for the test case of advection of circular column in rotational flow

	MOS	TCS	TCF	QMA	MSQ
CPU time [s]	182	595	606	275	159

$\Delta t = 50$ s.

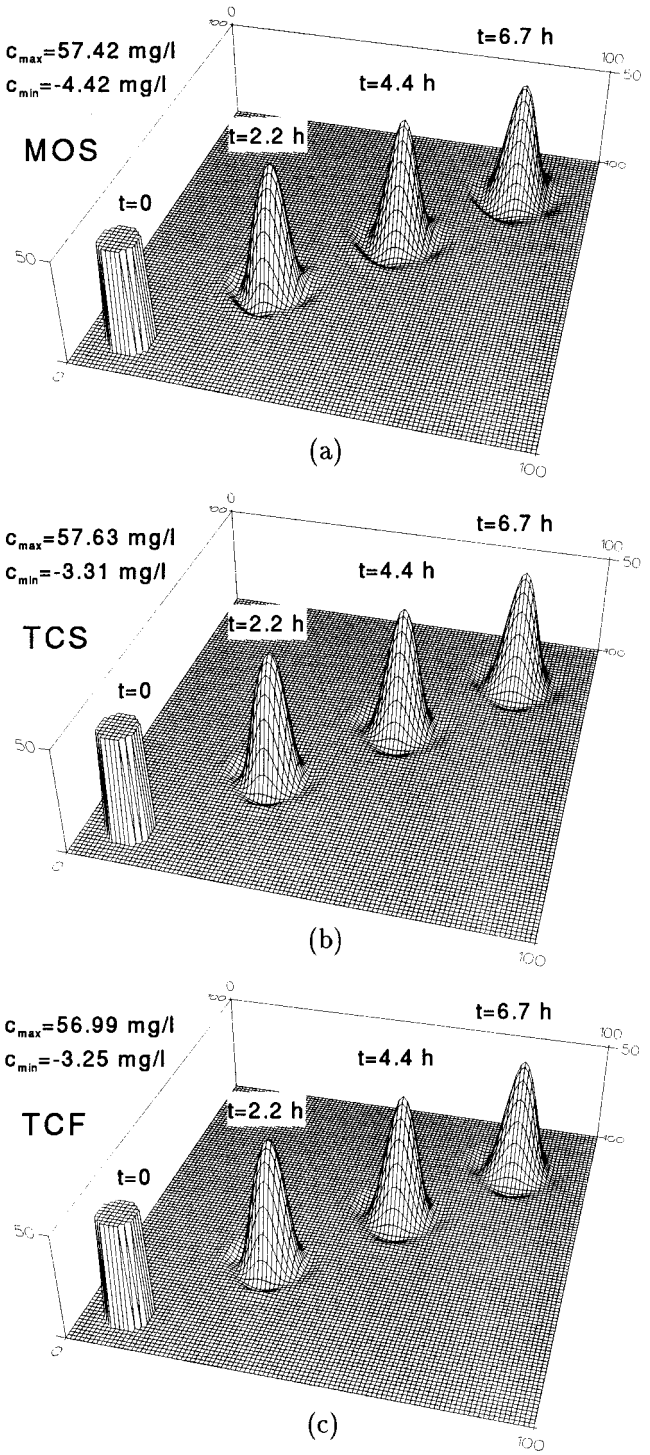

Figure 6. 2D advection of a circular column source in a uniform flow using (a) MOS, (b) TCS, and (c) TCF schemes.

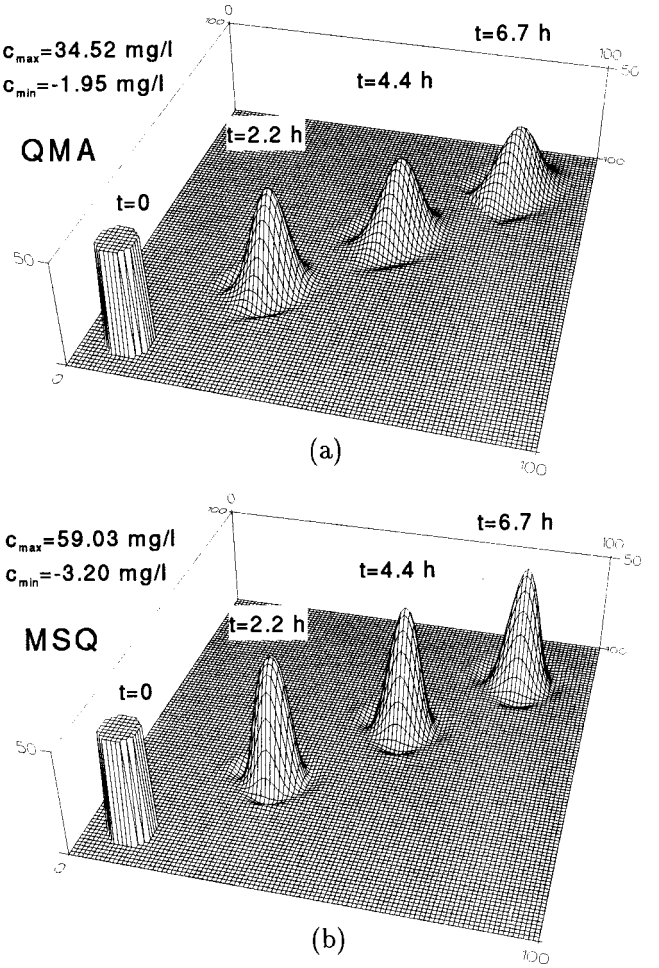

Figure 7. 2D advection of a circular column source in a uniform flow using (a) QMA and (b) MSQ schemes.

It is to be noted that MOS introduces numerical diffusion of order $0(\Delta t)$ in the solution of steady state problems as a consequence of the method derivation, while, being time centred, TCS, TCF and MSQ do not. However, in this case, the short computational time required by MOS makes feasible in practice an appropriate reduction of the time step in order to limit the numerical diffusion to acceptable values. Also, in principle, the method derivation itself could be adapted for the steady state by neglecting the higher-order time derivatives resulting from the Taylor series development of the discretized first-order time derivative in the expression of the truncation error, Equation (4). In fact, this derivative should be identically zero for the steady state [25].

5. CONCLUSIONS

An explicit 2D scheme for numerical simulation of advection (MOSQUITO, MOS), representing an extension of the 1D QUICKEST scheme, has been presented. Like the 1D QUICKEST

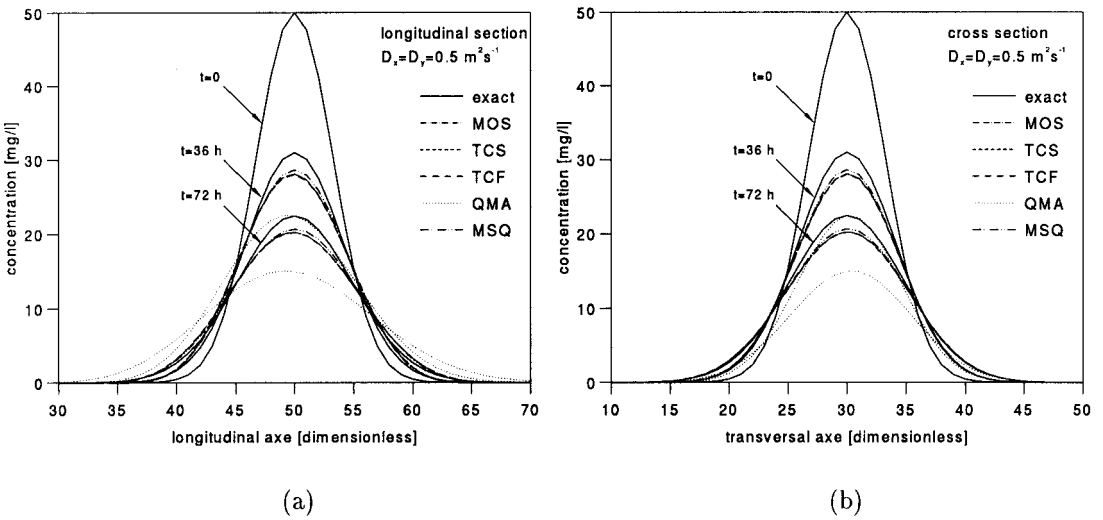

Figure 8. 2D advection–diffusion of a Gaussian source in a rotational flow with diffusion coefficients $D_x = D_y = 0.5$ $m^2\,s^{-1}$: (a) longitudinal and (b) cross-section of the concentration distribution.

scheme, MOS is a method for unsteady state problems. Although with truncation error of formal order $0(\Delta x/\Delta y, \Delta y \Delta t, \Delta t^2)$, the scheme has been shown to be actually of an accuracy comparable with schemes of third-order in space.

Compared with MSQ, MOS is about 20% slower; however, it has better stability properties and is free from computational modes. Compared with TCS and TCF, MOS is considerably faster and is thus a valuable alternative to those schemes. Consequently, MOS is also to be preferred to other popular finite difference schemes, e.g. the ADI QUICK and the two-point fourth-order Eulerian–Lagrangean, and all the schemes that were proved to be less accurate than TCS and TCF in [20]. The slight difference in accuracy among MOS, TCS, TCF and MSQ is further reduced in the presence of physical diffusion. Moreover, in the case of steady state problems, the short computational time required by the method seems to make it feasible, in practice, to reduce appropriately the time step in order to limit the first-order in time numerical diffusion introduced. Also, extension to the 3D case is straightforward in principle.

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