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A high-order splitting scheme for the advection-diffusion equation

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Abstract: A high-order splitting scheme for the advection-diffusion equation of pollutants is proposed in this paper. The multidimensional advection-diffusion equation is splitted into several one-dimensional equations that are solved by the scheme. Only three spatial grid points are needed in each direction and the scheme has fourth-order spatial accuracy. Several typically pure advection and advection-diffusion problems are simulated. Numerical results show that the accuracy of the scheme is much higher than that of the classical schemes and the scheme can be efficiently solved with little programming effort.

Keywords: pollutants; advection-diffusion equation; high-order scheme; numerical modelling

Introduction

With the development of modern industry, various pollutants discharge into the air, rivers, lakes and oceans, which makes the environmental qualities worsen and has bad effect on the mankind's health and the sustained development of industry and agriculture. The environmental pollution has been a worldwide problem that has drawn more and more attention. The thorough studies on the activities and the fate of the harmful pollutants have important theoretical and practical meanings for the establishment of the accurate environmental protection strategy, for the guaranty of the sustained development of national economic, and for the improvement of mankind living environment.

The changes of pollutants in the air or in the water consist of the physical, chemical and biochemical processes, and so on. The physical changes of pollutants involve two main important processes, that is, advection and diffusion. The mathematical model describing these two processes is the well-known advection-diffusion equation. Numerical methods should be used at present to obtain the solution to a complicated advection-diffusion problem although the solution to a simple advection-diffusion problem can be obtained analytically. The numerical methods for the advection-diffusion equation are much more (Fletcher, 1991; Leonard, 1988; Noye, 1988; 1989, Sankaranarayanan, 1998; Shi, 1996; Sobey, 1983). In these methods, some show low accuracy, some are accurate enough but deal with many grids points, which makes them difficult to extended to be applied to practical problems. For this purpose a high-order splitting scheme is proposed and used to simulate three classical pure advection and advection-diffusion problems in the paper. The results are satisfactory.

1 Mathematical model

1.1 Basic equation

The method will be introduced in this paper by taking the two-dimensional advection-diffusion problem as an example. The two-dimensional advection-diffusion equation is:

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} + v\frac{\partial c}{\partial y} = \frac{\partial}{\partial x}\left(D_x\frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y\frac{\partial c}{\partial y}\right) + S_m, \tag{1}$$

where c is the concentration of pollutants; u and v are the velocities in the x and y direction, respectively; D_x and D_y are the diffusion coefficients; S_m is the source or sink; t is the time.

1.2 Numerical scheme

If the velocity field is known, the main difficulty of numerical solution of Eq.(1) lies in the simulation of the advection terms. If the advection term is not dominated, many of the existing schemes can give satisfactory results. Otherwise, they may cause large numerical errors. Based on the operator-splitting method, a high-order scheme is proposed by taking the two-dimensional advection-diffusion equation as an example. The extension of a two-dimensional treatment to a three-dimensional one is straightforward.

According to Szymkiewicz (Szymkiewicz, 1993), the solving of Eq.(1) is equivalent to the solving of the following one dimensional equations one by one, that is, Eq.(1) can be splitted into

$$\frac{\partial c^{(1)}}{\partial t} + u\frac{\partial c^{(1)}}{\partial x} = 0, \tag{2}$$

$$\frac{\partial c^{(2)}}{\partial t} + v\frac{\partial c^{(2)}}{\partial y} = 0, \tag{3}$$

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$$\frac{\partial c^{(3)}}{\partial t} = \frac{\partial}{\partial x}\left[D_x \frac{\partial c^{(3)}}{\partial x} \right], \tag{4}$$

$$\frac{\partial c^{(4)}}{\partial t} = \frac{\partial}{\partial y}\left[D_y \frac{\partial c^{(4)}}{\partial y} \right] + S_m. \tag{5}$$

The initial conditions for Eq. (2)—(5) are $c_t^{(1)} = c_t$, $c_t^{(2)} = c_{t+\Delta t}^{(3)}$, $c_t^{(1)} = c_{t+\Delta t}^{(2)}$ and $c_t^{(4)} = c_{t+\Delta t}^{(3)}$, respectively. The solution to Eq.(1) at time $t + \Delta t$, t is $c_{t+\Delta t} = c_{t+\Delta t}^{(4)}$. Clearly by the above splitting processes, the solving of a two-dimensional advection-diffusion equation is splitted into the solving of two one-dimensional pure advection equation, a one-dimensional pure diffusion equation and a one-dimensional diffusion equation including source or sink. So it is necessary to construct appropriate numerical schemes for these one-dimensional equations. For convenience, the superscripts in Eqs. (2)—(5) are omitted in the following sections.

If the Galerkin finite element method with linear interpolation is applied to Eq.(2), the following system of equations can be obtained (Fletcher, 1991):

$$M_x \left[\frac{\partial c}{\partial t} \right]_i + u \left. \frac{\partial c}{\partial x} \right|_i = 0, \tag{6}$$

where $M_x = (\delta, 1 - 2\delta, \delta)$ is the directional mass operator. The application of the Crank-Nicolson scheme to the above equation gives:

$$M_x \left[\frac{c_i^{n+1} - c_i^n}{\Delta t} \right] + \frac{u}{2} \left[\left. \frac{\partial c^{n+1}}{\partial x} \right|_i + \left. \frac{\partial c^n}{\partial x} \right|_i \right] = 0. \tag{7}$$

If the central difference is applied to the first order derivatives in the above equation, we can obtain after some arrangements

$$P_1 c_{i-1}^{n+1} + P_2 c_i^{n+1} + P_3 c_{i+1}^{n+1} = P_3 c_{i-1}^n + P_2 c_i^n + P_1 c_{i+1}^n, \tag{8}$$

where n and $n+1$ represent the time t and $t + \Delta t$, respectively; i is the spatial grid number; $P_1 = \delta - 0.25\alpha$; $P_2 = 1 - 2\delta$; $P_3 = \delta + 0.25\alpha$; $\alpha = u\Delta t/\Delta x$ is the Courant number. If $\delta = 0$, Eq. (8) is simplified to the Crank-Nicolson finite difference scheme.

Eq.(8) is unconditionally stable and has a truncation error of $O(\Delta t^2, \Delta x^4)$ when $\delta = 1/6 + \alpha^2/12$.

It should be noted that the time step in the numerical computation should not be too large although Eq. (8) is unconditionally stable. The reason is the accuracy of numerical results will decline if the time step is too large due to the second order accuracy in time.

Similarly, the numerical scheme for Eq.(3) can be easily obtained and will not be introduced here because of the space limit.

For Eq.(4) with constant D_x, Fletcher (Fletcher, 1991) gave several schemes and analyzed the stability, accuracy, and advantage and shortcomings of them in details. Of these schemes the highly accurate Crank-Nicolson finite element scheme is extended in this paper to the case with variable D_x.

The application of the Crank-Nicolson finite element method to Eq.(4) and making some arrangements yield

$$Q_1 c_{i-1}^{n+1} + Q_2 c_i^{n+1} + Q_3 c_{i+1}^{n+1} = Q_4 c_{i-1}^n + Q_5 c_i^n + Q_6 c_{i+1}^n, \tag{9}$$

where $Q_1 = \delta - 0.5S_{i-1/2}$, $Q_2 = 1 - 2\delta + 0.5S_{i-1/2} + 0.5S_{i+1/2}$, $Q_3 = \delta - 0.5S_{i+1/2}$, $Q_4 = \delta + 0.5S_{i-1/2}$, $Q_5 = 1 - 2\delta - 0.5S_{i-1/2} - 0.5S_{i+1/2}$, $Q_6 = \delta + 0.5S_{i+1/2}$, $S_{i-1/2} = \frac{0.5(D_{xi} + D_{xi-1})}{\Delta x^2}\Delta t$. Eq.(9) is neutrally stable with a truncation error of $O(\Delta t^2, \Delta x^2)$. If D_x is constant and $\delta = 1/12$, the scheme has fourth order accuracy (Flecther, 1991).

For Eq.(5) it is difficult to give a general scheme due to the different source or sink . If the special source or sink terms are given, a numerical scheme can be easily obtained by using the above method.

2 Examples and analysis

To illustrate the accuracy of the scheme given in the preceding section, we will apply it to several classical pure advection and advection-diffusion problems in the following.

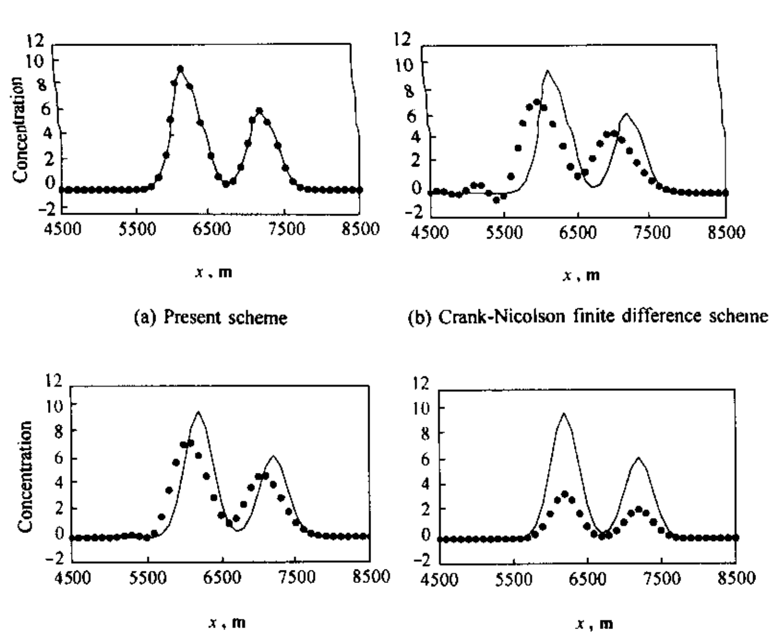
2.1 Calculation of two-dimensional pure advection in a uniform flow

In an infinite two-dimensional plane, a couple of Gaussian distributions are advected downstream at constant velocity $u = 0.5$ m/s, $v = 0.5$ m/s. The initial locations of each Gaussian distribution's center are $(x_1, y_1) = (1400\text{m}, 1400\text{m})$ and $(x_2, y_2) = (2400\text{m}, 2400\text{m})$. The initial values of peak concentrations are $c_1 = 10.0$ and $c_2 = 6.5$, and the standard deviations are $\sigma_1 = 264$m and $\sigma_2 = 264$m, respectively. The analytical solution to the problem is

$$c(x, y, t) = c_1 \exp\left[- \frac{(x - x_1 - ut)^2 + (y - y_1 - vt)^2}{2\sigma_1^2} \right] +$$

$$c_2 \exp\left[- \frac{(x - x_2 - ut)^2 + (y - y_2 - vt)^2}{2\sigma_2^2} \right].$$

Substituting $t = 0$ into the above equation gives the initial condition. In the numerical computation, the time step and the space step are taken to be 100s and 100m, respectively. Fig.1 shows the comparison of the numerical results obtained by four numerical schemes with the analytical solutions along the line $y = x$. It can be seen that the results obtained by the present scheme are almost the same as the analytical solutions, while the results obtained by the other classical schemes show



(a) Present scheme (b) Crank-Nicolson finite difference scheme

(c) Lax-Wendroff scheme (d) Two-point upwind difference

Fig.1 Cmparison of several schemes for two-dimensional pure advection in a uniform flow(along line $y = x$), $\Delta x = \Delta y = 100$m, $\Delta t = 100$s
· numerical solution —analytical solution

large discrepancy from the analytical solutions. Clearly the results obtained by the present scheme are much better.

2.2 Calculation of two-dimensional pure advection in a rotational flow

Suppose in a finite two-dimensional plane exists a rotational flow, the flow velocity is given by

$$u = -\omega(y - y_0), v = \omega(x - x_0),$$

where ω is the angular rotation rate; $\omega = 2\pi/12000$(rad/s); (x_0, y_0) are the coordinates of the rotational center, (x, y) are the coordinates in the plane. A Gaussian distribution centered at (x_1, y_1) is in the plane with the initial values given by

$$c(x,y,0) = 10\exp\left[-\frac{(x - x_1)^2 + (y - y_1)^2}{2 \times 200^2}\right].$$

The center of the Gaussian distribution does not coincide with the rotational center, that is, $x_0 = y_0 = 2400.0$m, $x_1 = y_1 = 1400$m. The computational domain is bounded by $0 \leqslant x \leqslant 5000$ m and $0 \leqslant y \leqslant 5000$m. The time step and the space step are taken to be 50.0s and 100m, respectively.

Fig.2 shows the comparison of the numerical results by four schemes with the analytical solutions after one turn of rotation. It can be seen that the results obtained by the present scheme are much closer to the analytical ones while the results obtained by the other three schemes show large discrepancy from the analytical solutions. Table 1 gives the relative errors between the calculated peak values and the analytical one. The results illustrate once more that the present scheme can give highly accurate results for two-dimensional pure advection problems.

Table 1 Relative errors between the calculated peak values and the analytical one

	Analytical solution	Present scheme	Crank-Nicolson finite difference	Lax-Wendroff scheme	Two-point upwind scheme
Peak value	10.0	9.6291	3.5188	3.8825	0.8973
Relative error, %		3.71	64.81	61.18	91.03

2.3 Two dimensional advection-diffusion problem

Here the two-dimensional advection-diffusion of a Gaussian pulse in a rectangular domain is simulated to investigate the accuracy of the present scheme. The Gaussian pulse of unit height is centered at (0.5m, 0.5m). The initial condition is given by

$$c(x,y,0) = \exp\left[-\frac{(x-0.5)^2}{D_x} - \frac{(y-0.5)^2}{D_y}\right].$$

The analytical solution to the problem is

$$c(x,y,t) = \frac{1}{4t+1}\exp\left[-\frac{(x - 0.5 - ut)^2}{D_x(4t+1)} - \frac{(y - 0.5 - vt)^2}{D_y(4t+1)}\right],$$

where, $D_x = D_y = 0.01$ m^2/s; $u = v = 0.8$ m/s. The computational domain is bounded by $0 \leqslant x \leqslant 2$ and $0 \leqslant y \leqslant 2$. The time

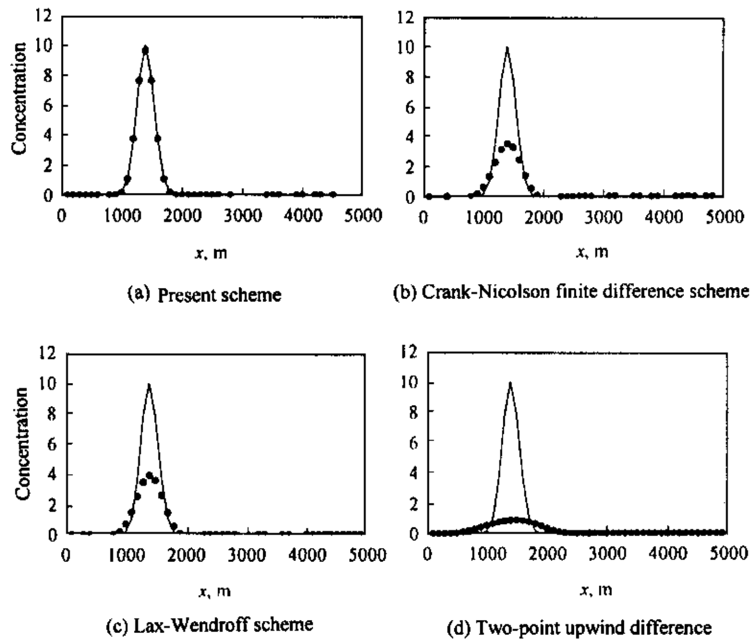


Fig.2 Comparison of several schemes for two-dimensional pure advection in a rotational flow(along line $y = x$), $\Delta x = \Delta y = 100\mathrm{m}$, $\Delta t = 50\mathrm{s}$
· numerical solution —analytical solution

step and the space step are 0.00625s and 0.05m, respectively. Fig.3 shows the comparison of the numerical results obtained by four numerical schemes with the analytical solutions at $t = 1.25\mathrm{s}$. It can be seen that the results given by the present scheme are almost the same as the analytical ones and the results given by the Crank-Nicolson finite difference scheme and Lax-Wendroff scheme are closer to the analytical solutions. There exists serious numerical diffusion in the results given by the two-point upwind scheme, the accuracy is very low. The results show further that the accuracy of the present scheme is high.

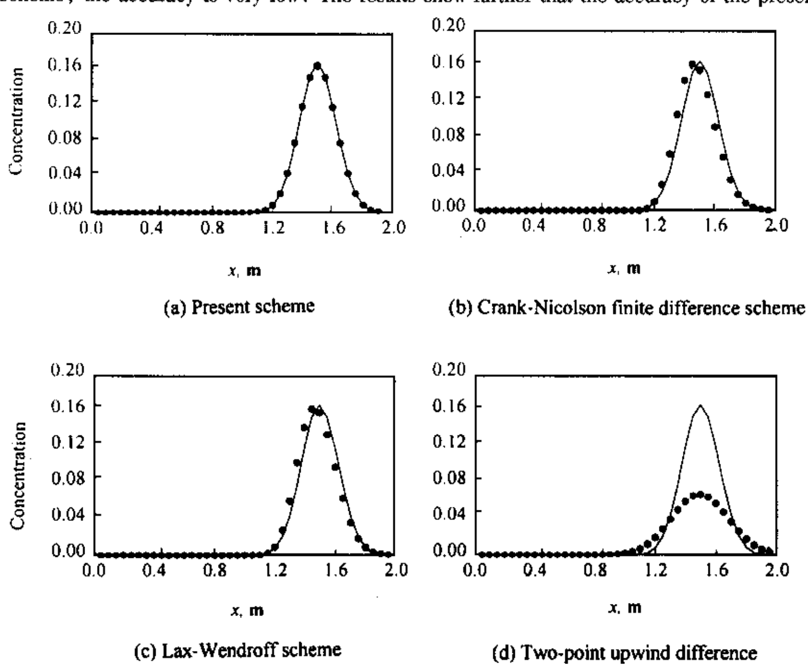


Fig.3 Numerical and analytical solutions to two-dimensional advection-diffusion problem(along line $y = x$), $\Delta x = \Delta y = 0.05\mathrm{m}$, $\Delta t = 0.00625\mathrm{s}$;

· numerical solution —analytical solution

3 Conclusions

A new high-order splitting scheme for the advection-diffusion equation of pollutants is proposed in this paper. Three classical pure advection and advection-diffusion problems are simulated. Comparisons of the numerical results with the analytical solutions and the results obtained by the other schemes show that the present scheme is highly accurate, can be easily programmed and extended to give refined prediction of the practical advection-diffusion problems.

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