INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN FLUIDS, VOL. 24, 169–183 (1997)

AN ACCURATE FINITE DIFFERENCE SCHEME FOR SOLVING CONVECTION-DOMINATED DIFFUSION EQUATIONS

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SUMMARY

Approximating convection-dominated diffusion equations requires a very accurate scheme for the convection term. The most famous is the method of backward characteristics, which is very precise when a good interpolation procedure is used. However, this method is difficult to implement in 2D or 3D. The goal of this paper is to show that it is possible to construct finite difference schemes almost as accurate as the method of characteristics. Starting from a family of second- and third-order Lax–Wendroff-type schemes, a TVD and L^{∞}-stable scheme that is easy to implement in higher dimensions is constucted. Numerical tests are performed on various model problems whose solution is known and on classical problems. Comparisons with some other limiter schemes and the method of characteristics are discussed.

KEY WORDS: convection-dominated diffusion equations; TVD schemes; antidiffusive schemes; flux limiter scheme

1. INTRODUCTION

The aim of this work is to construct efficient schemes to solve the dimensionless convection–diffusion equation of the form

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} - \nu\frac{\partial^2 C}{\partial x^2} = 0, \tag{1}$$

where u is a function depending only on the space and time variables and ν is a positive constant that is very small with respect to $\|u\|_{\infty}$. Such equations arise, for instance, when a contaminant is spread out in a porous medium; in this simplified model C is the concentration of the contaminant, u is the velocity of the saturation fluid and ν is the diffusion parameter.

During the last 15 years many authors have used the method of characteristics eventually combined with finite elements or finite differences to solve problems of miscible displacement in porous media.[1–4] This method is very accurate but difficult to implement in two or three dimensions. Thus our purpose is to introduce a new finite difference scheme that is easy to extend to higher dimensions, stable and accurate enough to avoid instabilities and numerical diffusion. To reach this goal, we build a TVD scheme following the ideas of Harten[5] and Van Leer[6] from a family of second- and third-order Lax–Wendroff-type schemes.

After giving the notation and the basis of TVD finite difference schemes, we show that the convection term must be discretized explicitly. In Section 3 we present the method of backward characteristics introduced by Holly and Preissmann.[7] Then we construct a TVD version of the

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CCC 0271–2091/97/020169–15

Received 27 October 1994
Revised 29 April 1996

QUICKTEST[8] or Takacs[9] scheme. Finally we give the extension to 2D and present some numerical experiments that show the efficiency of our scheme.

2. NOTATION AND PRELIMINARIES

For (x, t) in $]0, 1[\times \mathbb{R}^+$ we denote by δx and δt the space and time steps respectively and by C_i^n the approximation of $C(i\delta x, n\delta t)$. Let us approximate the equation

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = 0 \tag{2}$$

by an explicit scheme written as

$$C_i^{n+1} = C_i^n + D_{i+1/2}^+(C_{i+1}^n - C_i^n) - D_{i-1/2}^-(C_i^n - C_{i-1}^n). \tag{3}$$

We recall that a scheme is said to be TVD if

$$TV(C^{n+1}) \leqslant TV(C^n),$$

where

$$TV(C) = \sum_i |C_{i+1} - C_i|,$$

and is said to be L^∞-stable if there exists a constant d such that

$$\max_i |C_i^n| \leqslant d \max_i |C_i^0|.$$

Here the scheme (3) is TVD if

$$D_{i+1/2}^+ \geqslant 0 \quad \text{and} \quad D_{i-1/2}^- \geqslant 0, \quad \forall i,$$
$$D_{i+1/2}^+ + D_{i+1/2}^- \leqslant 1, \quad \forall i,$$

and is L^∞-stable if

$$D_{i+1/2}^+ \geqslant 0 \quad \text{and} \quad D_{i-1/2}^- \geqslant 0, \quad \forall i,$$
$$D_{i+1/2}^+ + D_{i-1/2}^- \leqslant 1, \quad \forall i.$$

Since an explicit scheme requires a CFL condition, it may be interesting to use an implicit scheme instead, as is done by several authors. However, this is not suitable because it adds some numerical viscosity. Indeed, let us discretize

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = 0,$$

where u is a positive constant, by

$$C_i^{n+1} = C_i^n - u\lambda(C_i^n - C_{i-1}^n) \tag{4a}$$

or

$$C_i^{n+1} = C_i^n - u\lambda(C_i^{n+1} - C_{i-1}^{n+1}) \tag{4b}$$

with a first-order upwind scheme, where $\lambda = \delta t/\delta x$.

The scheme (4a) is a second-order approximation at point $(i\delta x, (n + \frac{1}{2}\delta t)$ of the equation

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} - u\left(\frac{\delta x}{2} - u\frac{\delta t}{2}\right)\frac{\partial^2 C}{\partial x^2} = 0,$$

while the scheme (4b) is a second-order approximation at the same point of the equation

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} - u\left(\frac{\delta x}{2} + u\frac{\delta t}{2}\right)\frac{\partial^2 C}{\partial x^2} = 0.$$

In the first case the limiting CFL condition $\lambda u = 1$ gives the exact solution without any diffusion, whereas the diffusion term never vanishes but increases with δt in the second case. Thus the latter scheme is useless, since the space and time steps must be small enough in front of v to get a realistic solution. Therefore in this paper we approximate the convection term explicitly.

3. THE METHOD OF BACKWARD CHARACTERISTICS

We recall in this section the method of characteristics used for comparisons. First of all, equation (1) is split into

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = 0 \tag{5a}$$

and

$$\frac{\partial C}{\partial t} - v\frac{\partial^2 C}{\partial x^2} = 0 \tag{5b}$$

to show off the action of the different terms.

Then the transport equation is solved by the method of characteristics with $\bar{C}$ denoting the intermediate approximation.

To determine the value of the approximate solution $\bar{C}_i^{n+1}$ at point $(x_i = i\delta x, t^{n+1} = (n+1)\delta t)$, the idea is to seek the origin (x_{P}, t^n) of the characteristic curve passing by (x_i, t^{n+1}).

Equation (5a) can be rewritten as

$$\frac{\mathrm{d}}{\mathrm{d}t}\bar{C}(X, t) = 0,$$

where $X(t)$ is the characteristic curve given by

$$\frac{\mathrm{d}}{\mathrm{d}t}X(t) = u(X(t), t) \tag{6}$$

and

$$\bar{C}_i^{n+1} = C(x_{\mathrm{P}}, t^n).$$

Thus the algorithm consists of solving the differential equation (6) and then interpolating $C_{\mathrm{P}}^n = C(x_{\mathrm{P}}, t^n)$ from the known values C_i^n and the derivatives $(C_x)_i^n$, where $C_x = \partial C/\partial x$. Equation (6) can be solved by any appropriate method, e.g. a fourth-order Runge–Kutta algorithm. In contrast, the interpolation procedure is not straightforward. One of the best methods was introduced by Holly and Preissmann[7] and is described below.

Let us assume that x_{P} is located between x_{k-1} and x_k (Figure 1). The first step is to write a third-order interpolation as

$$C(x_{\mathrm{P}}, t^n) = \theta^2(3-2\theta)C_{k-1}^n + (1-\theta)C_k^n + \theta^2(1-\theta)\delta x(C_x)_{k-1}^n - \theta(1-\theta)^2\delta x(C_x)_k^n,$$

where $\theta = (x_k - x_{\mathrm{P}})/\delta x$ and C_x denotes the first space derivative; an approximation of C_x is obtained by solving

$$\frac{\partial C_x}{\partial t} + u\frac{\partial C_x}{\partial x} + u_x C_x - v\frac{\partial^2 C_x}{\partial x_2} = 0, \tag{7}$$

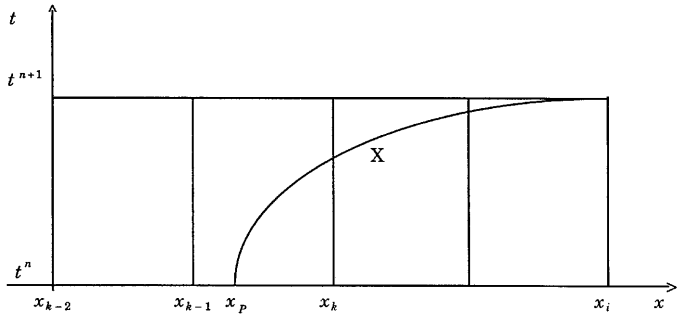

Figure 1. Characteristic curve for $u(x, t) \geqslant 0$

since C satisfies equation (1). Then equation (7) is solved in two fractional steps for the transport and the diffusion term:

$$\frac{\partial C_x}{\partial t} + u\frac{\partial C_x}{\partial x} = -u_x C_x, \tag{8a}$$

$$\frac{\partial C_x}{\partial t} - \nu\frac{\partial^2 C_x}{\partial x_2} = 0. \tag{8b}$$

Integrating (8a) by the characteristic method, one gets

$$(\tilde{C}_x)_k^{n+1} - (C_x)_\mathrm{P}^n = -\int_{x_\mathrm{P}}^{x_i} u_x C_x \mathrm{d}t,$$

where $(C_x)_\mathrm{P}^n$ is given by

$$(C_x)_\mathrm{P}^n = 6\theta(\theta-1)(C_{k-1}^n - C_k^n)/\delta x + \theta(3\theta-2)(C_x)_{k-1}^n + (1-\theta)(1-3\theta)(C_x)_k^n$$

and the integral is approximated by a linear quadrature formula; thus

$$(\tilde{C}_x)_k^{n+1} = (C_x)_k^{n+1} - \nu\delta t\big[(C_x)_{k-1}^{n+1} - 2(C_x)_k^{n+1} + (C_x)_{k+1}^{n+1}\big]/\delta x^2.$$

At the end the solution of (1) is given by

$$C_i^{n+1} - \nu\delta t(C_{i-1}^{n+1} - 2C_i^{n+1} + C_{i+1}^{n+1})/\delta x^2 = \bar{C}_i^{n+1}.$$

Remark

The choice of the interpolation technique to evaluate C_P^n determines the accuracy of the scheme. Indeed, the first idea is to interpolate linearly C_P^n with C_{k-1}^n and C_k^n, but the resulting scheme is a first-order diffusive scheme. Another way is to compute C_P^n from a second-order upwind interpolation using C_{k-2}^n, C_{k-1}^n and C_k^n, which gives a dissipative scheme, whereas the method of Holly and Preissman yields the optimal approximation (Figure 2). The numerical data are identical with those of Figure 7.

4. A NEW FLUX LIMITER SCHEME

In this section we construct a TVD and L^∞-stable scheme from a family of second- or third-order[8,9] schemes by introducing a new flux limiter, as has been done in previous works on the Lax–Wendroff scheme.

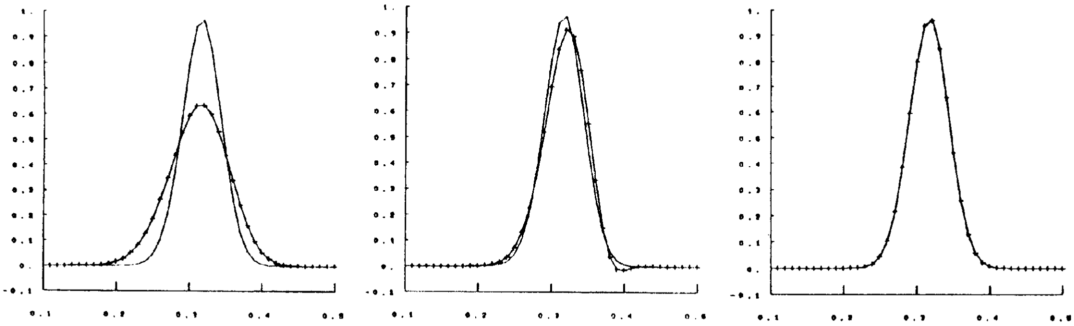

Figure 2. Comparison of first order (left), second-order (middle) and Holly–Preissmann (right) interpolations

Takacs[9] has built a family of second- and third-order upwind schemes for equation (2) by writing, when u is a positive constant,

$$C_i^{n+1} = \alpha_1 C_{i+1}^n + \alpha_0 C_i^n + \alpha_{-1} C_{i-1}^n + \alpha_{-2} C_{i-2}^n, \tag{9}$$

where the α_k are chosen such that the error

$$e = C(x, t + \Delta t) - \sum_{k=-2}^{1} \alpha_k C(x + k\Delta x, t)$$

is $\mathcal{O}(\delta t^3)$.

This is achieved by setting

$$C(x, t + \delta t) = C(x, t) - \delta t\, u \frac{\partial C}{\partial x}(x, t) + \frac{\delta t^2}{2} u^2 \frac{\partial^2 C}{\partial x^2}(x, t) - \frac{\delta t^3}{6} u^3 \frac{\delta^3 C}{\delta x^3}(x, t) + \mathcal{O}(\delta t^4) \tag{10}$$

and approximating the three derivatives on the four points chosen when u is positive as

$$\frac{\partial C}{\partial x}(x, t) = [C(x, t) - C(x - \delta x, t)]/\delta x + \frac{\delta x}{2}\frac{\partial^2 C}{\partial x^2}(x, t) - \frac{\delta x^2}{6}\frac{\partial^3 C}{\partial x^3}(x, t) + \mathcal{O}(\delta x^3),$$

$$\frac{\partial^2 C}{\partial x^2}(x, t) = [C(x + \delta x, t) - 2C(x, t) + C(x - \delta x, t)]/\delta x^2 + \mathcal{O}(\delta x^2),$$

$$\frac{\partial^3 C}{\partial x^3}(x, t) = [C(x + \delta x, t) - 3C(x, t) + 3C(x - \delta x, t) - C(x - 2\delta x, t)]/\delta x^3 + \mathcal{O}(\delta x).$$

This yields

$$\alpha_1 = \frac{\lambda u(\lambda u - 1)}{2} - \alpha_{-2}, \qquad \alpha_0 = 1 - (\lambda u)^2 + 3\alpha_{-2}, \qquad a_{-1} = \frac{\lambda u(\lambda u + 1)}{2} - 3\alpha_{-2},$$

where α_{-2} is determined in order to get the exact solution for $u = 0$ and $\lambda u = 1$, i.e.

$$\alpha_{-2} = \alpha\lambda u(\lambda u - 1),$$

with α a non-negative constant.

Thus the scheme (9) reads

$$\begin{aligned} C_i^{n+1} = C_i^n &- \frac{\lambda u}{2}(C_{i+1}^n - C_{i-1}^n) + \frac{(\lambda u)^2}{2}(C_{i+1}^n - 2C_i^n + C_{i-1}^n) \\ &- \alpha\lambda u(\lambda u - 1)(C_{i+1}^n - 3C_i^n + 3C_{i-1}^n - C_{i-2}^n) \end{aligned} \tag{11}$$

and is a third-order approximation of the equation

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}+\frac{\delta x^2}{6}u(1-\lambda u)(1+\lambda u-6\alpha)\frac{\partial^3 C}{\partial x^3}=0.$$

For $\alpha = 0$ we recognize the Lax–Wendroff scheme and for $\alpha = (1+\lambda u)/6$ we obtain a third-order approximation of equation (2). However, this scheme is neither TVD nor L^∞-stable and can generate some instabilities at singular points.[9] In this work we explain how we transform (11) to get a TVD and L^∞-stable scheme and we show in numerical tests the resulting improvement.

Let us rewrite (11) as

$$\begin{aligned}C_i^{n+1} &= C_i^n - \lambda u(C_i^n - C_{i-1}^n) - \frac{\lambda u(1-\lambda u)}{2}(C_{i+1}^n - 2C_i^n + C_{i-1}^n)\\ &\quad + \alpha\lambda u(1-\lambda u)[(C_{i+1}^n - C_i^n) - 2(C_i^n - C_{i-1}^n) + (C_{i-1}^n - C_{i-2}^n)]\end{aligned} \tag{12}$$

and let us set $\Delta C_{i+1/2}^n = C_{i+1}^n - C_i^n$ and $r_{i+1/2}^n = \Delta C_{i-1/2}^n/\Delta C_{i+1/2}^n$; we then obtain

$$\begin{aligned}C_i^{n+1} &= C_i^n - \lambda u\Delta C_{i-1/2}^n - \frac{\lambda u(1-\lambda u)}{2}(\Delta C_{i+1/2}^n - \Delta C_{i-1/2}^n)\\ &\quad + \alpha\lambda u(1-\lambda u)[(1-r_{i+1/2}^n)\Delta C_{i+1/2}^n - (1-r_{i-1/2}^n)\Delta C_{i-1/2}^n],\end{aligned} \tag{13}$$

since

$$\Delta C_{i+1/2}^n - 2\Delta C_{i-1/2}^n + \Delta C_{i-3/2}^n = (1-r_{i+1/2}^n)\Delta C_{i+1/2}^n - (1-r_{i-1/2}^n)\Delta C_{i-1/2}^n.$$

According to the sign of the coefficient $1 - r_{i+1/2}^n$, the last term is either a diffusive or an antidiffusive term added to the Lax–Wendroff scheme. To get a TVD scheme, we apply the technique of limiters used by Roe,[10] Sweby[11] or Van Leer[6] to transform the Lax–Wendroff scheme.

Thus we modify (11) as

$$\begin{aligned}C_i^{n+1} &= C_i^n - \lambda u\Delta C_{i-1/2}^n - \frac{\lambda u(1-\lambda u)}{2}(\Delta C_{i+1/2}n - \Delta C_{i-1/2}^n)\\ &\quad + \lambda u(1-\lambda u)[\bar{\alpha}_{i+1/2}^n(\Delta C_{i+1/2}^n - \Delta C_{i-1/2}^n) - \bar{\alpha}_{i-1/2}^n(\Delta C_{i-1/2}^n - \Delta C_{i-3/2}^n)],\end{aligned} \tag{14}$$

where the coefficients $\bar{\alpha}_{i\pm 1/2}^n$ are given by (15).

Proposition 1

If

$$\bar{\alpha}_{i\pm 1/2}^n = \min\left(\frac{|1-r_{i\pm 1/2}^n|}{2}, \frac{1}{2|1-r_{i\pm 1/2}^n|}\right), \tag{15}$$

then the scheme (14) is TVD and L^∞-stable under the CFL condition $0 \leqslant \lambda u \leqslant 1$.

Moreover, it is of second order when the solution is smooth enough except on a neighbourhood of the extremal points.

The proof is based on the classical results below.[12]

Lemma

The scheme defined by

$$C_i^{n+1} = C_i^n - \lambda u\Delta C_{i-1/2}^n - \frac{\lambda u(1-\lambda u)}{2}(\varphi_{i+1/2}\Delta C_{i+1/2}^n - \varphi_{i-1/2}\Delta C_{i-1/2}^n), \tag{16}$$

with

$$\varphi_{i+1/2} = \varphi(r_{i+1/2}),$$

is TVD and L^∞-stable under the CFL condition $0 \leqslant \lambda u \leqslant 1$ if φ satisfies

$$\varphi(r) = 0 \quad \text{if } r < 0, \qquad 0 \leqslant \varphi(r) \leqslant \min(2, 2r) \quad \text{otherwise.} \tag{17}$$

Moreover, if φ admits left and right derivatives at $r = 1$ and if $\varphi(1) = 1$, the scheme is of second order when the solution is smooth enough except on a neighbourhood of the extremal points.

Let us rewrite (14) as

$$\begin{aligned} C_i^{n+1} = C_i^n - \lambda u \Delta C_{i-1/2}^n - \frac{\lambda u(1-\lambda u)}{2}(\Delta C_{i+1/2}^n - \Delta C_{i-1/2}^n) \\ + \frac{\lambda u(1-\lambda u)}{2}[2\bar{\alpha}_{i+1/2}^n(1 - r_{i+1/2}^n)\Delta C_{i+1/2}^n - 2\bar{\alpha}_{i-1/2}^n(1 - r_{i-1/2}^n)\Delta C_{i-1/2}^n]. \end{aligned} \tag{18}$$

Then we find (16) be setting

$$\varphi_{i+1/2}^n = 1 - 2\bar{\alpha}_{i+1/2}^n(1 - r_{i+1/2}^n).$$

Further, if the coefficients $\bar{\alpha}_{i+1/2}^n$ are given by condition (15), then φ satisfies (17), since

$$\varphi(r) = \begin{cases} 2 & \text{if } r \geqslant 2, \\ 1 + (1-r)^2 & \text{if } 1 \leqslant r \leqslant 2, \\ 2r - r^2 & \text{if } 0 \leqslant r \leqslant 1, \\ 0 & \text{otherwise,} \end{cases} \tag{19}$$

$\varphi(1) = 1$ and $\varphi'(1^+) = \varphi'(1^-) = 0$.

The last step is to generalize the above scheme for the convection equation when u is a function of the space variable. In this case we write equation (2) as

$$\frac{\partial C}{\partial t} + u^+ \frac{\partial C}{\partial x} - u^- \frac{\partial C}{\partial x} = 0,$$

where $u(x) = u^+(x) - u^-(x)$, with u^+ and u^- two non-negative functions. Then we apply the discretization (9) for u^+ on points x_{i+1}, x_i, x_{i-1} and x_{i-2} and for u^- on points x_{i+2}, x_{i+1}, x_i and x_{i-1}. Indeed, when u is a function of x, equation (10) becomes

$$\begin{aligned} C(x, t+\delta t) = C(x,t) - \delta t u(x)\frac{\partial C}{\partial x}(x,t) + \frac{\delta t^2}{2}u(x)\frac{\partial}{\partial x}\left(u(x)\frac{\partial C}{\partial x}\right)(x,t) \\ - \frac{\delta t^3}{6}u(x)\frac{\partial}{\partial x}\left[u(x)\frac{\partial}{\partial x}\left(u(x)\frac{\partial C}{\partial x}\right)\right](x,t) + \mathcal{O}(\delta t^4) \end{aligned}$$

and the derivatives are approximated for u^+ by

$$\frac{\partial C}{\partial x}(x,t) = [C(x,t) - C(x-\delta x,t)]/\delta x + \frac{\delta x}{2}\frac{\partial^2 C}{\partial x^2}(x,t) - \frac{\delta x^2}{6}\frac{\partial^3 C}{\partial x^3}(x,t) + \mathcal{O}(\delta x^3),$$

$$\begin{aligned}\frac{\partial}{\partial x}\left(u^+(x)\frac{\partial C}{\partial x}\right)(x,t) = \Bigg[u^+\left(x+\frac{\delta x}{2}\right)&[C(x+\delta x,t) - C(x,t)]\\ - u^+\left(x-\frac{\delta x}{2}\right)&[C(x,t) - C(x-\delta x,t)]\Bigg]\Big/\delta x^2 + \mathcal{O}\big(\delta x^2\big),\end{aligned}$$

$$\begin{aligned}\frac{\partial}{\partial x}\left[u^+(x)\frac{\partial}{\partial x}\left(u^+(x)\frac{\partial C}{\partial x}\right)\right](x,t) = \Bigg\{&u^+(x)\Bigg[u^+\left(x+\frac{\delta x}{2}\right)[C(x+\delta x,t) - C(x,t)]\\ &- u^+\left(x-\frac{\delta x}{2}\right)[C(x,t) - C(x-\delta x,t)]\Bigg]\\ &- u^+(x-\delta x)\Bigg[u^+\left(x-\frac{\delta x}{2}\right)[C(x,t) - C(x-\delta x,t)]\\ &- u^+\left(x-\frac{3\delta x}{2}\right)[C(x-\delta x,t) - C(x-2\delta x,t)]\Bigg\}/\delta x^3\\ &+ \mathcal{O}(\delta x).\end{aligned}$$

Thus the third-order Takacs scheme reads

$$\begin{aligned}C_i^{n+1} = C_i^n &- \lambda u_i^+ \Delta C_{i-1/2}^n - \frac{\lambda}{2}u_i^+[(1-\lambda u_{i+1/2}^+)\Delta C_{i+1/2}^n - (1-\lambda u_{i-1/2}^+)\Delta C_{i-1/2}^n]\\ &+ \frac{\lambda}{6}u_i^+[(1-\lambda^2 u_i^+ u_{i+1/2}^+)\Delta C_{i+1/2}^n - (1-\lambda^2 u_i^+ u_{i-1/2}^+)\Delta C_{i-1/2}^n\\ &- (1-\lambda^2 u_{i-1}^+ u_{i-1/2}^+)\Delta C_{i-1/2}^n + (1-\lambda^2 u_{i-1}^+ u_{i-3/2}^+)\Delta C_{i-3/2}^n]\\ &+ \lambda u_i^- \Delta C_{i+1/2}^n - \frac{\lambda}{2}u_i^-[(1-\lambda u_{i+1/2}^-)\Delta C_{i+1/2}^n - (1-\lambda u_{i-1/2}^-)\Delta C_{i-1/2}^n]\\ &- \frac{\lambda}{6}u_i^-[(1-\lambda^2 u_{i+1}^- u_{i+3/2}^-)\Delta C_{i+3/2}^n - (1-\lambda^2 u_{i+1}^- u_{i+1/2}^-)\Delta_{i+1/2}^n\\ &- (1-\lambda^2 u_i^- u_{i+1/2}^-)\Delta C_{i+1/2}^n + (1-\lambda^2 u_i^- u_{i-1/2}^-)\Delta C_{i-1/2}^n].\end{aligned}$$

This scheme is neither TVD nor L^∞-stable and we need to introduce the second-order family scheme

$$\begin{aligned}C_i^{n+1} &= C_i^n - \lambda u_i^+ \Delta C_{i-1/2}^n - \frac{\lambda}{2}u_i^+[(1-\lambda u_{i+1/2}^+)\Delta C_{i+1/2}^n - (1-\lambda u_{i-1/2}^+)\Delta C_{i-1/2}^n]\\ &+ \lambda u_i^+[\alpha_{i+1/2}^+(1-\lambda u_{i+1/2}^+)\Delta C_{i+1/2}^n - \alpha_{i+1/2}^+(1-\lambda u_{i-1/2}^+)\Delta C_{i-1/2}^n - \alpha_{i-1/2}^+(1-\lambda u_{i-1/2}^+)\Delta C_{i-1/2}^n\\ &+ \alpha_{i-1/2}^+(1-\lambda u_{i-3/2}^+)\Delta C_{i-3/2}^n]\\ &+ \lambda u_i^- \Delta C_{i+1/2}^n - \frac{\lambda}{2}u_i^-[(1-\lambda u_{i+1/2}^-)\Delta C_{i+1/2}^n - (1-\lambda u_{i-1/2})\Delta C_{i-1/2}^n]\\ &- \lambda u_i^-[\alpha_{i+1/2}^-(1-\lambda u_{i+3/2}^-)\Delta C_{i+3/2}^n - \alpha_{i+1/2}^-(1-\lambda u_{i+1/2}^-)\Delta C_{i+1/2}^n\\ &- \alpha_{i-1/2}^-(1-\lambda u_{i+1/2}^-)\Delta C_{i+1/2}^n + \alpha_{i-1/2}^-(1-\lambda u_{i-1/2}^-)\Delta C_{i-1/2}^n].\end{aligned} \tag{20}$$

Thus, following the same procedure, equation (18) becomes

$$\begin{aligned}C_i^{n+1} = C_i^n - \lambda u_i^+ \Delta C_{i-1/2}^n - \frac{\lambda}{2} u_i^+ [(1-\lambda u_{i+1/2}^+)\Delta C_{i+1/2}^n - (1-\lambda u_{i+1/2}^+)\Delta C_{i-1/2}^n] \\ + \frac{\lambda}{2} u_i^+ [2\alpha_{i+1/2}^+ (1-\lambda u_{i+1/2}^+)(1-r_{i+1/2}^{+n})\Delta C_{i+1/2}^n - 2\alpha_{i-1/2}^+ (1-\lambda u_{i-1/2}^+)(1-r_{i-1/2}^{+n})\Delta C_{i-1/2}^n] \\ + \frac{\lambda}{2} u_i^- [2\alpha_{i+1/2}^- (1-\lambda u_{i+1/2}^-)(1-r_{i+1/2}^{-n})\Delta C_{i+1/2}^n - 2\alpha_{i-1/2}^- (1-\lambda u_{i-1/2}^-)(1-r_{i-1/2}^{-n})\Delta C_{i-1/2}^n],\end{aligned} \tag{21}$$

where

$$r_{i+1/2}^{+n} = \frac{(1-\lambda u_{i-1/2}^+)\Delta C_{i-1/2}^n}{(1-\lambda u_{i+1/2}^+)\Delta C_{i+1/2}^n}, \qquad r_{i+1/2}^{-n} = \frac{(1-\lambda u_{i+3/2}^-)\Delta C_{i+3/2}^n}{(1-\lambda u_{i+1/2}^-)\Delta C_{i+1/2}^n},$$

and we replace the $\alpha_{i+1/2}^{\pm}$ by some functions $\bar{\alpha}_{i+1/2}^{\pm n}$ depending on $r_{i+1/2}^{\pm n}$ to obtain a TVD and L^∞-stable scheme.

Proposition 2

If

$$\bar{\alpha}_{i\pm1/2}^{\pm n} = \min\left(\frac{|1-r_{i\pm1/2}^{\pm n}|}{2}, \frac{1}{2|1-r_{i\pm1/2}^{\pm n}|}\right),$$

then the resulting scheme is TVD and L^∞-stable under the CFL condition $\lambda\|u\|_\infty \leqslant 1$.

Proof. We write (21) as

$$\begin{aligned}C_i^{n+1} = C_i^n - \lambda u_i^+ \Delta C_{i-1/2}^n - \frac{\lambda}{2} u_i^+ [(1-\lambda u_{i+1/2}^+)\varphi_{i+1/2}^{+n}\Delta C_{i+1/2}^n - (1-\lambda u_{i-1/2}^+)\varphi_{i-1/2}^{+n}\Delta C_{i-1/2}^n] \\ + \lambda u_i^- \Delta C_{i+1/2}^n - \frac{\lambda}{2} u_i^- [(1-\lambda u_{i+1/2}^-)\varphi_{i+1/2}^{-n}\Delta C_{i+1/2}^n - (1-\lambda u_{i-1/2}^-)\varphi_{i-1/2}^{-n}\Delta C_{i-1/2}^n].\end{aligned}$$

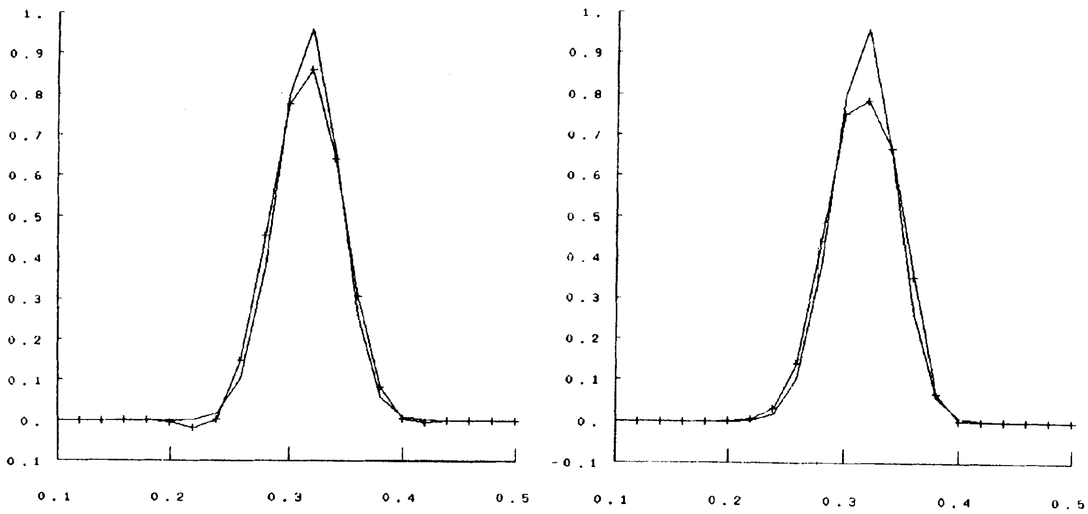

Figure 3. Solution on coarse mesh with third-order Takacs (left) and new (right) schemes

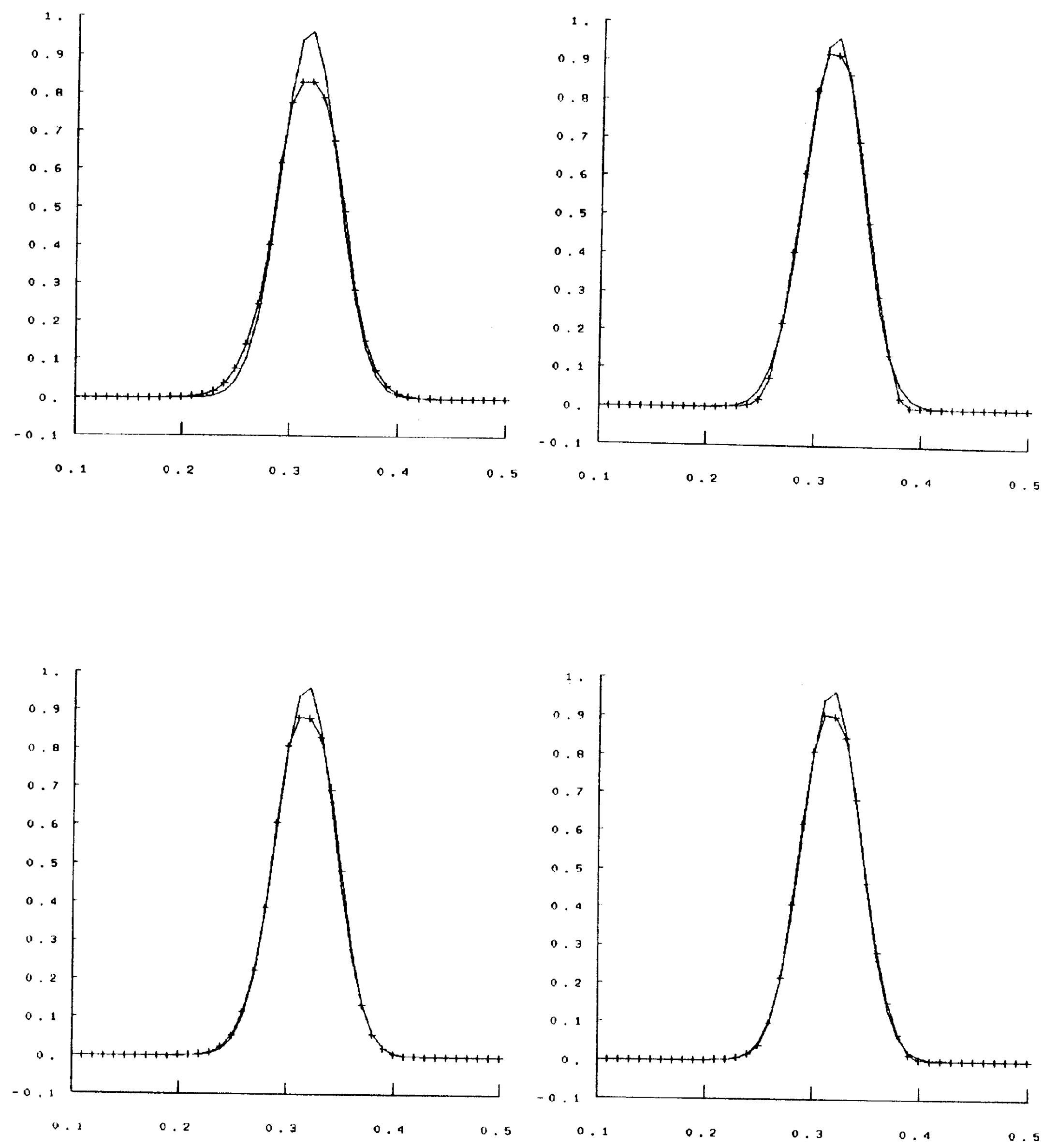

Figure 4. Comparison of results obtained with minmod (top left), superbee (top right), Van Leer (bottom left) and present (bottom right) limiters

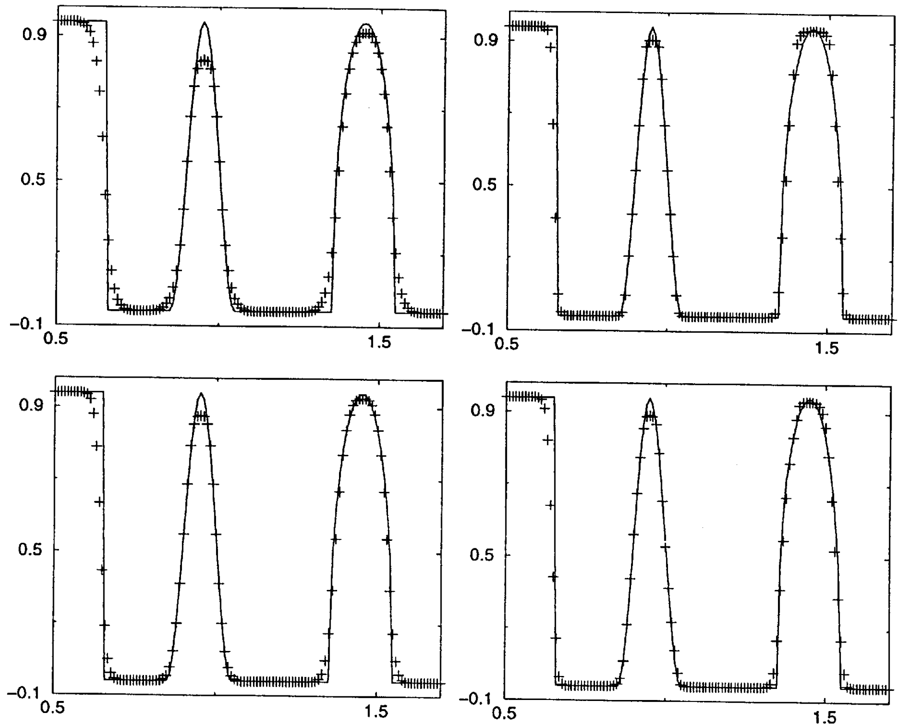

Figure 5. Comparison of results obtained on three benchmark problems at $N_{\mathrm{CFL}} = \frac{1}{2}$ with minmod (top left), superbee (top right), Van Leer (bottom left) and present (bottom right) limiters

Thus, using the Lemma, we can conclude as for the proof of Proposition 1 that the scheme is TVD and L^{∞}-stable under the CFL condition $\lambda\|u\|_{\infty} \leqslant 1$.

When using a coarse mesh, the third-order Takacs scheme can produce dispersive solutions, whereas the new scheme avoids non-expected negative values. This can be seen in Figure 3 for the same data as in Figure 2, except that $\delta x = 0{\cdot}02$ instead of $0{\cdot}01$.

Remark

Starting with the Lax–Wendroff scheme, several limiters have been found that satisfy the hypotheses of the Lemma, e.g.

$$\varphi_{\rho}(r) = \max[0, \min(\rho r, 1), \min(r, \rho)],$$

with $1 \leqslant \rho \leqslant 2$, which gives the well-known minmod and superbee limiters for $\rho = 1$ and 2 respectively,[12] or

$$\varphi(r) = \frac{r + |r|}{1 + |r|},$$

introduced by Van Leer.[12] Here the limiter $\varphi(r)$ is naturally derived from the Takacs scheme. Numerical test performed with the same data as in Figure 2 show that this limiter is better than the above three (Figure 4). To confirm this result, we performed some numerical experiments on three benchmark test problems gathered by Leonard.[13] They correspond to the transport of a unit step, an isolated sine-squared wave and a semi-ellipse with constant velocity $u = 1$. The results obtained with exactly the same parameters as used by Leonard are plotted in Figure 5. They show again the accuracy of the new limiter, which appears to be a good compromise between the Van Leer and superbee limiters.

5. THE 2D EXTENSION

We consider now the 2D transport equation for a uniform flow $U = (u_x, u_y)^T$, namely

$$\frac{\partial C}{\partial t} + U \cdot \nabla C = 0. \tag{22}$$

The two-dimensional scheme is derived by a Taylor expansion of the solution of (22) where the terms of order strictly greater, than two are neglected:

$$C(x, y, t + \delta t) = C(x, y, t) - \delta t U \cdot \nabla C(x, y, t) + \frac{\delta t^2}{2} \mathrm{div}[D^*(U) \cdot \nabla C(x, y, t)] + \mathcal{O}(\delta t^3),$$

with

$$D^*(U) = \begin{bmatrix} u_x^2 & u_x u_y \\ u_x u_y & u_y^2 \end{bmatrix}.$$

We point out that the extra-diagonal terms in the D^* tensor couple both directions and avoids strong grid orientation effects. Thus all fluxes are limited with (19) and we get for a positive velocity[14]

$$\begin{aligned} C_{i,j}^{n+1} = {} & C_{i,j}^n - \lambda_x u_x \left(1 - \frac{\lambda_y}{2} u_y\right) \Delta C_{i-1/2,j}^n - \lambda_y u_y \left(1 - \frac{\lambda_x}{2} u_x\right) \Delta C_{i,j-1/2}^n \\ & - \frac{\lambda_x \lambda_y}{2} u_x u_y (\Delta C_{i-1/2,j-1}^n \\ & + \Delta C_{i-1,j-1/2}^n) - \frac{\lambda_x}{2} (F_{i+1/2,j}^n - F_{i-1/2,j}^n) - \frac{\lambda_y}{2} (F_{i,j+1/2}^n - F_{i,j-1/2}^n), \end{aligned}$$

where $\lambda_x = \delta t / \delta x$, $\lambda_y = \delta t / \delta y$ and

$$F_{i+1/2,j}^n = u_x \left(1 - \max\left(\lambda_x u_x, \lambda_y u_y\right) - \frac{\lambda_y}{2} u_y\right) \varphi(r_{i+1/2,j}) \Delta C_{i+1/2,j}^n + \frac{\lambda_y}{2} u_x u_y \varphi(r_{i+1/2,j-1}) \Delta C_{i+1/2,j-1}^n,$$

$$F_{i,j+1/2}^n = u_y \left(1 - \max\left(\lambda_x u_x, \lambda_y u_y\right) - \frac{\lambda_x}{2} u_x\right) \varphi(r_{i,j+1/2}) \Delta C_{i,j+1,2}^n + \frac{\lambda_x}{2} u_x u_y \varphi(r_{i-1,j+1/2}) \Delta C_{i-1,j+1/2}^n,$$

with

$$r_{i+1/2,j} = \frac{\Delta C_{i-1/2,j}}{\Delta C_{i+1/2,j}}, \qquad r_{i,j+1/2} = \frac{\Delta C_{i,j-1/2}}{\Delta C_{i,j+1/2}}.$$

Remarks

This scheme is L^∞-stable under the CFL condition $\max(\lambda_x u_x, \lambda_y u_y) \leqslant \frac{2}{3}$. Moreover, the extension when U depends on (x, y) is straightforward.

6. NUMERICAL TESTS

The 1D numerical tests are discussed on a model problem whose solution is known in order to better compare the performance of the various schemes. We solve equation (1) in the domain $(-1, 1)$ with $u(x) = A(1 - Bx)$, where A and B are some constants and B is non-negative.

The initial data are given by

$$C(x, 0) = a_0 \exp[-(b_0 x + c_0)^2]$$

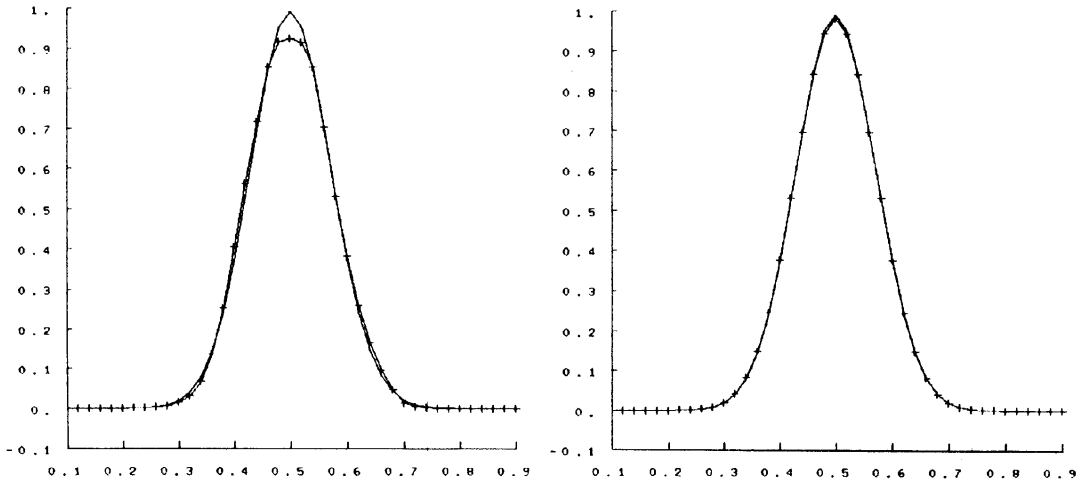

Figure 6. Numerical results with new flux limiter (left) and Holly–Preissmann (right) schemes

and the exact solution is written as

$$C(x, t) = a(t)\exp[-(b(t)x + c(t))^2],$$

where $a(t)$, $b(t)$ and $c(t)$ are three functions given by the system of differential equations

$$\begin{aligned}
&\frac{\mathrm{d}a}{\mathrm{d}t} - \left(2c\frac{\mathrm{d}c}{\mathrm{d}t} - 2Abc - 2\nu b^2 + 4\nu b^2 c^2\right)a = 0,\\
&\frac{\mathrm{d}b}{\mathrm{d}t} + ABb + 2\nu b^3 = 0,\\
&\frac{\mathrm{d}c}{\mathrm{d}t} + \left(b^{-1}\frac{\mathrm{d}b}{\mathrm{d}t} + AB + 4\nu b^2\right)c = Ab,
\end{aligned}$$

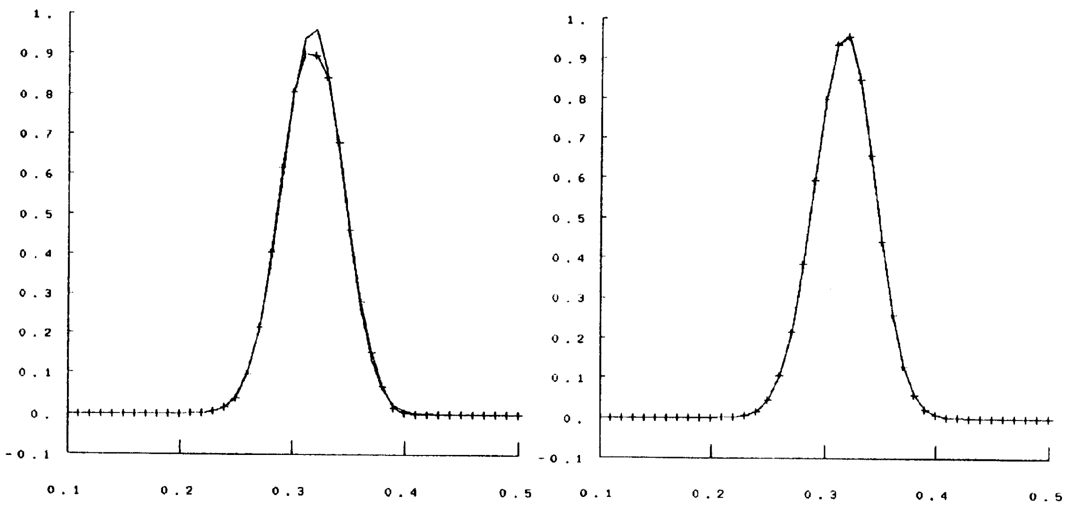

Figure 7. Numerical results with new flux limiter (left) and Holly–Preissmann (right) schemes

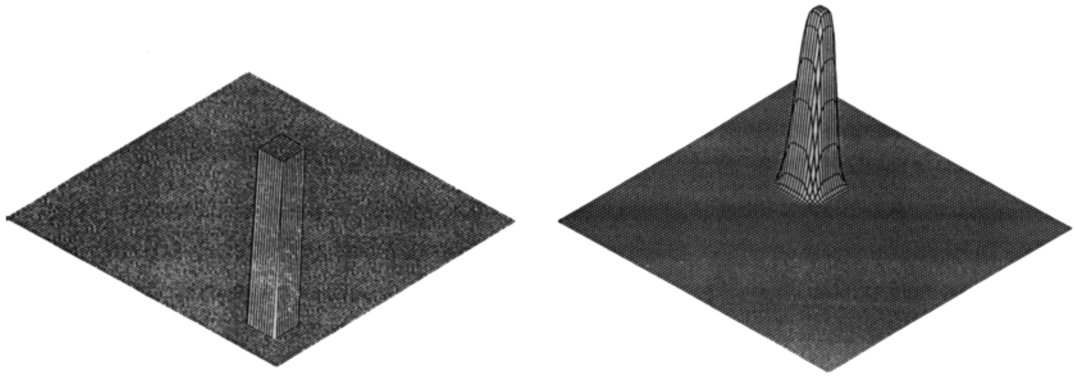

Figure 8. Transport of 2D square with new flux limiter scheme

with $a(0) = a_0 = 1$, $b(0) = b_0 = 10$ and $c(0) = c_0 = 1$. The solution of the above equations is

$$a(t) = \frac{(|A|B)^{1/2} \exp(ABt)}{|-200\nu + (200\nu + AB)\exp(2ABt)|^{1/2}},$$

$$b(T) = \frac{10(|A|B)^{1/2}}{|-200\nu + (200\nu + AB)\exp(2ABt)|^{1/2}},$$

$$c(t) = \frac{10|A|^{1/2}(-1 + \exp(ABt))}{|-200\nu + (200\nu + AB)\exp(2ABt)|^{1/2} B^{1/2}},$$

which reduces to

$$a(t) = 1/(400\nu t + 1)^{1/2}, \qquad b(t) = 10/(400\nu t + 1)^{1/2}, \qquad c(t) = Atb(t)$$

when $B = 0$ (u is a constant function).

For the tests we take ν small, i.e. $\nu \ll \|A(1 - Bx)\|_\infty \delta x/2$.

When u is a constant function, it is well known that all the schemes give the exact solution for a CFL number $N_{\mathrm{CFL}} = 1$. We take $u = 1$, ν small in front of u ($\nu = 10^{-4}$), a coarse mesh ($\delta x = 0{\cdot}02$) and $N_{\mathrm{CFL}} = \frac{1}{2}$. Our new scheme produces results close to those obtained by the Holly–Preissmann backward characteristics method (Figure 6).

When the function u is equal to $u(x) = 1 - 2x$, the results obtained with $N_{\mathrm{CFL}} = 1$ ($\max_{0 \leqslant x \leqslant 1} |u(x)|\delta t/\delta x \leqslant 1$) on a medium mesh ($\delta x = 0{\cdot}01$) and a small diffusion term ($\nu = 10^{-4}$) are very good. The new flux limiter scheme yields almost the exact solution except at the extrenum (Figure 7).

A 2D numerical test is performed on a domain $(0, 1) \times (0, 1)$ with $\delta x = \delta y = 0{\cdot}01$ A 2D square of size 10 δx is advected by a diagonal uniform flow $u_x = u_y = 0{\cdot}5$. Figure 8 shows the initial condition and the approximate solution at $t = 1{\cdot}3$ computed with $N_{\mathrm{CFL}} = 1$. We see that there are no grid orientation effects and only a weak diffusion.

7. CONCLUSIONS

From a family of second- and third-order Lax–Wendroff-type schemes we build a TVD scheme corresponding to a new limiter that is more efficient than the classical minmod, superbee and Van Leer limiters. The results obtained with this scheme are close to those produced by the Holly–Preissmann backward characteristic method. However, our scheme is much easier to extend to higher dimensions.

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