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An accurate integral-based scheme for advection–diffusion equation

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SUMMARY

This paper proposes an accurate integral-based scheme for solving the advection–diffusion equation. In the proposed scheme the advection–diffusion equation is integrated over a computational element using the quadratic polynomial interpolation function. Then elements are connected by the continuity of first derivative at boundary points of adjacent elements. The proposed scheme is unconditionally stable and results in a tridiagonal system of equations which can be solved efficiently by the Thomas algorithm. Using the method of fractional steps, the proposed scheme can be extended straightforwardly from one-dimensional to multi-dimensional problems without much difficulty and complication. To investigate the computational performances of the proposed scheme five numerical examples are considered: (i) dispersion of Gaussian concentration distribution in one-dimensional uniform flow; (ii) one-dimensional viscous Burgers equation; (iii) pure advection of Gaussian concentration distribution in two-dimensional uniform flow; (iv) pure advection of Gaussian concentration distribution in two-dimensional rigid-body rotating flow; and (v) three-dimensional diffusion in a shear flow. In comparison not only with the QUICKEST scheme, the fully time-centred implicit QUICK scheme and the fully time-centred implicit TCSD scheme for one-dimensional problem but also with the ADI-QUICK scheme, the ADI-TCSD scheme and the MOSQUITO scheme for two-dimensional problems, the proposed scheme shows convincing computational performances. Copyright © 2001 John Wiley & Sons, Ltd.

KEY WORDS: quadratic polynomial interpolation function; numerical model; advection–diffusion equation; integral-based scheme

1. INTRODUCTION

The advection–diffusion equation is one of the governing equations used for modelling solute transport processes and water quality in rivers, lakes, oceans and groundwater. Among

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various numerical methods available for the solution of the advection–diffusion equation, the conventional Crank–Nicolson second-order central difference scheme [1] is a relatively simple and convenient way. However, due to central discretization of advection processes, it suffers from severe numerical oscillation under large Peclet number (cell Reynolds number). This numerical oscillation can be vanished by using a first-order upwind-type finite difference scheme, but it induces excessive numerical damping. Thus, in order to tackle the numerical oscillation problem and reduce excessive numerical damping, several high-order upwind-type finite difference methods have been proposed, such as the quadratic upstream interpolation for convective kinematics (QUICK) scheme [2], the QUICK with estimated stream terms (QUICKEST) scheme [2] and the third-order convection second-order diffusion (TCSD) scheme [3]. These numerical schemes are all explicit formulations originally. Later on, some implicit forms of modified QUICK [4, 5] and TCSD [6] schemes were proposed. These high-order upwind-type finite difference schemes have been attractive for practical engineering applications. For example, the explicit QUICK scheme has been used for hydraulic and water quality studies in coastal and inland waters [7–9] and the implicit QUICK-based formulation has been applied to the investigations of unsteady flow [10].

In addition, the Eulerian–Lagrangian split operator approach in which advection and diffusion processes are computed independently for each step has been pursued by many numerical modellers. The split operator approach has the advantage of using different accurate schemes for each physical process. However, since the advection and diffusion processes are computed separately, the split operator approach is more complicated and expensive when applied to multi-dimensional problems, especially for the problems with complex flow pattern. Thus, as far as simplicity and efficiency is concerned, the numerical schemes without split operator approach are still very attractive for solving the advection–diffusion problems.

In this paper an accurate integral-based numerical scheme for solving the advection–diffusion equation is proposed. In the proposed scheme, the advection–diffusion equation is integrated over a computational element using the quadratic polynomial interpolation function. Then elements are connected by the continuity of first derivative between boundary points of adjacent elements. Using the method of fractional steps and the technique of linearization, the proposed scheme, originally developed for one-dimensional linear problems, can be extended straightforwardly to multi-dimensional and non-linear problems. Five numerical examples, including: (i) dispersion of Gaussian concentration distribution in one-dimensional uniform flow; (ii) one-dimensional viscous Burgers equation; (iii) pure advection of Gaussian concentration distribution in two-dimensional uniform flow; (iv) pure advection of Gaussian concentration distribution in two-dimensional rigid-body rotating flow; and (v) three-dimensional diffusion in a shear flow, are used to investigate the computational performances of the proposed scheme. The proposed scheme is compared not only with the QUICKEST scheme, the fully time-centred implicit QUICK scheme and the fully time-centred implicit TCSD scheme for one-dimensional problem but also with the ADI-QUICK scheme, the ADI-TCSD scheme and the modified second-order QUICKEST scheme (MOSQUITO) [11] for two-dimensional problems in terms of numerical damping and numerical oscillation.

2. DEVELOPMENT OF INTEGRAL-BASED SCHEME

2.1. Discretization

The transient one-dimensional advection–diffusion equation can be written as

$$\frac{\partial \Phi}{\partial t} + \frac{\partial (u\Phi)}{\partial x} = \frac{\partial}{\partial x}\left(\alpha \frac{\partial \Phi}{\partial x}\right) \tag{1}$$

where the scalar function $\Phi(x,t)$ may represent, for example, temperature or concentration at position x and time t in a fluid moving with a speed $u(x,t)$ and diffusion coefficient $\alpha(x,t)$.

First, Equation (1) is integrated over an interval from position x_i to position x_{i+1} and is expressed as

$$\int_{x_i}^{x_{i+1}} \frac{\partial \Phi}{\partial t}\,\mathrm{d}x + \int_{x_i}^{x_{i+1}} \frac{\partial (u\Phi)}{\partial x}\,\mathrm{d}x = \int_{x_i}^{x_{i+1}} \frac{\partial}{\partial x}\left(\alpha \frac{\partial \Phi}{\partial x}\right)\mathrm{d}x \tag{2}$$

By defining $\bar{\Phi}_{i+1/2}$, i.e. the average quantity over a computational element, as

$$\bar{\Phi}_{i+1/2} = \frac{1}{\Delta x}\int_{x_i}^{x_{i+1}} \Phi\,\mathrm{d}x \tag{3}$$

and adopting the quadratic polynomial interpolation function in the interval $[x_i, x_{i+1}]$, the first derivatives at point x_i and x_{i+1} can be expressed as

$$\left.\frac{\partial \Phi}{\partial x}\right|_{x_{i+1}} = \frac{1}{\Delta x}(4\Phi_{i+1} + 2\Phi_i - 6\bar{\Phi}_{i+1/2}) \tag{4}$$

$$\left.\frac{\partial \Phi}{\partial x}\right|_{x_i} = \frac{1}{\Delta x}(-2\Phi_{i+1} - 4\Phi_i + 6\bar{\Phi}_{i+1/2}) \tag{5}$$

with a uniform grid space, i.e. $\Delta x = x_{i+1} - x_i$, as shown in Figure 1. The detailed derivations of Equations (4) and (5) are given in the Appendix.

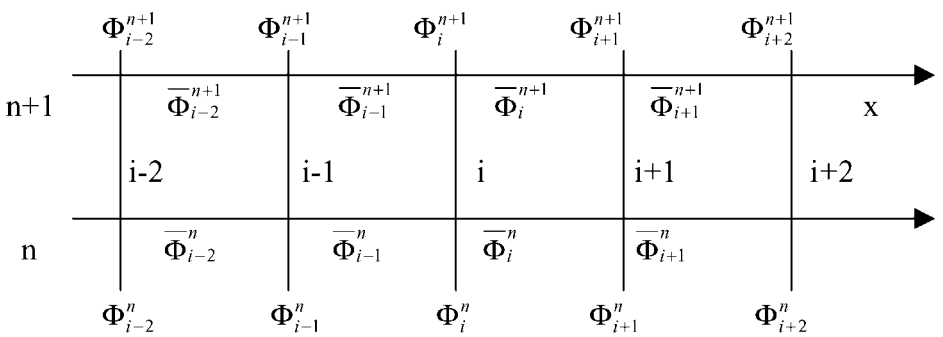

Figure 1. Sketch of grid representation of the proposed scheme.

Substituting Equations (3)–(5) into Equation (2) produces

$$\frac{\partial \bar{\Phi}_{i+1/2}}{\partial t} + \frac{1}{\Delta x}\left[u_{i+1}\Phi_{i+1} - u_i\Phi_i\right] = \frac{1}{\Delta x^2}[\alpha_{i+1}(4\Phi_{i+1} + 2\Phi_i - 6\bar{\Phi}_{i+1/2}) - \alpha_i(-2\Phi_{i+1} - 4\Phi_i + 6\bar{\Phi}_{i+1/2})] \tag{6}$$

Using the Crank–Nicholson method to Equation (6), one obtains

$$\begin{aligned}\frac{\bar{\Phi}^{n+1}_{i+1/2} - \bar{\Phi}^{n}_{i+1/2}}{\Delta t} &+ \frac{1}{2\Delta x}\left[\left(u^{n+1}_{i+1}\Phi^{n+1}_{i+1} + u^{n}_{i+1}\Phi^{n}_{i+1}\right) - \left(u^{n+1}_{i}\Phi^{n+1}_{i} + u^{n}_{i}\Phi^{n}_{i}\right)\right] \\ &= \frac{1}{2\Delta x^2}\left[\alpha^{n+1}_{i+1}\left(4\Phi^{n+1}_{i+1} + 2\Phi^{n+1}_{i} - 6\bar{\Phi}^{n+1}_{i+1/2}\right) + \alpha^{n}_{i+1}\left(4\Phi^{n}_{i+1} + 2\Phi^{n}_{i} - 6\bar{\Phi}^{n}_{i+1/2}\right)\right] \\ &\quad - \frac{1}{2\Delta x^2}\left[\alpha^{n+1}_{i}\left(-2\Phi^{n+1}_{i+1} - 4\Phi^{n+1}_{i} + 6\bar{\Phi}^{n+1}_{i+1/2}\right) + \alpha^{n}_{i}\left(-2\Phi^{n}_{i+1} - 4\Phi^{n}_{i} + 6\bar{\Phi}^{n}_{i+1/2}\right)\right]\end{aligned} \tag{7}$$

where Δt is the time step. Rearranging Equation (7), the average quantity over the interval $[x_i, x_{i+1}]$ at $n+1$ time step, i.e. $\bar{\Phi}^{n+1}_{i+1/2}$, can be expressed as

$$\bar{\Phi}^{n+1}_{i+1/2} = (a_{-1})_i\Phi^{n+1}_i + (a_1)_i\Phi^{n+1}_{i+1} + (b_{-1})_i\Phi^{n}_i + (b_0)_i\bar{\Phi}^{n}_{i+1/2} + (b_1)_i\Phi^{n}_{i+1} \tag{8}$$

with

$$(a_{-1})_i = \frac{0.5(Cr_i^{n+1} + 2D_{i+1}^{n+1} + 4D_i^{n+1})}{1 + 3D_{i+1}^{n+1} + 3D_i^{n+1}}$$

$$(a_1)_i = \frac{-0.5(Cr_{i+1}^{n+1} - 4D_{i+1}^{n+1} - 2D_i^{n+1})}{1 + 3D_{i+1}^{n+1} + 3D_i^{n+1}}$$

$$(b_{-1})_i = \frac{0.5(Cr_i^{n} + 2D_{i+1}^{n} + 4D_i^{n})}{1 + 3D_{i+1}^{n+1} + 3D_i^{n+1}}$$

$$(b_0)_i = \frac{1 - 3D_{i+1}^{n} - 3D_i^{n}}{1 + 3D_{i+1}^{n+1} + 3D_i^{n+1}}$$

$$(b_1)_i = \frac{0.5(-Cr_{i+1}^{n} + 4D_{i+1}^{n} + 2D_i^{n})}{1 + 3D_{i+1}^{n+1} + 3D_i^{n+1}}$$

where the Courant numbers, $Cr_i^n = u_i^n\Delta x/\Delta t$ and $Cr_i^{n+1} = u_i^{n+1}\Delta x/\Delta t$ and diffusion numbers, $D_i^n = \alpha_i^n\Delta t/\Delta x^2$ and $D_i^{n+1} = \alpha_i^{n+1}\Delta t/\Delta x^2$, have been introduced. It must be noticed that in Equation (8) $\bar{\Phi}^{n+1}_{i+1/2}$ is explicitly related to Φ^{n+1}_i, Φ^{n+1}_{i+1}, Φ^{n}_i, Φ^{n}_{i+1} and $\bar{\Phi}^{n}_{i+1/2}$.

Assuming the first derivative of the scalar tracer distribution is continuous at any grid point, the continuity of the solution at point x_i and $n+1$ time step is imposed by satisfying the

following condition:

$$2\Phi_i^{n+1} + \Phi_{i-1}^{n+1} - 3\bar{\Phi}_{i-1/2}^{n+1} = -\Phi_{i+1}^{n+1} - 2\Phi_i^{n+1} + 3\bar{\Phi}_{i+1/2}^{n+1} \tag{9}$$

By substituting Equation (8) into Equation (9), the discretization form of the advection–diffusion equation becomes

$$A_{-1}\Phi_{i-1}^{n+1} + A_0\Phi_i^{n+1} + A_1\Phi_{i+1}^{n+1} = B_{-1}\Phi_{i-1}^{n} + \overline{B_{-1}}\bar{\Phi}_{i-1}^{n} + B_0\Phi_i^{n} + \overline{B_1}\bar{\Phi}_i^{n} + B_1\Phi_{i+1}^{n} \tag{10}$$

where

$$\begin{aligned}
A_{-1} &= 1 - 3(a_{-1})_{i-1} \\
A_0 &= 4 - 3(a_1)_{i-1} - 3(a_{-1})_i \\
A_1 &= 1 - 3(a_1)_i \\
B_{-1} &= 3(b_{-1})_{i-1} \\
\overline{B_{-1}} &= 3(b_0)_{i-1} \\
B_0 &= 3(b_1)_{i-1} + 3(b_{-1})_i \\
\overline{B_1} &= 3(b_0)_i \\
B_1 &= 3(b_1)_i
\end{aligned}$$

If the diffusion coefficient $\alpha(x,t) = \alpha$ is constant, Equation (10) can be reduced to

$$A_{-1}^*\Phi_{i-1}^{n+1} + A_0^*\Phi_i^{n+1} + A_1^*\Phi_{i+1}^{n+1} = B_{-1}^*\Phi_{i-1}^{n} + B_0^*\Phi_i^{n} + B_i^*\Phi_{i+1}^{n} \tag{11}$$

where

$$\begin{aligned}
A_{-1}^* &= 1 - 1.5Cr_{i-1}^{n+1} - 3D \\
A_0^* &= 4 + 1.5Cr_{i-1}^{n+1} - 1.5Cr_{i+1}^{n+1} + 6D \\
A_1^* &= 1 + 1.5Cr_{i+1}^{n+1} - 3D \\
B_{-1}^* &= 1 + 1.5Cr_{i-1}^{n} + 3D \\
B_0^* &= 4 - 1.5Cr_{i-1}^{n} + 1.5Cr_{i+1}^{n} - 6D \\
B_1^* &= 1 - 1.5Cr_{i+1}^{n} + 3D
\end{aligned}$$

with the diffusion number being $D = \alpha\Delta t/\Delta x^2$.

2.2. Solution procedure

From Equation (10) the proposed scheme would result in a tridiagonal system of algebraic equations which can be solved efficiently by the Thomas algorithm [12]. The boundary condition of Dirichlet type can be applied to the proposed scheme directly, whereas for the Neumann boundary condition the discretization technique of finite difference method may be introduced to keep the tridiagonal structure of the system unchanged.

If the diffusion coefficient is constant, one can directly apply Equation (11) to solve the advection–diffusion equation without computing the average quantity of every element. For the non-constant diffusion coefficient the solution procedure of the proposed scheme is depicted as follows:

1. Specify initial value, Φ_i^0, at every grid point and compute initial average value, $\bar{\Phi}_{i+1/2}^0$, for every interval from the initial condition.
2. Use Equation (10) along with the boundary conditions to solve for the unknown, Φ_i^{n+1}, at every grid point in space at next time step.
3. Use Equation (8) to explicitly compute the unknown, $\bar{\Phi}_{i+1/2}^{n+1}$, at every space interval at next time step.
4. Repeat steps 3 and 4 to the end of time of simulation.

2.3. Stability analysis

The stability of any numerical schemes is one of the main properties first needing to be investigated before those can be favourably considered for application. The matrix and von Neumann methods are two commonly used ways for analysing the stability of any numerical scheme. In this study the von Neumann stability analysis is conducted by assuming that the velocity and diffusion coefficient are constant and positive. The von Neumann stability analysis shows that the proposed scheme is unconditionally stable.

2.4. Extension to multi-dimensional problems

The proposed scheme is originally developed for one-dimensional linear advection–diffusion equation. Using the method of fractional steps [13], the proposed scheme can be extended straightforwardly to multi–dimensional advection–diffusion problems without much complication and difficulty. The two-dimensional advection–diffusion equation can be written as

$$\Phi_t + U\Phi_x + V\Phi_y = D_x\Phi_{xx} + D_y\Phi_{yy} \tag{12}$$

where U, V, D_x and D_y represent the flow velocity and diffusion coefficient in x and y directions, respectively. Dividing the two-dimensional advection and diffusion processes into two successive steps in x and y directions, respectively, Equation (12) can be approximated with a series of one-dimensional advection–diffusion equation as

$$\Phi_t + U\Phi_x = D_x\Phi_{xx} \tag{13}$$

and

$$\Phi_t + V\Phi_y = D_y\Phi_{yy} \tag{14}$$

Equations (13) and (14) can be solved by the proposed scheme as shown in Figure 2. The three-dimensional problems can also be formulated and solved in the same manner by adding z directional advection and diffusion as the third processes. In addition, the non-linear problems can also be solved iteractively by the proposed scheme with the technique of linearization.

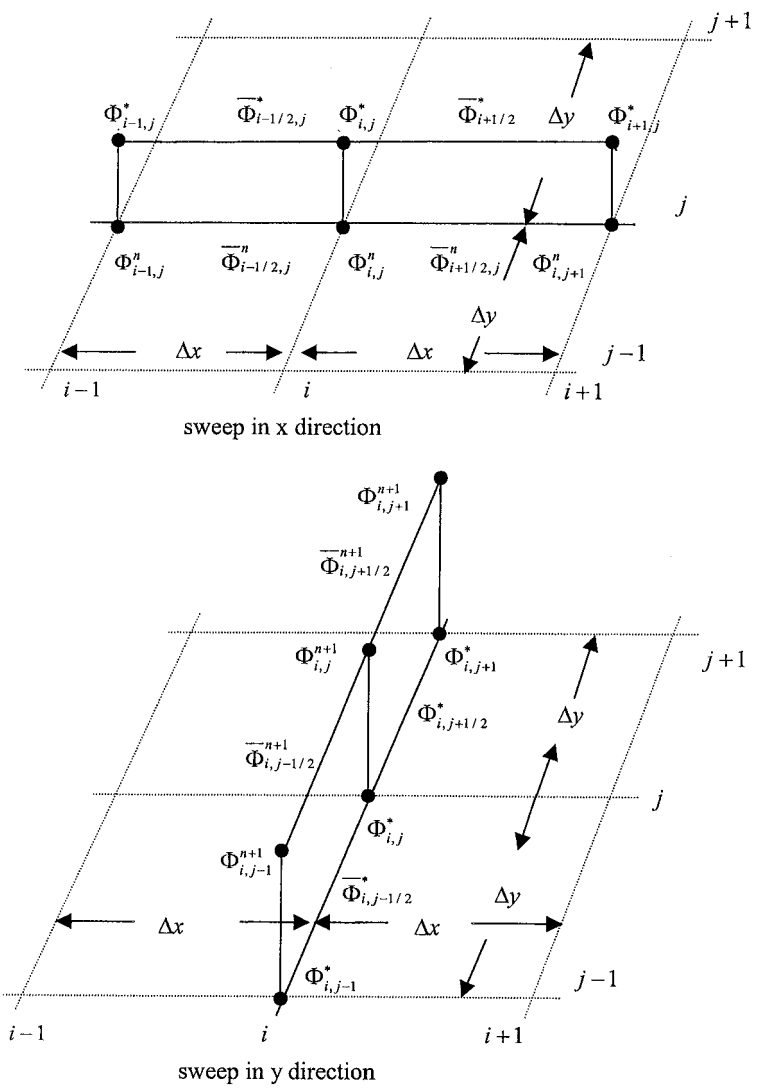

Figure 2. Sketch of two-dimensional integral-based scheme.

3. NUMERICAL EXAMPLES

3.1. One-dimensional problems

3.1.1. Calculation of advection and diffusion. To investigate the computational performances of the proposed scheme, the advection and diffusion of a Gaussian concentration distribution with the peak value 16.71 and a standard deviation of 280 m is considered with constant velocity $u = 0.3$ m s^{-1} and diffusion coefficient $\alpha = 1.0$ m^2 s^{-1}. In this example, with time

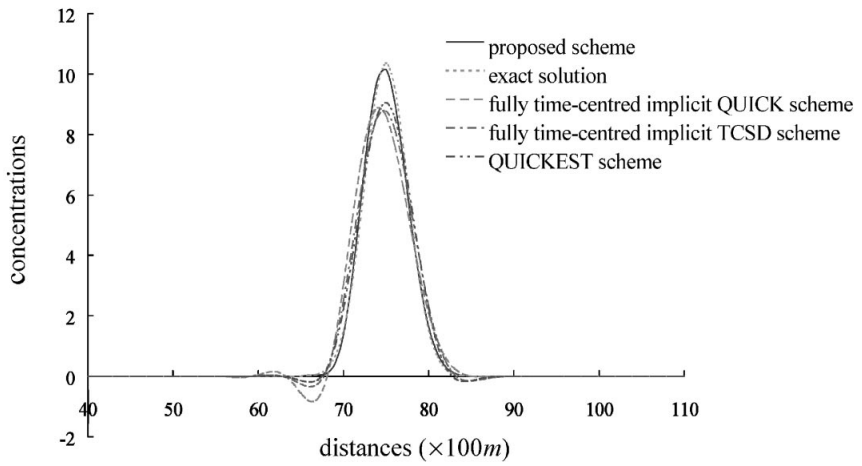

Figure 3. Comparison of various schemes for dispersion of Gaussian concentration distribution ($Cr = 0.3,\ D = 0.01$).

step size $\Delta t = 100$ s and grid space $\Delta x = 100$ m, the Courant number, Cr, and the diffusion number, D, are 0.3 and 0.01, respectively. The computed results are shown in Figure 3 for the simulation time of 20 000 s. From Figure 3, one can find that the proposed scheme induces the least numerical oscillation and diffusion in comparison with the QUICKEST scheme, the fully time-centred implicit QUICK scheme and the fully time-centred implicit TCSD scheme.

3.1.2. Calculation of viscous Burgers equation. To further investigate the capability of the proposed scheme for solving non-linear problems, a viscous Burgers equation is considered. The viscous Burgers equation can be expressed as

$$u_t + uu_x = \alpha u_{xx} \tag{15}$$

with the initial and boundary conditions

$$\begin{aligned} u(x,0) &= 1, \quad x \leqslant 0 \\ &= 0, \quad x > 0 \\ u(-\infty, t) &= 1, \quad u(\infty, t) = 0, \quad t > 0 \end{aligned} \tag{16}$$

The exact solution for the above problem is

$$u(x,t) = \left[1 + \exp\left[\frac{1}{2\alpha}\left(x - \frac{1}{2}t\right)\right] \frac{\operatorname{erfc}(-x/2\sqrt{\alpha t})}{\operatorname{erfc}[(x-t)/2\sqrt{\alpha t}]}\right]^{-1} \tag{17}$$

where erfc is the complementary error function. Using the technique of linearization, the viscous Burgers equation can be solved iteractively by the proposed scheme. The numerical solution of the proposed scheme at time $t = 2$ s is depicted in Figure 4 with the grid space of 0.01 m, time step of 0.01 s and diffusion coefficient of 0.01 $m^2\ s^{-1}$. The range of Courant

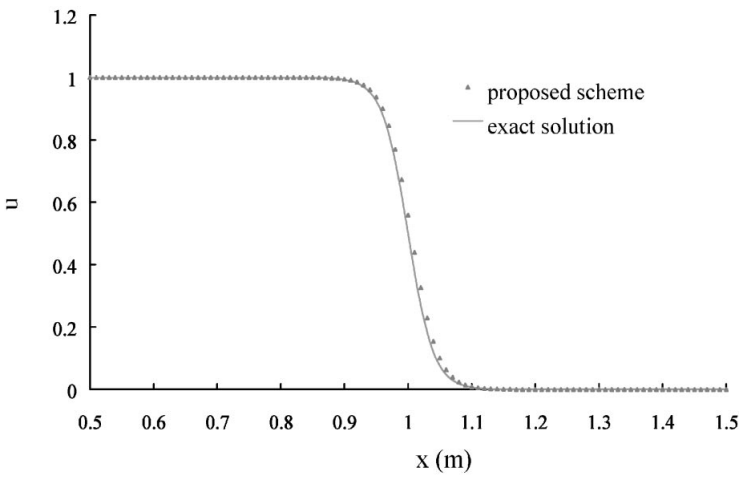

Figure 4. Computational results of the proposed scheme for Burges equation.

Table I. Performances of various schemes in two-dimensional pure advection test ($Cr = 0.5$).

Scheme	Max.	Min.	RMS error
Exact solution	10.00	0.0	0.0
Proposed scheme	9.51	−0.01	0.0057
MOSQUITO scheme	7.74	−0.56	0.0141
ADI-QUICK scheme	7.89	−0.57	0.0170
ADI-TCSD scheme	8.00	−1.04	0.0244

number used in this example is from zero to unity, whereas the constant diffusion number is 0.01. Figure 4 shows that the simulated results of the proposed scheme are very close to the exact solution. This numerical example demonstrates that the proposed scheme also performs well for the nonlinear problem.

3.2. Two-dimensional problems

3.2.1. Calculation of pure advection in uniform flow. The Gaussian concentration distribution with the peak value of 10 and a standard deviation of 220 m is advected for 5000 s at constant velocity of $U = 0.5$ m s^{-1} and $V = 0.5$ m s^{-1}. The grid size of 100 m $\times$ 100 m and time step of 100 s are used. Thus, the Courant numbers in x and y directions are all 0.5. The computed results in terms of maximum, minimum values and RMS error by using the proposed scheme, ADI-QUICK scheme, ADI-TCSD scheme and the MOSQUITO scheme are displayed in Table I. From Table I, one can find that the proposed scheme yields the best results among those schemes considered, whereas the ADI-TCSD scheme induces the largest numerical oscillation and RMS error. In this numerical example, the computational time of the proposed scheme is about 4 times greater than that of the MOSQUITO scheme.

This is so happened because the latter scheme is an explicit-type scheme in which there is no need to solve the system of equations simultaneously. On the other hand, based on the method of fractional steps and the implicit-type schemes, the proposed scheme, the ADI scheme and the ADI-TCSD scheme have competitive computational efficiency. The computational time of the MOSQUITO scheme is less than that of the proposed scheme, but it must be noticed that the explicit-type scheme usually need smaller time step than that of the implicit-type scheme to keep the stability. Thus, generally speaking, the implicit-type scheme is more efficient than the explicit-type scheme for the simulation of practical problems.

3.2.2. Calculation of pure advection in rigid-body rotating flow. Another numerical example of pure advection of Gaussian concentration distribution in rigid-body rotating flow in an infinite two-dimensional domain is adopted to investigate the application of the proposed scheme to the flow field with non-uniform velocity. The peak value and standard deviation of Gaussian distribution are 10 and 250 m, respectively. In the simulation of this example, a finite square computational domain of 80 000 m $\times$ 80 000 m is used. The rigid-body spends 80 000 s rotating around the center of the computational domain one turn. With the grid size of 100 m $\times$ 100 m and time step of 50 s, the ranges of Courant numbers used in x and y directions are all from $-\pi/2$ to $\pi/2$. In addition, the radius of circular trajectory of the centroid of the Gaussian distribution is 2000 m. The maximum, minimum values and RMS error of simulated results by using the proposed scheme, the ADI-QUICK scheme and the ADI-TCSD scheme after one turn of rotation are $(9.78, -0.02, 0.00035)$, $(6.63, -0.57, 0.0054)$ and $(6.46, -0.18, 0.0045)$, respectively.

3.3. Three-dimensional problem

In order to investigate the capability of the proposed scheme for solving three-dimensional problems with complex flow field, diffusion in the shear flow is considered. The velocity shear plays an important role in the diffusion of a patch of passive contaminant from an instantaneous source in natural streams such as oceans, lakes and estuaries. The governing equation for shear diffusion can be expressed by

$$\frac{\partial \Phi}{\partial t} + (V_0 + \Omega_y y + \Omega_z z)\frac{\partial \Phi}{\partial x} = \alpha_x \frac{\partial^2 \Phi}{\partial x^2} + \alpha_y \frac{\partial^2 \Phi}{\partial y^2} + \alpha_z \frac{\partial^2 \Phi}{\partial z^2} \tag{18}$$

where x, y and z is the co-ordinate system; Φ represents the concentration of contaminant; V_0 is the mean velocity in the x direction; Ω_y and Ω_z represent the horizontal and vertical shears. In addition, α_x, α_y and α_z are the eddy diffusivities in the x, y and z directions, respectively. The analytical solution for an instantaneous point source of mass M released at $x = y = z = 0$ was obtained by Carter and Okubo [14] as follows:

$$\Phi = \frac{M}{8\pi^{3/2}(\alpha_x \alpha_y \alpha_z)^{1/2} t^{3/2}(1 + \beta^2 t^2)^{1/2}} \exp - \left[\frac{(x - V_0 t - 0.5(\Omega_y y + \Omega_z z)t)^2}{4\alpha_x t(1 + \beta^2 t^2)} + \frac{y^2}{4\alpha_y t} + \frac{z^2}{4\alpha_z t} \right] \tag{19}$$

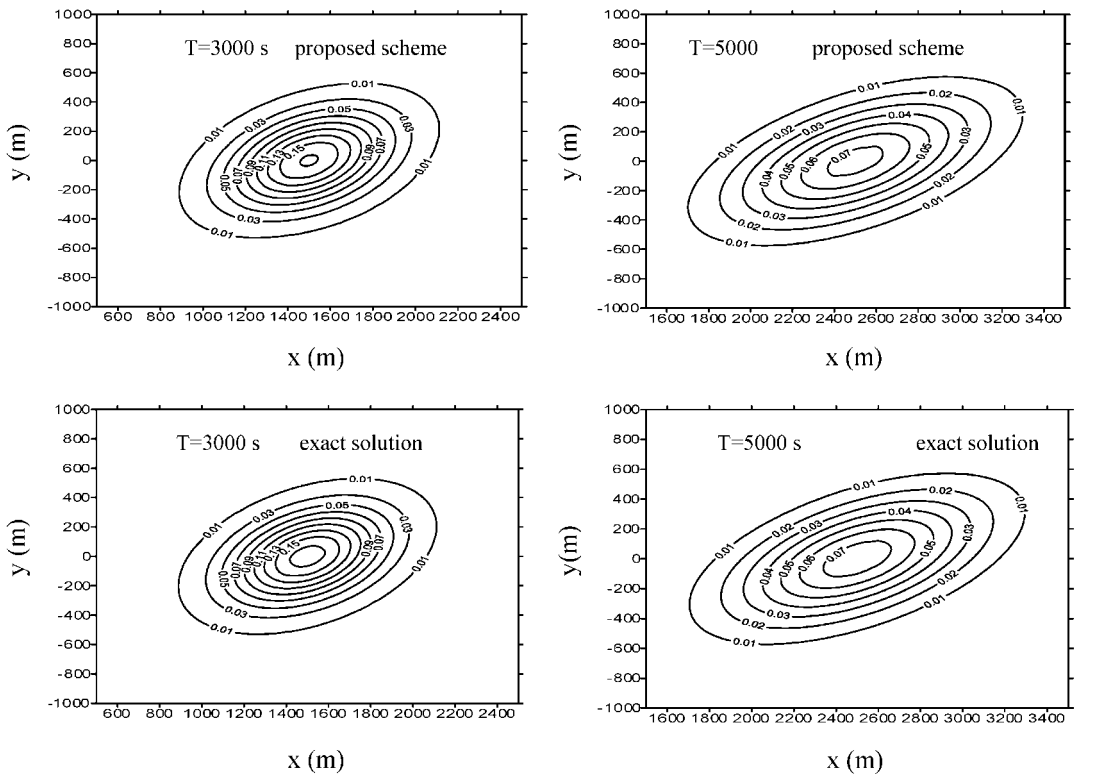

Figure 5. Comparison of contour plots of diffusion in shear flow on plane $z = 0$ at time = 3000 s and 5000 s by using proposed scheme and exact solution.

where

$$\beta^2 = \frac{\lfloor (\Omega_y^2 \alpha_y / \alpha_x) + (\Omega_z^2 \alpha_z / \alpha_x) \rfloor}{12} \tag{20}$$

To allow numerical solution having an initial peak concentration of unity, calculation begins at time $t = t_0$. Thus, the point source of mass M can be specified as

$$M = 8\pi^{3/2} (\alpha_x \alpha_y \alpha_z)^{1/2} t^{3/2} (1 + \beta^2 t_0^2)^{1/2} \tag{21}$$

The following parameters are used in this numerical example: $t_0 = 1000$ s, $V_0 = 0.5$ m s^{-1}, $\Omega_y = \Omega_z = 0.0003$ s^{-1}, $\alpha_x = \alpha_y = \alpha_z = 8.0$ m^2 s^{-1}, time step size $\Delta t = 100$ s and grid space $\Delta x = \Delta y = \Delta z = 100$ m. Thus, the Courant number in x direction is 0.5, whereas the ranges of the equivalent Courant numbers in y and z directions, causing by the shear flow, are all from -0.3 to 0.3 for the computational domain used in this example. In addition, the diffusion numbers in three directions are all 0.08. Figure 5 depicts the contour plots as simulated by the proposed scheme and analytical solution at time $t = 3000$ and 5000 s on the plan $z = 0$, respectively. It is apparent that the proposed scheme yields computational results which are good in agreement with the exact solution.

4. CONCLUSIONS

In this paper an accurate integral-based numerical scheme for solving the advection–diffusion equation is proposed. The proposed scheme is unconditionally stable and results in a tridiagonal system of equations which can be solved efficiently by the Thomas algorithm. By using the method of fractional steps and the technique of linearization, the proposed scheme that was originally developed for one-dimensional linear problem can be extended straightforwardly to multi-dimensional and nonlinear problems. Some one-, two- and three-dimensional numerical examples are used to investigate the computational performances of the proposed scheme. In comparison with the QUICKEST scheme, the fully time-centred implicit QUICK scheme, the fully time-centred implicit TCSD scheme, the ADI-QUICK scheme, the ADI-TCSD scheme, the MOSQUITO scheme and the exact solutions, the proposed scheme yields convincing simulated results.

APPENDIX. DERIVATION OF FIRST DERIVATIVES

The appendix shows the derivation of first derivatives at boundary points in each computational element.

By adopting the quadratic polynomial interpolation function in each computed element, Φ in the interval $[x_i, x_{i+1}]$ can be represented as

$$\Phi(x) = a + bx + cx^2 \tag{A1}$$

Using the two nodal values of Φ at the boundary points in a computed element, namely,

$$\Phi(x = 0) = a = \Phi_i \tag{A2}$$

$$\Phi(x = \Delta x) = a + b\Delta x + c\Delta x^2 = \Phi_{i+1} \tag{A3}$$

and the definition of $\bar{\Phi}_{i+1/2}$, i.e.,

$$\frac{1}{\Delta x}\int_0^{\Delta x}(a + bx + cx^2)\,\mathrm{d}x = \bar{\Phi}_{i+1/2} \tag{A4}$$

the coefficients a, b, and c in Equation (A1) can be specified as follows:

$$a = \Phi_i \tag{A5}$$

$$b = \frac{1}{\Delta x}(-2\Phi_{i+1} - 4\Phi_i + 6\bar{\Phi}_{i+1/2}) \tag{A6}$$

$$c = \frac{1}{\Delta x^2}(3\Phi_{i+1} + 3\Phi_i - 6\bar{\Phi}_{i+1/2}) \tag{A7}$$

where the node x_i is taken as the origin and $\Delta x = x_{i+1} - x_i$. Thus, the first derivatives at the boundary points x_i and x_{i+1} can be expressed as

$$\left.\frac{\partial \Phi}{\partial x}\right|_{x_{i+1}} = \frac{1}{\Delta x}(4\Phi_{i+1} + 2\Phi_i - 6\bar{\Phi}_{i+1/2}) \tag{A8}$$

$$\left.\frac{\partial \Phi}{\partial x}\right|_{x_i} = \frac{1}{\Delta x}(-2\Phi_{i+1} - 4\Phi_i + 6\bar{\Phi}_{i+1/2}) \tag{A9}$$

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