Hybrid Finite-Difference Scheme for Solving the Dispersion Equation

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Abstract: An efficient hybrid finite-difference scheme capable of solving the dispersion equation with general Peclet conditions is proposed. In other words, the scheme can simultaneously deal with pure advection, pure diffusion, and/or dispersion. The proposed scheme linearly combines the Crank–Nicholson second-order central difference scheme and the Crank–Nicholson Galerkin finite-element method with linear basis functions. Using the method of fractional steps, the proposed scheme can be extended straightforwardly from one-dimensional to multidimensional problems without much difficulty. It is found that the proposed scheme produces the best results, in terms of numerical damping and oscillation, among several non-split-operator schemes. In addition, the accuracy of the proposed scheme is comparable with a well-known and accurate split-operator approach in which the Holly–Preissmann scheme is used to solve the pure advection process while the Crank–Nicholson second-order central difference scheme is applied to the pure diffusion process. Since the proposed scheme is a non-split-operator approach, it does not compute the two processes separately. Therefore, it is simpler and more efficient than the split-operator approach.

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Introduction

The dispersion equation is one of the governing equations in solute transport and water quality models in rivers, lakes, and oceans. It involves two types of processes, advection and diffusion. Generally, the numerical schemes available for solving the dispersion equation could be classified into two types: split-operator and non-split-operator approaches. By the split-operator approach, the advection and diffusion processes are separately computed using different numerical schemes, whereas the non-split-operator approach simulates the dispersion equation without separating the two processes.

In the split-operator approach, the diffusion process can be accurately computed by several numerical schemes, such as the Crank–Nicholson central difference scheme and the Crank–Nicholson Galerkin finite-element method. Thus, the accuracy of solving the dispersion equation mainly depends on the computed results of the advection process. Among the procedures for solving the pure advection equation, several accurate monotonic schemes have been proposed, such as the MPL scheme (Van Leer 1977), the MSOU scheme (Roe 1981), the SHARP scheme (Leonard 1988), the SMART scheme (Gaskell and Lau 1988), and the TVD scheme (Wang and Windhopf 1989). In addition, the characteristic-based Holly–Preissmann two-point scheme (Holly and Preissmann 1977) is one of the best in terms of less numerical oscillation and damping in modeling the advection process along a river channel or coastal area. Although the split-operator approach clearly has considerable advantages, it is computationally more intensive and complicated when applied to multidimensional flow problems because the advection and diffusion processes must be handled separately (Li et al. 1992; Chen and Falconer 1994).

The non-split-operator approach offers an alternative to the split-operator approach due to its simplicity and efficiency. To tackle the numerical oscillation problem and to eliminate excessive numerical damping, several nonsplit, high-order upwind-type explicit finite-difference methods have been proposed, such as the QUICKEST scheme (Leonard 1979) and the third-order convection second-order diffusion (TCSD) scheme (Bradley and Missaghi 1988). Some implicit forms of the modified QUICK scheme (Leonard and Noye 1990; Chen and Falconer 1992) and the TCSD scheme (Chen and Falconer 1994) have also been proposed. These schemes, however, could not accurately compute pure advection, pure diffusion, and dispersion simultaneously.

This article proposes a hybrid finite-difference scheme capable of solving the dispersion equation without Peclet number limitations. In other words, the proposed scheme can simultaneously deal with pure advection, pure diffusion, and dispersion. Based on the fact that both the Crank–Nicholson second-order central difference (CNSOCD) scheme and the Crank–Nicholson Galerkin finite-element method with linear basis functions (CNGFEMLF) are excellent for solving the pure diffusion process, the proposed scheme linearly combines the two to solve the dispersion equation. Using the method of fractional steps (Yanenko 1971), the proposed scheme, originally developed for one-dimensional (1D) flow problems, can be extended straightforwardly to multidimensional flow problems without much difficulty. Several numerical

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examples, including (1) pure advection and dispersion in 1D uniform flow; (2) 1D viscous Burgers equation; (3) pure advection and dispersion in two-dimensional (2D) uniform flow; (4) pure advection in 2D rigid-body rotating flow; and (5) three-dimensional (3D) diffusion in a shear flow, are used to examine the capabilities of the proposed scheme.

Development of Proposed Scheme

Consider the transient 1D dispersion equation with constant coefficients as

$$\Phi_t + U\Phi_x = D\Phi_{xx} \tag{1}$$

where the scalar function $\Phi(x,t)$ may represent, for example, temperature or concentration at position x and time t with flow velocity U and diffusion coefficient D. This article proposes a finite-difference scheme to solve Eq. (1) using a linear combination of the CNSOCD scheme and the CNGFEMLF. The comparisons of the two schemes for solving the dispersion equation have been discussed in detail by Gersho and Sani (1998). From the viewpoint of the finite-element method, the only difference between the two schemes is the treatment of the mass term, whether it is lumped or consistent. A brief review of the two schemes will be given prior to the introduction of the proposed finite-difference scheme.

Crank–Nicholson Second-Order Central Difference Scheme

By the Crank–Nicholson second-order central difference (CNSOCD) scheme, the discretized equation of Eq. (1) can be written as

$$\left(-\frac{c}{4}-\frac{s}{2}\right)\Phi_{i-1}^{n+1}+(1+s)\Phi_i^{n+1}+\left(\frac{c}{4}-\frac{s}{2}\right)\Phi_{i+1}^{n+1}-\left(\frac{c}{4}+\frac{s}{2}\right)\Phi_{i-1}^{n}$$
$$-(1-s)\Phi_i^n-\left(-\frac{c}{4}+\frac{s}{2}\right)\Phi_{i+1}^n=0 \tag{2}$$

where $c=U\Delta t/\Delta x$ is the Courant number; $s=D\Delta t/\Delta x^2$ is the diffusion number; $\Delta t=$time step; $\Delta x=$grid size; and $\Phi_i^{n+1}=$the value of Φ at grid point i for time level $t=(n+1)\Delta t$. The modified equation (Warming and Hyett 1974) corresponding to Eq. (2) is

$$\Phi_t+U\Phi_x-\Delta\Phi_{xx}+U\frac{\Delta x^2}{12}(2+c^2)\Phi_{xxx}+O[\Delta x^2]=0. \tag{3}$$

Crank–Nicholson Galerkin Finite-Element Method

The discretized form of Eq. (1) by the Crank–Nicholson Galerkin finite-element method with linear basis functions (CNGFEMLF) can be expressed as

$$\left(\frac{1}{6}-\frac{c}{4}-\frac{s}{2}\right)\Phi_{i-1}^{n+1}\left(\frac{2}{3}+s\right)\Phi_i^{n+1}+\left(\frac{1}{6}+\frac{c}{4}-\frac{s}{2}\right)\Phi_{i+1}^{n+1}$$
$$-\left(\frac{1}{6}+\frac{c}{4}+\frac{s}{2}\right)\Phi_{i-1}^{n}-\left(\frac{2}{3}-s\right)\Phi_i^n$$
$$-\left(\frac{1}{6}-\frac{c}{4}+\frac{s}{2}\right)\Phi_{i+1}^n=0 \tag{4}$$

Similarly, the modified equation corresponding to Eq. (4) can be written as

$$\Phi_t+U\Phi_x-D\Phi_{xx}+U\frac{\Delta x^2}{12}c^2\Phi_{xxx}+O[\Delta x^2]=0 \tag{5}$$

As shown in Eqs. (3) and (5), it is clearly seen that the errors of these two numerical schemes for solving the dispersion equation are dominated by the third-order derivative terms. If the leading truncation error term in the modified equation is an odd derivative, the numerical solution will exhibit dispersive errors. In other words, these two numerical schemes will produce numerical oscillations when the dispersion equation is solved. Thus, a numerical scheme without error term dominated via the third-order derivative would be desirable. This can be simply achieved by a linear combination of the two schemes. In addition, the proposed scheme, as shown later, preserves the capability of solving a pure diffusion process since the coefficients of the third-order derivative in Eqs. (3) and (5) involve the Courant number but not the diffusion number.

A mathematical proof for a general two-level numerical scheme is given in Appendix I to show that the equation resulting from a linear combination of two discretized equations, which are each consistent with the dispersion equation, is still consistent with the dispersion equation. In addition, the relations between the modified equations corresponding to the proposed scheme and any selected two-level numerical schemes are also shown in Appendix I. There, one can observe that the coefficients of not only the first- and second-order spatial derivatives, but also the first-order time derivative in the modified equation corresponding to the proposed scheme, are the sum of those in the two selected numerical schemes. Furthermore, the coefficient of the third-order spatial derivative can be obtained in the same manner under a sufficient condition, i.e., $2a_1+a_2-a_4-2a_5=2c_1+c_2-c_4-2c_5$, where a_1, c_1; a_2, c_2; a_4, c_4; and a_5, c_5 are, respectively, the weights at nodes $i-2$, $i-1$, $i+1$, and $i+2$ for the new time step in the two discretized equations [see Eq. (52) in the Appendix].

Proposed Scheme

Referring to Eqs. (3) and (5), the coefficients of the third-order spatial derivatives are $U\Delta x^2(2+c^2)/12$ and $U\Delta x^2c^2/12$, respectively. Taking the linear combination of Eqs. (2) and (4) as $0.5[\text{Eq. }(4)\times(2+c^2)-\text{Eq. }(2)\times c^2]$ yields a new finite-difference scheme without an error term that is dominated by the third-order derivative. Hence, the discretized equation of the proposed scheme for solving the dispersion equation can be expressed as

$$\left(\frac{1}{6}+\frac{c^2}{12}-\frac{c}{4}-\frac{s}{2}\right)\Phi_{i-1}^{n+1}+\left(\frac{2}{3}-\frac{c^2}{6}+s\right)\Phi_i^{n+1}$$
$$+\left(\frac{1}{6}+\frac{c^2}{12}+\frac{c}{4}-\frac{s}{2}\right)\Phi_{i+1}^{n+1}-\left(\frac{1}{6}+\frac{c^2}{12}+\frac{c}{4}+\frac{s}{2}\right)\Phi_{i-1}^{n}$$
$$-\left(\frac{2}{3}-\frac{c^2}{6}-s\right)\Phi_i^n-\left(\frac{1}{6}+\frac{c^2}{12}-\frac{c}{4}+\frac{s}{2}\right)\Phi_{i+1}^n=0 \tag{6}$$

The corresponding modified equation is

$$\Phi_t+U\Phi_x-D\Phi_{xx}+U\frac{\Delta x^2}{12}(1-2c^2)\Phi_{xxxx}+O(\Delta x^4)=0 \tag{7}$$

The only difference between Eqs. (4) and (6) is the presence of the Courant-number-squared terms in the weights. The effect of these new weights is to eliminate the dominant error term associated with the third-order derivative from Eq. (4) to reduce the

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numerical oscillation in solving the dispersion equation. In addition, the proposed scheme is identical to Eq. (4) when the Courant number is equal to zero. In other words, it preserves the ability to solve a pure diffusion process. One can observe from Eq. (7) that the proposed scheme has fourth-order accuracy for the pure advection process, whereas Eq. (4) only has second-order accuracy.

The proposed scheme can be applied directly to cases of nonconstant U, D, and Δx by adopting the representative velocity, diffusion coefficient, and grid space as follows:

$$U=U_i, \quad D=D_i \tag{8}$$

and

$$\Delta x=\frac{\Delta x_{i-1,i}+\Delta x_{i,i+1}}{2} \tag{9}$$

where $\Delta x_{i-1,i}=x_i-x_{i-1}$; U_i, and D_i represent the velocity and diffusion coefficient of flow field at grid point i, respectively.

Extension to Multidimensional Problems

The above derivation for 1D problems can be extended by the method of fractional steps (Yanenko 1971) to multidimensional problems without much difficulty. The 2D dispersion equation can be written as

$$\Phi_t+U\Phi_x+V\Phi_y=D_x\Phi_{xx}+D_y\Phi_{yy} \tag{10}$$

where U, V, D_x, and D_y represent the velocity and diffusion coefficient in the x and y directions, respectively. Dividing the 2D dispersion process into two successive steps in the x and y directions, respectively, Eq. (10) can be approximated with a series of 1D dispersion equations as

$$\Phi_t+U\Phi_x=D_x\Phi_{xx} \tag{11}$$

and

$$\Phi_t+V\Phi_y=D_y\Phi_{yy} \tag{12}$$

Eqs. (11) and (12) can each be solved by the proposed scheme. The 3D problems can also be formulated and solved in the same manner by adding z-directional dispersion as an additional term.

Stability Analysis

The stability of any numerical scheme must be examined before it can be considered for application. The matrix and von Neumann methods are two commonly used ways for analyzing the stability of any numerical scheme. In this study, the von Neumann stability analysis is applied.

Analysis of Amplification Factor

Suppose that the solution to Eq. (1) can be expressed as a complex Fourier series (Komatsu et al. 1997), that is,

$$\Phi(x,t)=\sum_{m=-\infty}^{\infty} W_m \exp(-j\sigma_m t)\exp(jk_m x) \tag{13}$$

where σ_m, k_m = angular frequency and wave number of an mth wave component, respectively; j = imaginary unit. Because Eq. (1) is linear, each component of Eq. (13), that is,

$$\Phi(x,t)=W\exp(-j\sigma t)\exp(jkx) \tag{14}$$

is also a solution of Eq. (1). Substituting Eq. (14) into (6), one obtains

$$e^{-j\sigma\Delta t}=\frac{Z_1+jZ_2}{\overline{Z}_1+j\overline{Z}_2} \tag{15}$$

where

$$Z_1=(2+\cos k\Delta x)/3-c^2(1-\cos k\Delta x)/6-s(1-\cos k\Delta x)$$

$$\overline{Z}_1=(2+\cos k\Delta x)/3-c^2(1-\cos k\Delta x)/6+s(1-\cos k\Delta x)$$

$$Z_2=(-c^2\sin k\Delta x)/2$$

$$\overline{Z}_2=(c^2\sin k\Delta x)/2$$

Therefore, the amplification factor of the proposed scheme is

$$|e^{-j\sigma\Delta t}|=\sqrt{\frac{Z_1^2+Z_2^2}{\overline{Z}_1^2+\overline{Z}_2^2}} \tag{16}$$

The amplification factor depends on three quantities: Courant number, c; diffusion number, s; and wavelength to the grid size ratio, $L/\Delta x$. One can clearly see from Eqs. (15) and (16) that the amplification factor of the proposed scheme is less than or equal to unity when the Courant number is less than or equal to unity. In other words, it is a conditionally stable scheme when the Courant number is less than or equal to unity. Figs. 1(a and b) compare the amplification factor of the proposed scheme with that of several schemes for the pure advection case with $c=0.8$, and the dispersion case with $c=0.6, s=0.06$, respectively. Fig. 1(a) indicates that the proposed scheme, the Noye scheme (Noye 1990), and the CNGFEMLF have no numerical damping for the pure advection process, whereas the fully time-centered implicit QUICK (FTC-QUICK) scheme and the fully time-centered implicit TCSD (FTC-TCSD) scheme produce large numerical diffusion. In addition, Fig. 1(b) shows that the proposed scheme and the CNGFEMLF scheme have less numerical damping than all other schemes considered to solve the dispersion equation.

Analysis of Phase Error Factor

Substituting the complex angular frequency

$$\sigma=\mathrm{Re}(\sigma)+j\,\mathrm{Im}(\sigma) \tag{17}$$

into Eq. (6) and considering the real parts of both sides, the propagation velocity of the proposed scheme is

$$\frac{\mathrm{Re}(\sigma)}{k}=\frac{1}{k\Delta x}\tan^{-1}\left(\frac{\overline{Z}_2Z_1-\overline{Z}_1Z_2}{\overline{Z}_1Z_1+\overline{Z}_2Z_2}\right) \tag{18}$$

The phase error factor, defined as the ratio of the propagation velocity of the proposed scheme to the real velocity U of the analytical solution, becomes

$$\frac{\mathrm{Re}(\sigma)}{kU}=\frac{1}{2\pi c}\frac{L}{\Delta x}\tan^{-1}\left(\frac{\overline{Z}_2Z_1-\overline{Z}_1Z_2}{\overline{Z}_1Z_1+\overline{Z}_2Z_2}\right) \tag{19}$$

Like the amplification factor, the phase error factor is also dependent on Courant number, diffusion number, and the wavelength to grid size ratio. The phase error factors of some schemes considered for the pure advection equation with $c=0.8$ and the dispersion equation with $c=0.6, s=0.06$ are displayed in Figs. 1(c and d), respectively. One can observe from Figs. 1(c and d) that the phase performance of the proposed scheme is the best among the schemes considered. In addition, the Noye scheme generates leading phase errors, whereas the others have lagging ones.

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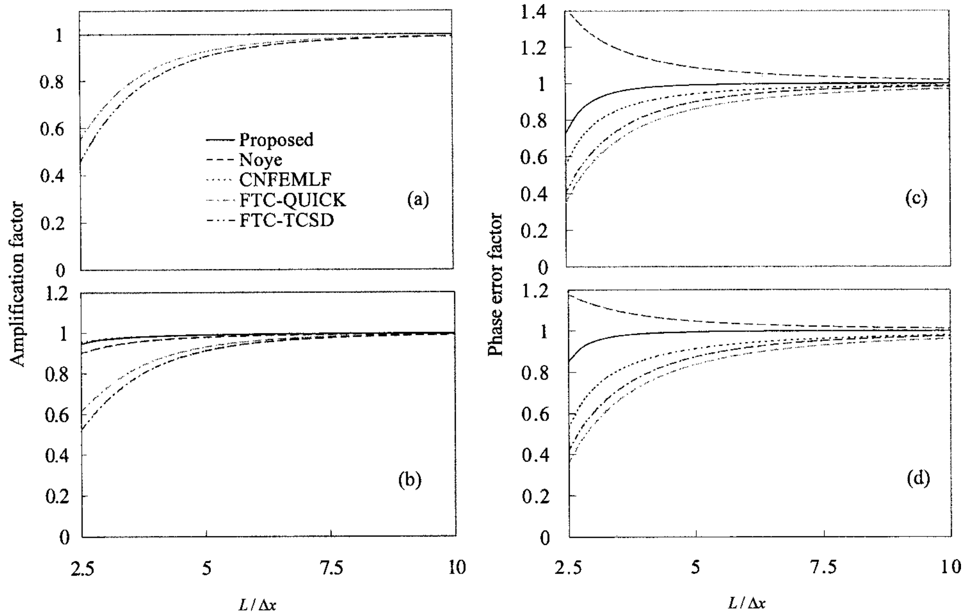

Fig. 1. (a) Amplification factor portraits $c=0.8$; (b) amplification factor portraits $c=0.6$, $s=0.006$; (c) phase error factor portraits $c=0.8$; and (d) phase error portraits $c=0.6$, $s=0.06$

Numerical Results

To investigate the computational performances of the proposed scheme, the dispersion equation in various dimensions is solved and compared with other existing numerical schemes.

One-Dimensional Examples

Pure Advection in Uniform Flow

A Gaussian concentration distribution is advected for 10,000 s with a uniform velocity $U=0.8$ m/s. A grid space of 100 m and time interval of 100 s are used in this example. The domain of simulation is long enough so that the boundary effect can be ignored. The computed results of various numerical schemes and the exact solution are depicted in Fig. 2 and Table 1 in terms of the maximum and minimum values and the rms errors. From Fig. 2 and Table 1, one can observe that the simulated results by the proposed scheme and the Holly–Preissmann scheme are almost identical to the exact solution. On the other hand, the other schemes produce large numerical oscillation. Furthermore, the Noye scheme yields leading phase error as shown in the previous stability analysis. The FTC-TCSD scheme and the FTC-QUICK scheme appear to induce large numerical damping.

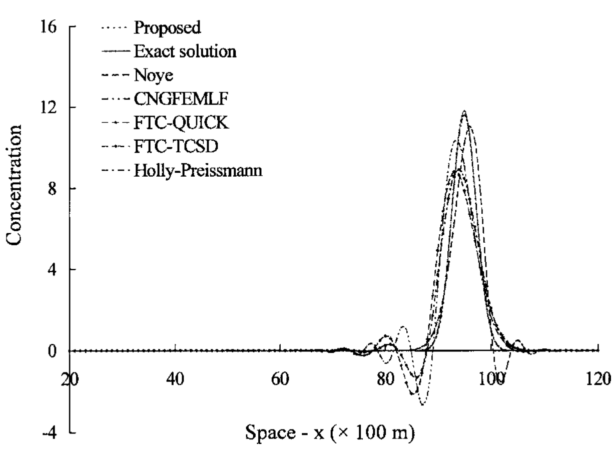

Fig. 2. Comparison of various schemes for 1D pure advection of Gaussian concentration distribution

Dispersion in Uniform Flow

The dispersion of a Gaussian concentration distribution with a velocity $U=0.8$ m/s and a diffusion coefficient $D=0.8$ m^2/s is simulated for 10,000 s with a grid space of 100 m and time interval of 100 s. Fig. 3 and Table 2 show the proposed scheme produces comparable results compared with a split-operator approach in which the Holly–Preissmann scheme is applied to solve the advection process while the CNSOCDC scheme is applied to the diffusion process. The split-operator CNSOCDC approach used has no numerical oscillation, but its numerical diffusion is larger than that of the proposed scheme. In addition, in comparison with the other schemes, the proposed scheme has the best computational results.

Advection or Dispersion with Variable Velocity

For flow fields with variable velocity, two examples are shown. The first is from Morton and Parrott (1980) with the following pure advection equation:

Table 1. Performances of Various Schemes in 1D Pure Advection Test

Scheme	Max.	Min.	rms error
Exact solution	11.81	0.0	0.0
Proposed	11.77	−0.002	0.0046
Holly–Preissmann	11.59	−0.003	0.0056
Noye	11.03	−1.540	0.0961
CNGFEMLF	10.24	−2.666	0.1692
FTC-QUICK	8.78	−2.098	0.1948
FTC-TCSD	8.88	−1.324	0.1374

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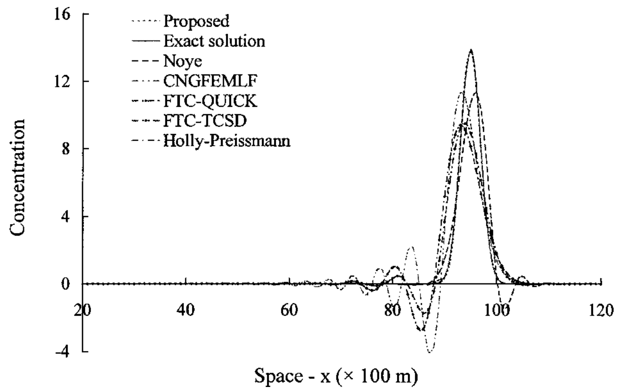

Fig. 3. Comparison of various schemes for 1D dispersion of Gaussian concentration distribution

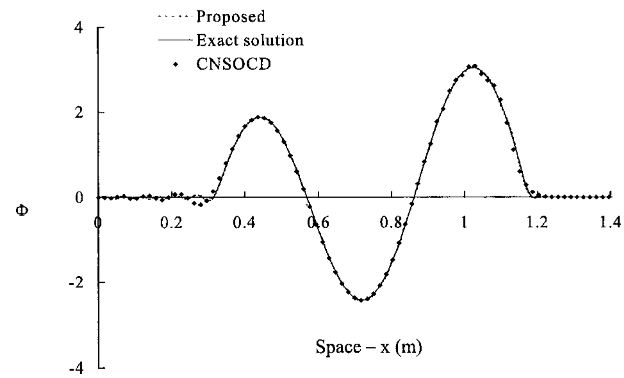

Fig. 4. Computational results of pure advection equation with variation of velocity

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$$\frac{\partial \Phi}{\partial t}+\frac{\partial}{\partial x}\left(\frac{\Phi}{1+2x}\right)=0 \quad x\in[0,\pi] \tag{20}$$

With the following initial and boundary conditions:

$$\Phi(0,t)=0;\quad \Phi(x,0)=(1+2x)\sin 9x,\quad x\in[0,\pi/3];$$
$$\Phi(x,0)=0,\quad x\in[\pi/3,\pi] \tag{21}$$

the exact solution for Eq. (20) can be derived as

$$\Phi(x,t)=(1+2x)\sin 9\{[x^2+x-t+\tfrac{1}{4}]^{1/2}-\tfrac{1}{2}\},$$
$$\text{for}\ \ 0\leqslant x^2+x-t\leqslant[\pi/3(1+\pi/3)]$$
$$\Phi(x,t)=0,\quad \text{for elsewhere} \tag{22}$$

With $\Delta x=\pi/180$ and $\Delta t=0.3\Delta x$, simulation results of 80 time steps from the proposed scheme and the CNSOCD scheme, along with the exact solution, are displayed in Fig. 4. Fig. 4 reveals that, despite of little numerical oscillation, the computed results by the proposed scheme are better than those of the CNSOCD scheme.

A second example considers the viscous Burgers equation

$$\Phi_t+\Phi\Phi_x=D\Phi_{xx} \tag{23}$$

Under the initial and boundary conditions of

$$\Phi(x,0)=1 \quad x\leqslant 0$$
$$\Phi(x,0)=0,\quad x>0 \tag{24}$$
$$\Phi(-\infty,t)=1,\quad \Phi(\infty,t)=0,\quad t>0$$

the exact solution to Eq. (23) is

$$\Phi(x,t)=\left\{1+\exp\left[\frac{1}{2\alpha}\left(x-\frac{1}{2}t\right)\right]\frac{\operatorname{erfc}(-x/2\sqrt{Dt})}{\operatorname{erfc}[(x-t)/2\sqrt{Dt}]}\right\}^{-1} \tag{25}$$

Table 2. Performances of Various Schemes in 1D Dispersion Test

Scheme	Max.	Min.	rms error
Exact solution	13.91	0.0	0.0
Proposed	13.81	−0.057	0.0123
Holly–Preissmann+CNSOCD	13.75	0.0	0.0065
Noye	11.32	−1.401	0.1127
CNGFEMLF	11.31	−3.996	0.2648
FTC-QUICK	9.38	−2.680	0.2490
FTC-TCSD	9.48	−1.755	0.1837

in which erfc represents the complementary error function. After linearization, the Burgers equation can be solved by the proposed scheme and the numerical simulation results at time $t=2$ s are shown in Fig. 5 under $\Delta x=0.01$ m, $\Delta t=0.01$ s, and $D=0.01\ m^2/s$. Fig. 5 shows that the proposed scheme has satisfactory simulation results despite small deviations from the exact solution. It is clearly seen, from the above two numerical examples, that the proposed scheme performs well in flow fields with variable velocity.

Two-Dimensional Examples

Pure Advection in Uniform Flow

A Gaussian concentration distribution with a peak value of 10 and a standard deviation of 220 m is advected for 10,000 s under a constant velocity $U=0.5$ m/s and $V=0.5$ m/s in a two-dimensional infinite domain. The initial central position of this Gaussian distribution is at $(x,y)=(1{,}400\ \text{m},1{,}400\ \text{m})$. A grid size of 100 m×100 m and time step of 100 s are used to conduct the simulation. Figs. 6(a–h) show the bird's-eye view of the computed results from several numerical schemes. Table 3 displays the maximum and minimum values and the rms errors for each scheme used. In addition, the computed concentration profiles by different schemes along the line $y=x$ are shown in Fig. 7. It is observed that the computed results by the proposed scheme [Fig. 6(a)] and the Holly–Preissmann scheme [Fig. 6(g)] almost agree with the exact solution. The Holly–Preissmann scheme has the

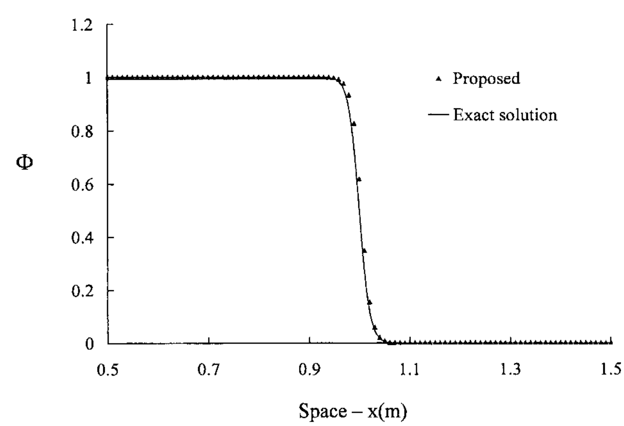

Fig. 5. Computational results of 1D viscous Burgers equation using the proposed scheme

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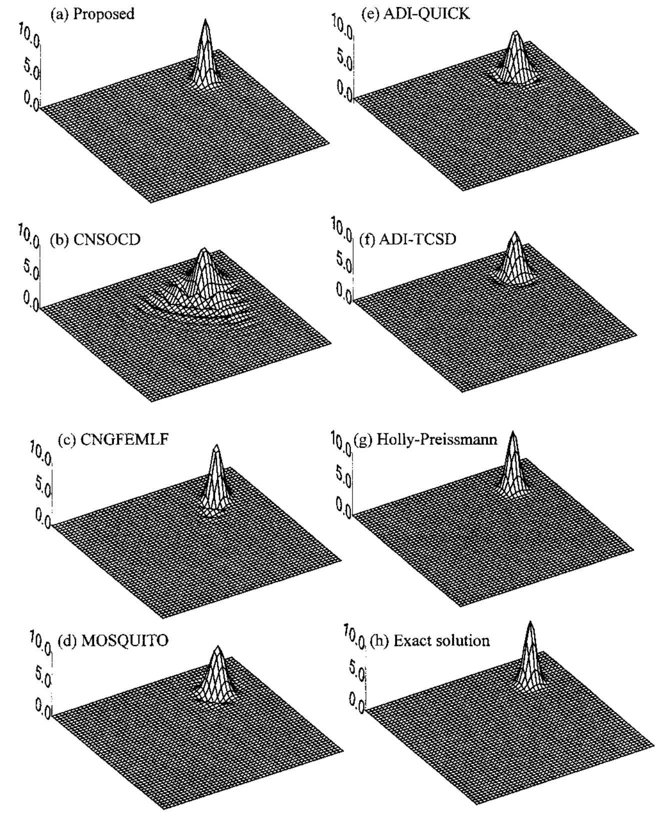

Fig. 6. Comparison of various schemes for 2D pure advection with uniform flow

least numerical oscillation among all the schemes considered, however, its numerical damping is larger than that of the proposed scheme. The CNSOCD scheme [Fig. 6(c)] produces very severe numerical oscillation that rapidly spreads over the modeling domain. The ADI-QUICK scheme (Chen and Falconer 1992) [Fig. 6(e)], the ADI-TCSD scheme (Chen and Falconer 1994) [Fig. 6(f)], and the MOSQUITO scheme [Fig. 6(d)] (Balzano 1999) seem to produce results with large numerical damping. The CNGFEMLF scheme [Fig. 6(b)] has smaller numerical diffusion than those of the ADI-QUICK scheme, the ADI-TCSD scheme, and the MOSQUITO scheme. However, its numerical oscillation is large in comparison with the other three schemes.

Dispersion in Uniform Flow

Consider a 2D nondimensional dispersion equation with uniform flow velocity as

$$\Phi_t+\Phi_x+\Phi_x=D(\Phi_{xx}+\Phi_{yy}) \tag{26}$$

Table 3. Performances of Various Schemes in 2D Pure Advection Test

Scheme	Max.	Min.	rms error
Exact solution	10.00	0.0	0.0
Proposed	9.87	−0.010	0.0017
Holly–Preissmann	9.60	−0.008	0.0017
CNSOCD	5.94	−2.517	0.1000
CNGFEMLF	9.05	−1.719	0.0195
MOSQUITO	6.62	−0.959	0.0261
ADI-QUICK	6.96	−0.957	0.0278
ADI-TCSD	6.81	−0.431	0.0173

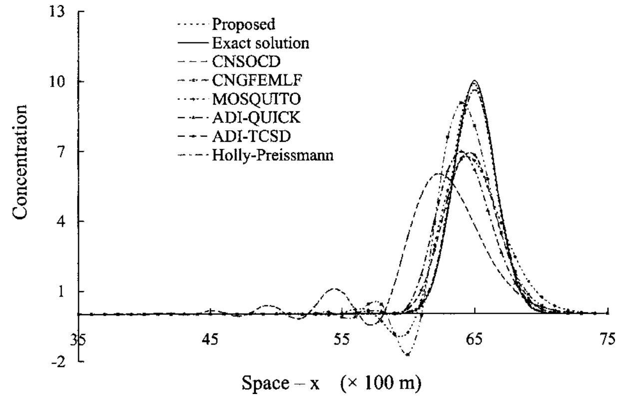

Fig. 7. Comparison of various schemes for 2D pure advection with uniform flow (along line $y=x$)

where D = inverse of the Reynolds number. Under the initial condition

$$\Phi(x,y,0)=\sin(\pi x)+\sin(\pi y). \tag{27}$$

and the boundary conditions

$$\begin{aligned}\Phi(0,y,t)&=[\sin(-\pi t)+\sin\pi(y-t)]\exp(-D\pi^2 t)\\ \Phi(1,y,t)&=[\sin(1-t)+\sin\pi(y-t)]\exp(-D\pi^2 t)\\ \Phi(x,0,t)&=[\sin(x-t)+\sin(-\pi t)]\exp(-D\pi^2 t)\\ \Phi(x,1,t)&=[\sin(x-t)+\sin\pi(1-t)]\exp(-D\pi^2 t)\end{aligned} \tag{28}$$

the exact solution to Eq. (26) is

$$\Phi(x,y,t)=[\sin\pi(x-t)+\sin\pi(y-t)]\exp(-D\pi^2 t) \tag{29}$$

Numerical results by the proposed scheme and a split-operator approach are shown in Figs. 8(a and b) at $t=2$ and $t=3$ along the line $y=x$ with $D=0.0002$, a uniform grid size of 0.02×0.02, and time step of 0.01. In the split-operator approach, the Holly–Preissmann scheme and the Crank–Nicholson second-order central difference scheme are used to solve the advection and the diffusion processes, respectively. Figs. 8(a and b) demonstrate that the simulated results by the proposed scheme and the split-operator approach are almost identical to the exact solution. It must be noticed that the use of the proposed scheme to the 2D dispersion equation is straightforward by adopting the method of fractional steps. However, the application of a split-operator approach is more expensive and complicated since the advection and diffusion processes are computed separately. Furthermore, the additional equations of spatial derivative must be computed in the Holly–Preissmann scheme for solving the dispersion equation.

Pure Advection in Rigid-Body Rotating Flow

A pure advection of a Gaussian concentration distribution with a rigid-body rotating flow in a two-dimensional infinite domain is considered. This problem has a flow field of variable velocity. The maximum value and the standard deviation of this Gaussian concentration distribution are unity and 250 m, respectively. The rigid body spends 20,000 s rotating one turn. A grid size of 100 m×100 m and time step of 50 s are used in numerical simulation. After one rotation, the maximum and minimum values of the computational results by the proposed scheme are 0.986 and −0.012, respectively. This numerical example shows that the proposed scheme also has good capability to accurately solve the two-dimensional problem with variable velocity.

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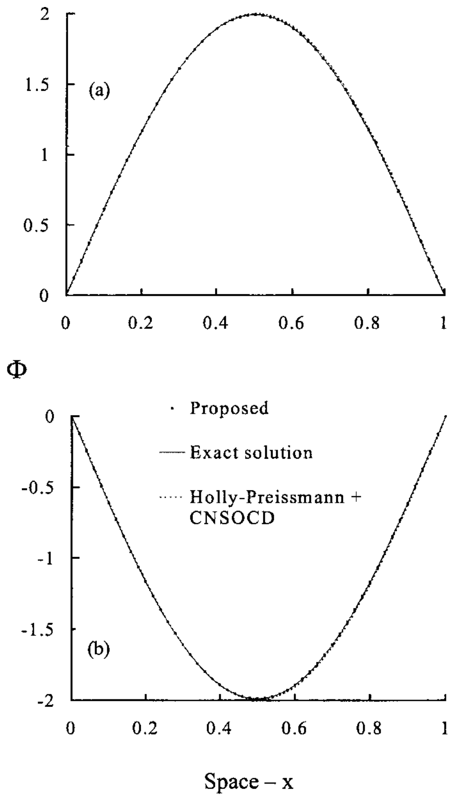

Fig. 8. Computational results of 2D dispersion equation (along line $y=x$): (a) $t=2$ and (b) $t=3$

Three-Dimensional Example

Three-Dimensional Diffusion in A Shear Flow

To investigate the capability of the proposed scheme for solving three-dimensional problems, diffusion in a shear flow is considered. The velocity shear in the diffusion of a patch of passive contaminant from an instantaneous source plays an important role in groundwater flow or natural streams such as ocean, lake, and estuaries. The governing equation for shear diffusion can be expressed as

$$\Phi_t+(V_0+\Omega_y y+\Omega_z z)\Phi_x=D_x\Phi_{xx}+D_y\Phi_{yy}+D_z\Phi_{zz} \quad (30)$$

where V_0 = mean velocity in the x direction; Ω_y and Ω_z = horizontal and vertical shear, respectively; and D_x, D_y, and D_z = eddy diffusivities in 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 (1965) as

$$\Phi(x,y,z,t)=\frac{M}{8\pi^{3/2}(D_xD_yD_z)^{1/2}t^{3/2}(1+\beta^2t^2)^{1/2}}\exp\left\{-\left[\frac{(x-V_0t-0.5(\Omega_y y+\Omega_z z)t)^2}{4D_xt(1+\beta^2t^2)}+\frac{y^2}{4D_yt}+\frac{z^2}{4D_zt}\right]\right\} \quad (31)$$

where

$$\beta^2=\frac{\lfloor(\Omega_y^2D_y/D_x)+(\Omega_z^2D_z/D_x)\rfloor}{12} \quad (32)$$

Allowing numerical solution having an initial peak concentration of unity, simulation begins at time $t=t_0$ having the point source of mass M as

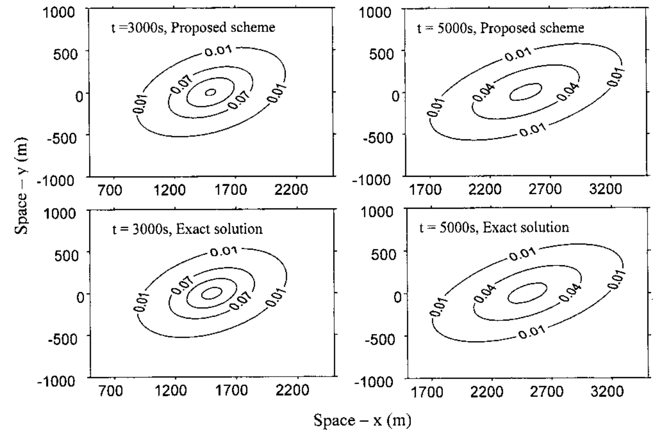

Fig. 9. Comparison of contour plots of diffusion in shear flow on plane $z=0$ at $t=3000$ and 5000 s

$$M=8\pi^{3/2}(D_xD_yD_z)^{1/2}t^{3/2}(1+\beta^2t_0{}^2)^{1/2} \quad (33)$$

In the numerical simulation the following parameters are used: $t_0=1000$ s, $V_0=0.5$ m/s, $\Omega_y=\Omega_z=0.0003$ 1/s, $D_x=D_y=D_z=5.0$ m^2/s, $\Delta t=100$ s, and grid space $\Delta x=\Delta y=\Delta z=100$ m. Fig. 9 shows the contour plots of the proposed scheme and the analytical solution at $t=3{,}000$ and 5,000 s on the plane $z=0$, respectively. The proposed scheme yields the results that are almost in excellent agreement with the exact solution.

Conclusions

In this article, a hybrid finite-difference scheme capable of solving pure advection, pure diffusion, and dispersion processes is proposed. The proposed scheme combines two well-known schemes, namely, the Crank–Nicholson second-order central difference scheme and the Crank–Nicholson Galerkin finite-element method with linear basis functions. The consistency and stability of the proposed scheme are investigated. In addition, the relations between the modified equations corresponding to the proposed scheme and the two selected schemes are obtained. Employing the method of fractional steps, the proposed scheme that was originally developed for one-dimensional problems can be applied straightforwardly to multidimensional ones without much difficulty. The proposed scheme has the best performance in several examples among some non-split-operator schemes. In addition, the proposed scheme yields comparable results in comparison with a well-known and accurate split-operator approach in which the Holly–Preissmann scheme and the Crank–Nicholson second-order central difference scheme were used to solve advection and diffusion processes, respectively. The proposed scheme is a non-split-operator approach and, therefore, it has the advantage of being simpler and more efficient than the split-operator approach.

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Appendix: Consistency and Modified Equation

Consistency

Applying any two-level numerical schemes to Eq. (1), one may obtain the following discretization equations:

$$a_1\Phi_{i-2}^{n+1}+a_2\Phi_{i-1}^{n+1}+a_3\Phi_{i}^{n+1}+a_4\Phi_{i+1}^{n+1}+a_5\Phi_{i+2}^{n+1}$$
$$=b_1\Phi_{i-2}^{n}+b_2\Phi_{i-1}^{n}+b_3\Phi_{i}^{n}+b_4\Phi_{i+1}^{n}+b_5\Phi_{i+2}^{n} \quad (34)$$

and

$$c_1\Phi_{i-2}^{n+1}+c_2\Phi_{i-1}^{n+1}+c_3\Phi_{i}^{n+1}+c_4\Phi_{i+1}^{n+1}+c_5\Phi_{i+2}^{n+1}$$
$$=d_1\Phi_{i-2}^{n}+d_2\Phi_{i-1}^{n}+d_3\Phi_{i}^{n}+d_4\Phi_{i+1}^{n}+d_5\Phi_{i+2}^{n} \quad (35)$$

where $a_1+a_2+a_3+a_4+a_5=c_1+c_2+c_3+c_4+c_5=1$. The Φ_i^{n+1} represents the value of Φ at grid point i for time level $t=(n+1)\Delta t$ and Δt is the time step. The terms Φ_{i+1}^{n+1}, Φ_{i}^{n+1}, Φ_{i-1}^{n+1}, Φ_{i+1}^{n}, and Φ_{i-1}^{n} can be expanded in Taylor series as

$$\Phi_{i+j_1}^{n+k_1}=\sum_{m=0}^{\infty}\frac{1}{m!}\left(k_1\Delta t\frac{\partial}{\partial t}+j_1\Delta x\frac{\partial}{\partial x}\right)^m\Phi_i^n \quad k_1,j_1=-1,0,1 \quad (36)$$

where $\Delta x=$ grid size. Substitution of Eq. (36) into Eqs. (34) and (35) yields

$$\Phi_t=A_1\Phi_x+A_2\Phi_{tt}+A_3\Phi_{tx}+A_4\Phi_{xx}+A_5\Phi_{ttt}+A_6\Phi_{ttx}+A_7\Phi_{txx}$$
$$+A_8\Phi_{xxx}+\cdots \quad (37)$$

and

$$\Phi_t=B_1\Phi_x+B_2\Phi_{tt}+B_3\Phi_{tx}+B_4\Phi_{xx}+B_5\Phi_{ttt}+B_6\Phi_{txx}+B_7\Phi_{txx}$$
$$+B_8\Phi_{xxx}+\cdots \quad (38)$$

where the superscript n and the subscript i for Φ are eliminated. The terms $A_1\sim A_8$ and $B_1\sim B_8$ are functions of a_1-a_5, b_1-b_5 and c_1-c_5, d_1-d_5, respectively. For example, A_2 and A_3 can be expressed as

$$A_2=\frac{-\Delta t}{2}(a_1+a_3+a_4+a_5)=\frac{-\Delta t}{2} \quad (39)$$

$$A_3=\Delta x(2a_1+a_2-a_4-2a_5) \quad (40)$$

As far as the accuracy is concerned, both A_1 and B_1 are equal to $-U$. In addition, because of the consistency, the terms $A_2\sim A_8$ and $B_2\sim B_8$, except A_4 and B_4, are all equal to zeros when Δt and Δx approach zero. However, A_4 and B_4 satisfy the following condition:

$$A_4=B_4=D \quad (41)$$

where $D=$ diffusion coefficient. Now, taking the linear combination of Eqs. (34) and (35) as α [Eq. (34)]+β [Eq. (35)], one obtains

$$(\alpha a_1+\beta c_1)\Phi_{i-2}^{n+1}+(\alpha a_2+\beta c_2)\Phi_{i-1}^{n+1}+(\alpha a_3+\beta c_3)\Phi_{i}^{n+1}$$
$$+(\alpha a_4+\beta c_4)\Phi_{i+1}^{n+1}+(\alpha a_5+\beta c_5)\Phi_{i+2}^{n+1}$$
$$=(\alpha b_1+\beta d_1)\Phi_{i-2}^{n}+(\alpha b_2+\beta d_2)\Phi_{i-1}^{n}+(\alpha b_3+\beta d_3)\Phi_{i}^{n}$$
$$+(\alpha b_4+\beta d_4)\Phi_{i+1}^{n}+(\alpha b_5+\beta d_5)\Phi_{i+2}^{n} \quad (42)$$

where α and β are constants. Similarly, substitution of Taylor series expansion (36) into Eq. (42) yields

$$\Phi_t=-U\Phi_x+\frac{1}{\alpha+\beta}[(\alpha A_2+\beta B_2)\Phi_{tt}+(\alpha A_3+\beta B_3)\Phi_{tx}$$
$$+(\alpha A_4+\beta B_4)\Phi_{xx}+(\alpha A_5+\beta B_5)\Phi_{ttt}(\alpha A_6+\beta B_6)\Phi_{ttx}$$
$$+(\alpha A_7+\beta B_7)\Phi_{txx}+(\alpha A_8+\beta B_8)\Phi_{xxx}]+\cdots \quad (43)$$

One can clearly see from Eq. (43) that Eq. (42) is also consistent with the dispersion equation (1).

Modified Equation

By eliminating pure and cross time derivatives with repeatedly differentiating Eqs. (37) and (38), the modified equation corresponding to Eqs. (37) and (38) can, respectively, be expressed as

$$\Phi_t=-U\Phi_x+E_2\Phi_{xx}+E_3\Phi_{xxx}+\cdots \quad (44)$$

and

$$\Phi_t=-U\Phi_x+F_2\Phi_{xx}+F_3\Phi_{xxx}+\cdots \quad (45)$$

where

$$E_2=U^2A_2-UA_3+A_4$$
$$E_3=-2U^3A_2^2+3U^2A_2A_3-2UA_2A_4-UA_3^2+A_3A_4-U^3A_5$$
$$+U^2A_6-UA_7+A_8 \quad (46)$$

and

$$F_2=U^2B_2-UB_3+B_4$$
$$F_3=-2U^3B_2^2+3U^2B_2B_3-2UB_2B_4-UB_3^2$$
$$+B_3B_4-U^3B_5+U^2B_6-UB_7+B_8 \quad (47)$$

Similarly, the modified equation corresponding to Eq. (43) is

$$\Phi_t=-U\Phi_x+\frac{G_2}{\alpha+\beta}\Phi_{xx}+\frac{G_3}{\alpha+\beta}\Phi_{xxx}+\cdots \quad (48)$$

where

$$G_2=U^2(\alpha A_2+\beta B_2)-U(\alpha A_3+\beta B_3)+(\alpha A_4+\beta B_4)$$
$$G_3=\frac{1}{\alpha+\beta}[-2U^3(\alpha A_2+\beta B_2)^2+3U^2(\alpha A_2+\beta B_2)$$
$$\times(\alpha A_3+\beta B_3)-2U(\alpha A_2+\beta B_2)(\alpha A_4+\beta B_4)$$
$$-U(\alpha A_3+\beta B_3)^2+(\alpha A_3+\beta B_3)(\alpha A_4+\beta B_4)]$$
$$-U^3(\alpha A_5+\beta B_5)+U^2(\alpha A_6+\beta B_6)$$
$$-U(\alpha A_7+\beta B_7)+(\alpha A_8+\beta B_8) \quad (49)$$

It is obvious that G_2, E_2, and F_2 satisfy

$$G_2=\alpha E_2+\beta F_2 \quad (50)$$

In addition, if A_2, B_2, A_3, and B_3 satisfy the following conditions:

$$A_2=B_2 \quad (51)$$

and

$$A_3=B_3 \quad (52)$$

one can obtain

$$G_3=\alpha E_3+\beta F_3 \quad (53)$$

In other words, Eq. (48) can be rewritten as

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$$(\alpha+\beta)\Phi_t = -U(\alpha+\beta)\Phi_x + (\alpha E_2 + \beta F_2)\Phi_{xx} + (\alpha E_3 + \beta F_3)\Phi_{xxx} + \cdots \quad (54)$$

It is necessary to point out that condition (51) is always satisfied due to Eq. (39). Eq. (52) is a sufficient condition for Eq. (53). Although the above derivation is only up to the third-order derivative, the higher-order derivative can also be executed in the same manner.

Notation

The following symbols are used in this paper:

$a_1 - a_3, b_1 - b_3, c_1 - c_3, d_1 - d_3$ = coefficients of discretized equation;
$A_1 - A_8, B_1 - B_8, E_1 - E_8, F_1 - F_8$ = function of $a_1 - a_3, b_1 - b_3, c_1 - c_3, d_1 - d_3$;
c = Courant number;
D, D_x, D_y, D_z = diffusion coefficient or the inverse of Reynolds number;
$G_2 G_3$ = function of $A_1 - A_8, B_1 - B_8$;
j = an imaginary unit;
k = wave number;
L = wavelength;
M = mass of concentration;
s = diffusion number;
U, V = velocity component;
W = amplitude of wave;
$Z_1, Z_2, \overline{Z}_1, \overline{Z}_2$ = function of c, s, k, and Δx;
α, β = constant;
Δt = time increment;
Δx = computational grid interval;
Φ = temperature or concentration; and
Ω_y, Ω_z = horizontal and vertical shears.

Subscripts

i = x-directional computational point index; and
m = index of an mth wave component.

Superscripts

n = time step index.

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