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MODIFIED BOX SCHEMES FOR POLLUTANT TRANSPORT IN RIVERS WITH DEAD ZONES

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SUMMARY

Several difference schemes approximating a mathematical model of river pollution are investigated and their truncation error, stability and monotonicity conditions are shown. Based on numerical experiments, the classical six-point schemes and some new modified box schemes are compared. The latter proved to be not only faster but also more accurate for practically used step lengths.

KEY WORDS: dead zone model; finite difference; modified box schemes; classical six-point schemes; truncation error; monotonicity condition

1. INTRODUCTION

In this paper we numerically investigate a mathematical model describing the transport of pollution in rivers (or in soil). The essence of this so-called dead zone model (which became of interest in connection with the SANDOZ accident) is that if a great amount of pollution is transported in a short time through the main river, then a small amount of soluble matter remains in the dead zones of the river (mud, holes, breakwaters) and decreases only slowly. This behaviour can be modelled by the system of differential equations

$$\frac{\partial c_1(x,t)}{\partial t} + v\frac{\partial c_1(x,t)}{\partial x} - D\frac{\partial^2 c_1(x,t)}{\partial x^2} = \frac{1}{\tau_1}[c_2(x,t) - c_1(x,t)] - kc_1(x,t), \tag{1}$$

$$\frac{\partial c_2(x,t)}{\partial t} = \frac{1}{\tau_2}[c_1(x,t) - c_2(x,t)] - kc_2(x,t), \tag{2}$$

where

x	distance measured from beginning of river reach (m), $0 \leqslant x \leqslant L$
t	time (s), $0 \leqslant t$
$c_1(x, t)$	concentration of pollution in main flow (g m^{-3})
$c_2(x, t)$	concentration of pollution in dead zones (g m^{-3})
v	velocity of main flow (m s^{-1})
D	coefficient of longitudinal dispersion in main flow (m^2 s^{-1})
τ_1	characteristic time of back diffusion from dead zones into main flow (s)
τ_2	characteristic time of diffusion from main flow into dead zones (s)
k	chemical decay constant (s^{-1})
L	considered length of river
T	considered time of pollution event.

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The initial and boundary conditions are

$$c_i(x,t) = c_i^0(x), \quad 0 \leqslant x \leqslant L, \quad t = 0, \quad i = 1, 2,$$

$$c_1(x,t) = l(t), \quad x = 0, \qquad \frac{\partial c_1(x,t)}{\partial x} = 0, \quad x = L, \quad t \geqslant 0. \tag{3}$$

Here $L \gg 1$ (say $L = 10^5$ m), i.e. $D/vL \ll 1$, but the considered time T is large too (say 2×10^5 s), hence the diffusion cannot be neglected.

In this paper we use the finite difference method to solve problem (1)–(3).

We investigate several difference schemes, their truncation error, stability and monotonicity conditions. We report on numerical experiments to check and compare the accuracy of these schemes. We will show that modified box schemes give better results for practically used step lengths than classical six-point schemes. Therefore, in solving (1)–(3), we are able to avoid the solution of tridiagonal systems. Our work is based on References 1 and 2.

2. NUMERICAL METHODS

2.1.

A simple way to solve the above system is to approximate all the terms of both equations (1) and (2) by finite differences (classical six-point schemes). By making use of this approximation, we get a system of linear algebraic equations with a block-tridiagonal coefficient matrix to determine the solution at the jth time step.

One of these approximations is the weighted difference scheme

$$c_{1t,i} + v\sigma c_{1\mathring{x},i}^{j+1} + v(1-\sigma)\, c_{1\mathring{x},i}^{j} - D\sigma c_{1\bar{x}x,i}^{j+1} - D(1-\sigma) c_{1\bar{x}x,i}^{j}$$

$$= \frac{1}{\tau_1}[\sigma(c_2 - c_1)^{j+1} + (1-\sigma)(c_2 - c_1)^j]_i - k[\sigma c_{1,i}^{j+1} + (1-\sigma) c_{1,i}^{j}], \tag{4}$$

$$c_{2t,t} = \frac{1}{\tau_2}[\sigma(c_1 - c_2)^{j+1} + (1-\sigma)(c_1 - c_2)^j]_i - k[\sigma c_{2,i}^{j+1} + (1-\sigma) c_{2,i}^{j}]. \tag{5}$$

Here the following notation has been used:

$$\Omega := \{0 \leqslant x \leqslant L, 0 \leqslant t \leqslant T\}, \quad T > 0,$$

$$\omega_{h\tau} := \{(x_i, t_j) \in \Omega | h = L/N;\ \tau = T/M;\ N, M \in \mathbb{N};\ x_i = ih;\ t_j = j\tau;\ i = 0, \dots, N, j = 0, \dots, M\},$$

$$c_{1,i}^j ;= c_1(x_i, t_j), \qquad c_{2,i}^j := c_2(x_i, t_j), \qquad (x_i, t_j) \in \omega_{h\tau},$$

$$c_{1t,i} := \frac{c_{1,i}^{j+1} - c_{1,i}^j}{\tau}, \qquad c_{2t,i} := \frac{c_{2,i}^{j+1} - c_{2,i}^j}{\tau},$$

$$c_{1\mathring{x},i}^j := \frac{c_{1,i+1}^j - c_{1,i-1}^j}{2h} \quad \text{(central difference)},$$

$$c_{1\bar{x}x,i}^j := \frac{c_{1,i+1}^j - 2c_{1,i}^j + c_{1,i-1}^j}{h^2} \quad \text{(second-order divided difference)}$$

and σ is a weighting factor satisfying $0 \leqslant \sigma \leqslant 1$.

Equations (4) and (5) represent an approximation of order $O(\tau\,|\,\sigma-\frac{1}{2}\,|+\tau^2+h^2)$ and can be shown to be stable in a mean square sense if the weighting factor σ is not less than $\frac{1}{2}$.[3,4] Here the case $\sigma=\frac{1}{2}$ is investigated. Hence the approximate solution according to (4) and (5) converges to the exact solution of (1) and (2) at least to second order. However, it is well-known that this scheme may lead to oscillations when $|vh/2D|>1$. In what follows this scheme will be called the 'weighted' difference scheme.

We mention another well-known difference scheme which differs from (4) and (5) in the approximation of the advection term by a backward difference, namely

$$\frac{\partial c_1}{\partial x}(x_{i+1/2},t_{j+1/2})\approx\sigma c^j_{1\bar{x},i}+(1-\sigma)c^{j+1}_{1\bar{x},i},$$

where

$$c^j_{1\bar{x},i}:=\frac{c^j_{1,i}-c^j_{1,i-1}}{h}.$$

This is only a first-order approximation in h but is stable without the condition $|vh/2D|\leqslant 1$. Based on our numerical experiments, we know it to be much less accurate than (4) and (5). Therefore, it is not investigated later in Section 3. (The condition of mean square stability here is also $\sigma\geqslant\frac{1}{2}$.)

2.2.

A new way to solve (1) and (2) is the following:[1,2] instead of (1) we approximate the equation

$$\frac{\partial c_1(x,t)}{\partial t}+v\frac{\partial c_1(x,t)}{\partial x}=\frac{1}{\tau_1}[c_2(x,t)-c_1(x,t)]-kc_1(x,t),\tag{6}$$

where we take the boundary conditions into consideration only at $x=0$.

Our approximate solution will contain a certain numerical diffusion D^*. This coefficient can be expressed by the discretization parameters h, τ, velocity v and by the weighting factors of the scheme used. We select the weighting factors of the approximation in such a way that D^* equals the given physical diffusion. Using such an approximation, we can get a modified box scheme involving only the four points (x_i,t_j), (x_{i-1},t_j), (x_i,t_{j+1}) and (x_{i-1},t_{j+1}). Then, to determine the numerical solution at the jth time step, a 2×2 system of linear algebraic equations with a constant coefficient matrix has to be solved. This system can be solved exactly and the solution can be expressed explicitly. Therefore the number of operations here is less than in the case of the scheme (4), (5).

In this paper two such schemes will be analysed. Based on our numerical experiments, these schemes may be considered as the two most accurate ones.

In what follows we investigate the approximation error and the monotonicity conditions of these difference schemes. In Section 3 we compare their accuracy and convergence with the scheme (4), (5). In Reference 2 only the case $k=0$ has been considered (but a source term f has been added to the right-hand side of equation (1)). In our analysis we admit $k\geqslant 0$.

Consider the difference scheme

$$\begin{aligned}\alpha c_{1t,i-1}+(1-\alpha)c_{1t,i}+\beta vc^j_{1\bar{x},i}+(1-\beta)\,vc^{j+1}_{1\bar{x},i}\\=\frac{1}{\tau_1}[\delta(\bar{c}_2-\bar{c}_1)_i+(1-\delta)(\bar{c}_2-\bar{c}_1)_{i-1}]-k[\delta\bar{c}_{1,i}+(1-\delta)\bar{c}_{1,i-1}],\end{aligned}\tag{7}$$

$$c_{2t,i}=\frac{1}{\tau_2}[\sigma(c_1-c_2)^j+(1-\sigma)(c_1-c_2)^{j+1}]_i-k[\sigma c^j_{2,i}+(1-\sigma)c^{j+1}_{2,i}],\tag{8}$$

where

$$\bar{c}_{1,i} := \frac{1}{2}(c_{1,i}^{j} + c_{1,i}^{j+1}), \qquad \bar{c}_{2,i} := \frac{1}{2}(c_{2,i}^{j} + c_{2,i}^{j+1})$$

and α, β, δ and σ are weighting factors in the interval [0, 1].

Since

$$c_{1t,i-1} = c_{1t,i} - \frac{h}{\tau}(c_{1\bar{x},i}^{j+1} - c_{1\bar{x},i}^{j}),$$

equation (7) can be written as

$$c_{1t,i} + \rho v\, c_{1\bar{x},i}^{j} + (1-\rho)\, v c_{1\bar{x},i}^{j+1} = \frac{1}{\tau_1}[\delta(\bar{c}_2 - \bar{c}_1)_i + (1-\delta)(\bar{c}_2 - \bar{c}_1)_{i-1}] - k[\delta\bar{c}_{1,i} + (1-\delta)\bar{c}_{1,i-1}], \tag{9}$$

where

$$\rho := \frac{1}{p}(\alpha + \beta p),$$

with $p := \tau v/h$ being the Courant number.

First we determine the coefficient of numerical diffusion and the truncation error of equation (9). For this we expand (9) into a Taylor series at the point $(x_{i-1/2}, t_{j+1/2})$:

$$\left(\frac{1}{\tau_1} + k\right)c_1 + \frac{\partial c_1}{\partial t} + \left(v + \frac{(2\delta-1)h(1+k\tau_1)}{2\tau_1}\right)\frac{\partial c_1}{\partial x} + \frac{h}{2}[1 + p(1-2\rho)]\frac{\partial^2 c_1}{\partial x \partial t} - \frac{1}{\tau_1}c_2$$
$$- \frac{(2\delta-1)h}{2\tau_1}\frac{\partial c_2}{\partial x} + O(\tau^2 + h^2) = 0. \tag{10}$$

Differentiating (1) with respect to x, we obtain

$$\frac{\partial^2 c_1}{\partial x \partial t} = -v\frac{\partial^2 c_1}{\partial x^2} + D\frac{\partial^3 c_1}{\partial x^3} - \left(\frac{1}{\tau_1} + k\right)\frac{\partial c_1}{\partial x} + \frac{1}{\tau_1}\frac{\partial c_2}{\partial x}. \tag{11}$$

Substituting (11) into (10), we get

$$\left(\frac{1}{\tau_1} + k\right)c_1 - \frac{1}{\tau_1}c_2 + \frac{\partial c_1}{\partial t} + \left(v + \frac{(2\delta-1)h(1+k\tau_1)}{2\tau_1} - \frac{1+k\tau_1}{\tau_1}\frac{h}{2}[1 + p(1-2\rho)]\right)\frac{\partial c_1}{\partial x}$$
$$-\left(\frac{(2\delta-1)h}{2\tau_1} - \frac{1}{\tau_1}\frac{h}{2}[1 + p(1-2\rho)]\right)\frac{\partial c_2}{\partial x} - v\frac{h}{2}[1 + p(1-2\rho)]\frac{\partial^2 c_1}{\partial x^2}$$
$$+D\frac{h}{2}[1 + p(1-2\rho)]\frac{\partial^3 c_1}{\partial x^3} + O(h^2 + \tau^2) = 0. \tag{12}$$

Thus the coefficient of numerical diffusion is

$$D^* = v\frac{h}{2}[1 + p(1-2\rho)]$$

and the velocity coefficients are $v + (1 + k\tau_1)V$ and $-V$, where

$$V := \frac{h}{2\tau_1}\{2\delta - 1 - [1 + p(1-2\rho)]\}.$$

Accordingly, if we choose the weighting factors ρ and δ to satisfy the two criteria (i) $D=D^*$, i.e. $p\rho=\frac{1}{2}(1+p-1/q)$, where $q:=vh/2D$ is the discrete Reynolds number, and (ii) $V=0$, i.e. $\delta=\frac{1}{2}(1+1/q)$, then we get that the truncation error is

$$\psi=\frac{D^2}{v}\frac{\partial^3 c_1}{\partial x^3}+O(h^2+\tau^2).$$

Our numerical experiments show that the value of the term $\partial^3 c_1/\partial x^3$ multiplying D^2/v is only weakly dependent on D and v. After transforming the $[0, L]$ interval to unit length, the truncation error is

$$\psi=O(D^2/vL^3+h^2+\tau^2).$$

In Section 3 we will show the effect of this fact on the convergence of the numerical solution.

If $\sigma=\frac{1}{2}$, equation (8) is the trapezium rule and hence of second order.

Further on we consider (8) and (9) with weighting factors which satisfy the criteria (i) and (ii) above and with $\sigma=\frac{1}{2}$. In what follows this scheme will be called the 'straight' box scheme. For practical computations the monotonicity (i.e. non-negativity) of the scheme is important. To analyse the monotonicity conditions of the 'straight' box scheme, we express $c_{1,i}^{j+1}$ and $c_{2,i}^{j+1}$ explicitly by $c_{1,i}^{j}$, $c_{1,i-1}^{j}$, $c_{1,i-1}^{j+1}$ and $c_{2,i}^{j}$, $c_{2,i-1}^{j}$, $c_{2,i-1}^{j+1}$ respectively. If the coefficients of these linear expressions are non-negative, when the scheme is monotone. In this way we get the monotonicity conditions

$$T_1\leqslant\tau\leqslant\min\left(\frac{2\tau_2}{1+k\tau_2},T_2\right),$$

$$\max\left(\frac{2D}{v},\frac{-2v\tau\tau_1(2\tau_2+\tau+k\tau\tau_2)}{[k(\tau_2+\tau_1)+k^2\tau_1\tau_2]\tau^2+2(\tau_2-\tau_1)\tau-4\tau_1\tau_2}-\frac{2D}{v}\right)\leqslant h\leqslant\frac{v\tau}{k\tau/2+\tau/2\tau_1+1}+\frac{2D}{v},$$

where

$$T_1:=\begin{cases}\dfrac{2(\tau_2-\tau_1)+\sqrt{[4(\tau_2-\tau_1)^2+16(k\tau_1+k\tau_2+k^2\tau_1\tau_2)\tau_1\tau_2]}}{-2(k\tau_1+k\tau_2+k\tau_1\tau_2)}, & \text{if } k>0,\\ 0, & \text{if } k=0,\end{cases}$$

$$T_2:=\begin{cases}\dfrac{2(\tau_2-\tau_1)-\sqrt{[4(\tau_2-\tau_1)^2+16(k\tau_1+k\tau_2+k^2\tau_1\tau_2)\tau_1\tau_2]}}{-2(k\tau_1+k\tau_2+k\tau_1\tau_2)}, & \text{if } k>0,\\ \infty, & \text{if } k=0 \text{ and } \tau_1\geq\tau_2,\\ \dfrac{2\tau_1\tau_2}{\tau_2-\tau_1}, & \text{if } k=0 \text{ and } \tau_1<\tau_2.\end{cases}$$

These conditions mean essentially that the Courant number p is close to unity. Using the maximum principle, the scheme can be shown to be maximum norm stable with these conditions.[4,5]

Another difference scheme of this modified box type is

$$\alpha c_{1t,i-1}+(1-\alpha)c_{1t,i}+\beta vc_{1\bar{x},i}^{j}+(1-\beta)vc_{1\bar{x},i}^{j+1}$$

$$=\frac{1}{\tau_1}[\delta(\bar{c}_2-\bar{c}_1)+(1-\delta)(\bar{c}_{2,i}-\bar{c}_{1,i})]-k[\delta\bar{c}_1+(1-\delta)\bar{c}_{1,i}], \quad (13)$$

$$c_{2t,i}=\frac{1}{\tau_2}[\sigma(c_1-c_2)^j+(1-\sigma)(c_1-c_2)^{j+1}]_i-k[\sigma c_{2,i}^j+(1-\sigma)c_{2,i}^{j+1}], \quad (14)$$

where

$$\tilde{c}_1 := \frac{1}{2}(c^j_{1,i-1} + c^{j+1}_{1,i}), \qquad \tilde{c}_2 = \frac{1}{2}(c^j_{2,i-1} + c^{j+1}_{2,i}).$$

If the weighting factors are chosen to satisfy

$$\alpha + \beta p = \frac{1}{2}(1 + p - 1/q), \qquad \delta := 1 - 1/q, \qquad \sigma := \frac{1}{2}, \tag{15}$$

then similarly as above it can be shown that the truncation error is again

$$\psi = O(D^2/vL^3 + h^2 + \tau^2).$$

In what follows this scheme will be called the 'skew' box scheme. Here the conditions of monotonicity are

$$0 \leqslant \tau \leqslant \min\left(\frac{\tau_1}{1 + k\tau_1}, \frac{2\tau_2}{1 + k\tau_2}\right),$$

$$\max\left(\frac{2D}{v}, \frac{(2\tau_2 + \tau + k\tau\tau_2)[v^2\tau\tau_1 + 2D(-\tau_1 + \tau + k\tau\tau_1)]}{v[\tau_1(2\tau_2 + \tau + k\tau\tau_2) + \tau^2]}\right) \leqslant h \leqslant v\tau + \frac{2D}{v}$$

or

$$\frac{\tau_1}{1 + k\tau_1} < \tau \leqslant \frac{2\tau_2}{1 + k\tau_2},$$

$$\max\left(\frac{2D}{v}, \frac{(2\tau_2 + \tau + k\tau\tau_2)[v^2\tau\tau_1 + 2D(-\tau_1 + \tau + k\tau\tau_1)]}{v[\tau_1(2\tau_2 + \tau + k\tau\tau_2) + \tau^2]}\right) \leqslant h \leqslant \min\left(v\tau + \frac{2D}{v}, \frac{v\tau}{\tau(1/\tau_1 + k) - 1} + \frac{2D}{v}\right).$$

The following assertion can be proved: if $\tau \leqslant 4\tau_1/(1 + k\tau_1)$, then the monotonicity conditions of the 'skew' box scheme are less restrictive than those of the 'straight' box scheme, i.e. the 'skew' box scheme is monotone in a larger domain of the spatial and time steps (h and τ) than the 'straight' box scheme.

When $\tau > 4\tau_1/(1 + k\tau_1)$, our numerical experiments show that the same assertion holds.

In Section 3 we will show that from the viewpoint of the reliability of the numerical solution it is very important to choose such h and τ which satisfy the monotonicity conditions.

2.3.

The following difference scheme is also mentioned in Section 3:

$$\frac{1}{2}c_{1t,i-1} + \frac{1}{2}c_{1t,i} + \frac{1}{2}vc^j_{1\bar{x},i} + \frac{1}{2}vc^{j+1}_{1\bar{x},i} = \frac{1}{\tau_1}(\hat{c}_2 - \hat{c}_1) - k\hat{c}_1, \tag{16}$$

$$c_{2t,i} = \frac{1}{\tau_2}(\bar{c}_{1,i} - \bar{c}_{2,i}) - k\bar{c}_{2,i}, \tag{17}$$

where

$$\hat{c}_1 := \tfrac{1}{4}(c^j_{1,i-1} + c^{j+1}_{1,i-1} + c^j_{1,i} + c^{j+1}_{1,i}), \qquad \hat{c}_2 := \tfrac{1}{4}(c^j_{2,i-1} + c^{j+1}_{2,i-1} + c^j_{2,i} + c^{j+1}_{2,i}).$$

This is the 'simple' box scheme approximating (6) and (2) by neglecting the physical diffusion. (In the case of $\tau_1 = \tau_2 = \infty$ and $k = 0$ it is the Wendroff scheme.[6]) We use this scheme for comparison only.

3. NUMERICAL EXPERIMENTS

3.1.

The following statement can be proved. The general solution of the ordinary differential equation (18) gives a particular solution of the system (1), (2):

$$D\dddot{F}(\xi) - \frac{D}{v}\left(\frac{1}{\tau_2} + k - \alpha\right)\ddot{F}(\xi) + \left(\alpha - \frac{1}{\tau_1} - k\right)\dot{F}(\xi) + \frac{k-\alpha}{v}\left(\frac{1}{\tau_1} + \frac{1}{\tau_2} + k - \alpha\right)F(\xi) = 0, \quad (18)$$

where $\xi := x - vt$, $c_1(x, t) := e^{-\alpha t}F(\xi)$ and α is an arbitrary parameter. Having fixed α and the parameters of the general solution of (18) in different ways, we can get some exact solutions of the system (1), (2) with corresponding initial and boundary conditions. The concentration c_2 is obtained from the expressions

$$c_2(x, t) = e^{-\alpha t}G(\xi), \qquad G(\xi) = \tau_1\left(k + \frac{1}{\tau_1} - \alpha\right)F(\xi) - \tau_1 D\ddot{F}(\xi).$$

In this part of the paper these exact solutions are used for comparison with the approximate solutions produced by the difference schemes described above. We investigate the accuracy and convergence of these numerical solutions. In the experiments, several exact solutions and choices of parameters of (1) and (2) have been evaluated. Since the results were similar to each other, we show only one case here.

The exact solution used is

$$c_1(x, t) = e^{-kt}e^{\lambda_2(x-vt)}, \; c_2(x, t) = e^{-kt}e^{\lambda_2(x-vt)}(1 - \lambda_2^2\tau_1 D),$$

where

$$\lambda_2 = \frac{1}{2v\tau_2} + \sqrt{\left(\frac{1}{4v^2\tau_2^2} + \frac{1}{D\tau_1}\right)}.$$

The corresponding initial and boundary conditions are

$$c_1(x, 0) = e^{\lambda_2 x}, \qquad c_2(x, 0) = e^{\lambda_2 x}(1 - \lambda_2^2\tau_1 D),$$

$$c_1(0, t) = e^{-kt}e^{\lambda_2(-vt)}, \qquad c_1(L, t) = e^{-kt}e^{\lambda_2(L-vt)}.$$

Remark. In further computations the following exact solution has been used and the qualitative results obtained are essentially the same:

$$c_1(x, t) = e^{-(k+1/\tau_1)t}\cos[\omega(x - vt)]e^{\mu(x-vt)},$$

$$c_2(x, t) = -\tau_1 De^{-(k+1/\tau_1)t}e^{\mu(x-vt)}\{(\mu^2 - \omega^2)\cos[\omega(x - vt)] - 2\mu\omega\sin[\omega(x - vt)]\},$$

where $\mu := \text{Re}\,\lambda_2$, $\omega := \text{Im}\,\lambda_2$ and λ_2 is a root of the equation

$$D\lambda^3 - \frac{D}{v}\left(\frac{1}{\tau_2} + \frac{1}{\tau_1}\right)\lambda^2 - \frac{1}{v\tau_1\tau_2} = 0 \quad (19)$$

if equation (19) has one real and two complex roots, i.e.

$$\lambda_1 \in \mathbb{R}, \qquad \lambda_2 = \bar{\lambda}_3 \in \mathbb{C}.$$

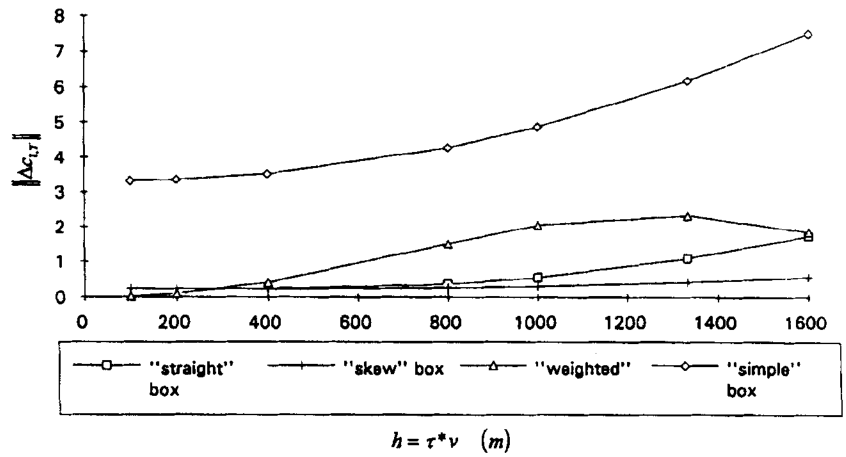

Figure 1. Relative error of $c_1(x, T)$ with respect to $h = \tau v$

When equation (19) has three real roots, the following solutions have been used:

$$c_1(x, t) = \mathrm{e}^{-(k+1/\tau_1)t}\mathrm{e}^{\lambda_2(x-vt)}, \qquad c_2(x, t) = -\tau_1 D\lambda_2^2\mathrm{e}^{-(k+1/\tau_1)t}\mathrm{e}^{\lambda_2(x-vt)},$$

where $\lambda_2 \in \mathbb{R}$ is one of the roots of equation (19).

Investigation of the convergence and accuracy. Figures 1 and 2 show the change in the relative error of each approximate solutions with respect to decreasing $\tau v = h$. These errors were calculated at a given time T in the discrete L_2-norm,

$$\|\Delta c_{l,T}\| := \frac{\sum_{i=0}^{N}(c_{l,i}^{M} - \tilde{c}_{l,i}^{M})^2 h}{\sum_{i=0}^{N}(c_{l,i}^{M})^2 h},$$

where c_l is the exact and $\tilde{c}_l$ is the computed solution, $l = 1, 2$, $T = M\tau$, $L = Nh$. The parameter of the system (1), (2) are here $\tau_1 = 2\times10^4$ s, $\tau_2 = 4\times10^3$ s, $k = 10^{-4}$ s^{-1}, $D = 150$ m^2 s^{-1}, $v = 1$ m s^{-1}, $L = 5\times10^4$ m and $T = 8\times10^3$ s. The data on τ_1, τ_2 and D correspond to the Rhine.

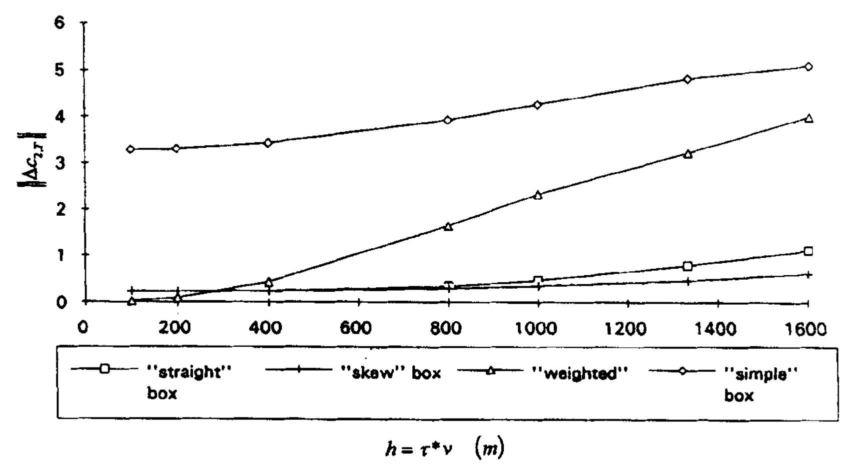

Figure 2. Relative error of $c_2(x, T)$ with respect to $h = \tau v$

Table I. Ratios of errors for decreasing h

Scheme	Error e	e_{1600}/e_{800}	e_{800}/e_{400}	e_{400}/e_{200}	e_{200}/e_{100}
'Weighted'	$\|\Delta c_{1,T}\|$	1·231	3·692	4·016	4·033
'Weighted'	$\|\Delta c_{2,T}\|$	2·441	3·809	4·055	4·079
'Straight' box	$\|\Delta c_{1,T}\|$	4·789	1·588	0·979	0·983
'Straight' box	$\|\Delta c_{2,T}\|$	3·214	1·409	1·024	1·000
'Skew' box	$\|\Delta c_{1,T}\|$	2·202	1·129	0·983	0·985
'Skew' box	$\|\Delta c_{2,T}\|$	2·073	1·215	1·035	1·001

These results are also illustrated in Table I. In this table we give the error ratios corresponding to various choices of $\tau v = h$ (e.g. e_{1600} is the error for $h = \tau v = 1600$ m).

An evaluation of the results is given in Table II.

3.2.

In addition to the comparison with the exact solutions, the behaviour of the computed solutions has been evaluated in two cases where the initial and boundary conditions were not continuous. In both cases the initial and boundary conditions on the grid points are

$$c_1(x, t) = \begin{cases} 1000/h & \text{if } x = 0,\ t = 0, \\ 0 & \text{if } x = 0,\ t \neq 0 \text{ or } x \neq 0,\ t = 0, \end{cases}$$

$$c_2(x, t) = 0 \qquad \text{if } x = 0 \text{ or } t = 0.$$

In case 1 the system parameters are $\tau_1 = 2\times10^4$ s, $\tau_2 = 4\times10^3$ s, $k = 0$ s^{-1}, $D = 150$ m^2 s^{-1}, $v = 1$ m s^{-1}, $L = 5\times10^4$ m and $T = 2\times10^4$ s. In case 2 the parameters are $\tau_1 = 2\times10^4$ s, $\tau_2 = 4\times10^3$ s, $k = 10^{-3}$ s^{-1}, $D = 150$ m^2 s^{-1}, $v = 1$ m s^{-1}, $L = 5\times10^4$ m and $T = 9\times10^3$ s.

In both cases the graph of the exact solution has a peak which decreases and spreads with time.

We investigate the shape and accuracy of the numerical solutions. A 'quasi-exact' solution was determined in both cases by using the 'weighted' scheme with 'small' time and space steps ($\tau = 50$ s, $h = 50$ m). The convergence of the solutions computed from the 'weighted' scheme for several decreasing values of τ and h has been evaluated and from there the 'quasi-exact' solution was found to be reliable. In what follows the various numerical solutions for $\tau = 1000$ s and $h = 1000$ m are compared with these 'quasi-exact' solutions.

Table II. Evaluation of results (based on comparison with five exact solutions, altogether about 150 test runs)

Scheme	Convergence	Accuracy	
		τ(s), h(m) > 300 (practical case)	τ(s), h(m) $\leqslant$ 300
'Weighted'	Second-order convergence	Less accurate than modified box schemes	Most accurate owing to its convergence
'Straight' box	No convergence for fixed D^2/vL^3, since the truncation error is $\psi = O(h^2 + \tau^2 + D^2/vL^3)$. However, this	Less accurate than 'skew' box scheme	Less accurate than 'weighted' scheme
'Skew' box	shows up only for τ and h much less than used in practice	Most accurate scheme	
'Simple' box	Approximates the equation only for $D = 0$	Significantly less accurate than the other schemes in all cases	

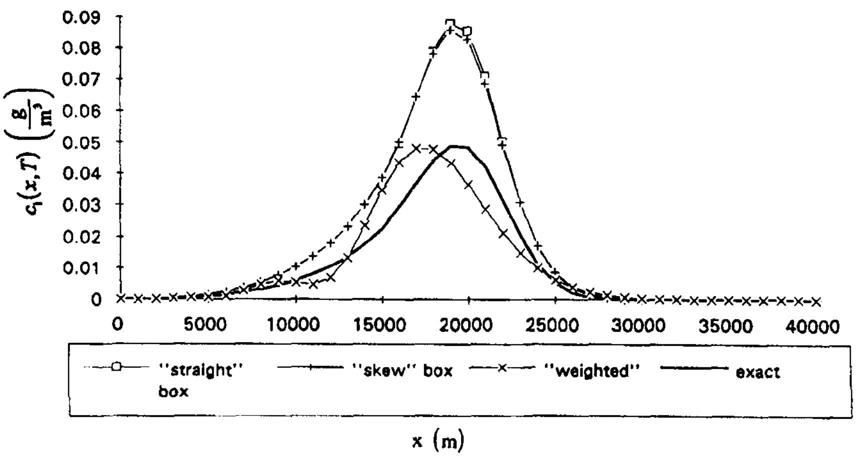

Figure 3. Comparison of 'quasi-exact' and numerical solutions, case 1

The solutions computed by the 'simple' box scheme (16), (17) are not shown in these figures because they are very inaccurate, with large oscillations in both cases.

The results for case 1 are shown in Figure 3. Only the approximations of $c_1(x, T)$ are displayed, but similar results were obtained for $c_1(x, T)$.

The results for case 2 show that neglect of the monotonicity conditions can result in serious distortions of the solution; see Figures 4 and 5.

An evaluation of the results is given in Table III. Finally, in Table IV the CPU times using the different schemes are compared with one other.

3.3.

In addition to the comparison with the classical six-point schemes, the modified box schemes were compared with the widely used QUICKEST scheme.[7,8] For this the sink terms have to be neglected, i.e. $1/\tau_1 = 1/\tau_2 = k = 0\ \mathrm{s}^{-1}$. (In this case the 'skew' and 'straight' box schemes are the same and therefore below we will speak only about the modified box scheme.)

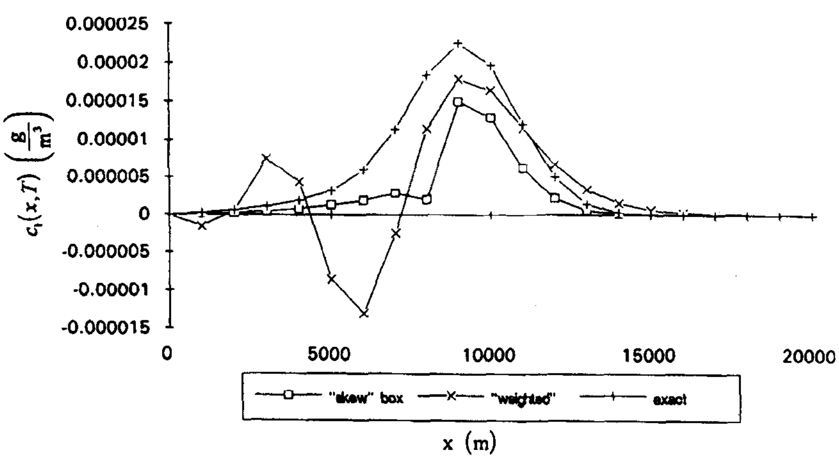

Figure 4. Comparison of 'quasi-exact' and numerical solutions, case 2

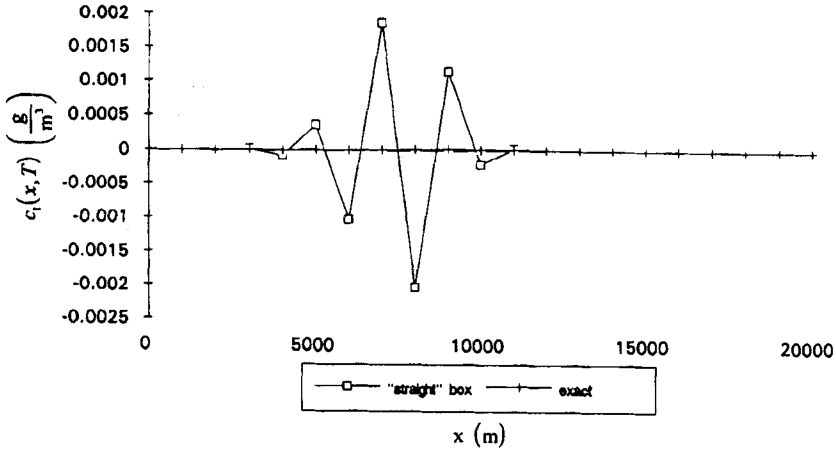

Figure 5. Comparison of 'quasi-exact' and numerical solutions ('straight' box scheme), case 2

A von Neumann linear stability analysis gives the following expression for the amplification factor $A(\alpha)$ of the modified box scheme:

$$A(\alpha)=\frac{1+(2\gamma^2/p^2-p^2/2-\frac{1}{2})(1-\cos\alpha)}{1+(2\gamma+2\gamma^2/p^2+p^2/2-\frac{1}{2})(1-\cos\alpha)}-i\frac{p\sin\alpha}{1+(2\gamma+2\gamma^2/p^2+p^2/2-\frac{1}{2})(1-\cos\alpha)},$$

where $\gamma:=D\tau/h^2$. From here one can prove straightforwardly that the modified box scheme is stable in the Neumann sense for every p, $\gamma>0$—which is not the case for the QUICKEST algorithm[7]

We compare the $c_1(x, T)$ solutions computed by the modified box scheme and the QUICKEST algorithm when the parameters of the differential equation are $D=150$ m^2 s^{-1}, $v=1$ m s^{-1}, $L=5\times10^4$ m and $T=1500$ s.

The initial and boundary conditions are

$$c_1(x,t)=\begin{cases}\frac{1}{2500}(x-22{,}500) & \text{if } 22{,}500<x\leqslant 25{,}000,\\ \frac{1}{2500}(27,000-x) & \text{if } 25{,}000<x<27{,}500,\\ 0 & \text{if } 0\leqslant x\leqslant 22{,}500,\ 27{,}500\leqslant x\leqslant L,\ t=0 \text{ or } x=0,\ t>0,\end{cases}$$

Table III. Evaluation of the results for discontinuous initial and boundary conditions

Case	Scheme	Oscillations	Peak height differs from exact one	Peak shift	Accuracy ($\|\Delta c_{1,T}\|$)	Remarks
1	'Weighted'	Small	No	Yes	0·28	—
	'Straight' box	No	Yes	No	0·73	τ and h satisfy the monotonicity conditions
	'Skew' box	No	Yes	No	0·70	
2	'Weighted'	Large	—	—	0·72	—
	'Straight' box	Large	—	—	79·78	τ and h are far from the monotonicity domain
	'Skew' box	Small	Small difference	No	0·57	τ and h are close to the monotonicity domain

Table IV. CPU times (s) for $L = 5 \times 10^4$ m and $T = 8 \times 10^3$ s (IBM/AT 386, 33 MHz, math coprocessor)

$h = \tau v$ (m)	'Weighted' scheme	Modified box schemes
1600	0·16	0·06
800	0·5	0·11
400	1·92	0·6
200	7·58	2·42
100	30·42	9·61
50	121·71	38·39

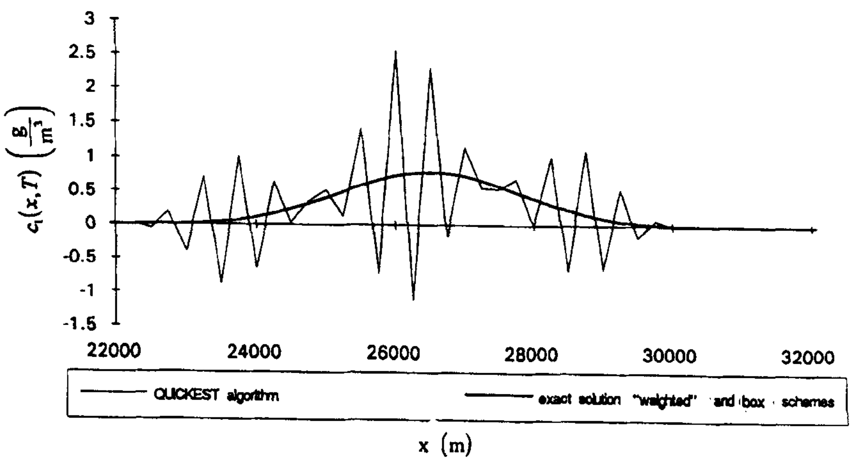

Figure 6. Comparison of 'quasi-exact' and numerical solutions of QUICKEST method and modified box scheme

$\tau = 300$ s and $h = 250$ m, i.e. $p = 1$, 2 and $\gamma := D\tau/h^2 = 0{\cdot}72$ are not in the stability range of the QUICKEST algorithm.

The results are illustrated in Figure 6. The QUICKEST algorithm gives large oscillations in this case, but the modified box scheme does not. The 'quasi-exact' solution was calculated with the 'weighted' scheme with $\tau = 60$ s and $h = 50$ m and the results computed in this way are almost indistinguishable from those of the modified box scheme or of the 'weighted' scheme with $\tau = 300$ s and $h = 250$ m.

Of course there are cases where the QUICKEST algorithm is better, e.g. for $p = 0{\cdot}5 = \gamma$, $\tau = 75$ s and $h = 150$ m the results of QUICKEST are four times more accurate.

4. CONCLUSIONS

In this paper we have investigated some difference schemes approximating the system (1)–(3). Two modified box schemes have been proposed which are favourable with respect to CPU time and proved to be more accurate for practically used step lengths than classical schemes. Of the two new schemes the 'skew' box scheme turned out to be more advantageous owing to its better accuracy and larger monotonicity domain. Both the monotonicity and small computing time of this scheme make it very useful in solving inverse problems connected with (1)–(3).

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