

# Fractional Steps Scheme of Finite Analytic Method for Advection–Diffusion Equation

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**Abstract:** For simply finding local analytic solution, the time derivative in the traditional finite analytic (FA) method is generally replaced with a first-order finite difference approximation as a source term. However, this may induce excessive numerical diffusion, especially for advection-dominated transport problems. In this paper, a fractional steps scheme of the FA method without using the finite difference approximation to time derivative is proposed by applying the one-dimensional FA method whose local analytic solution is obtained from both spatial and time domains, together with the method of fractional steps. Four hypothetical examples, including two-dimensional and three-dimensional cases, are employed to investigate this newly proposed method as compared with the traditional FA method, the optimal unsteady FA method, and the alternating direction scheme of the hybrid FA method. The results show that the fractional steps scheme of the FA method can greatly diminish numerical diffusion and is superior to the other methods compared herein.

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## Introduction

The finite analytic (FA) method, unlike the finite difference method which applies the Taylor series expansion formulation or the finite element method which uses the interpolation function and weighting function, was first proposed by Chen et al. (1981) and has been applied to many fields. Chen and Chen (1984), Chen et al. (1987), Aksoy and Chen (1992), and Chen et al. (1995), for example, used the FA method to compute Navier–Stokes equations. The FA method was also employed not only to the suspended sediment transport in river channel by Fang and Wang (2000) but also to the solute transport in two-dimensional (2D) groundwater flow by Hwang et al. (1985), Tsai et al. (1995), and Tsai et al. (2000).

The FA method is based on finding an analytic solution to a linear or linearized differential equation on a small subdomain of problem domain. For the one-dimensional (1D) case, two types of local analytic solutions could be found. With specifying proper initial and boundary conditions in a subdomain and applying the method of separation of variables, the first type of the local analytic solution is obtained by solving a partial differential equation. The second one is given by replacing the time derivative with a first-order finite difference approximation as a source term for

solving an ordinary differential equation. The major difference between these two types of local analytic solutions is that the former is found from both spatial and time domains, but the latter, namely the hybrid FA method, is only derived from spatial domain. However, for 2D and three-dimensional (3D) cases, only hybrid formulation could be applied to the FA method due to the difficulty in finding local analytic solution from both spatial and time domains.

In the FA method, the use of the first-order finite difference approximation to time derivative may deteriorate the computational results, especially for the large Péclet number. To tackle this problem, Tsai and Chen (1995) proposed an optimal unsteady FA method that introduced an optimal time-weighting factor to improve the approximation for the time derivative in the traditional FA method. The optimal time-weighting factor is obtained from the analytic solution of 1D linear advection and diffusion of a sharp front concentration following a uniform flow velocity and a constant diffusion coefficient in an infinite domain. However, with the use of the optimal time-weighting factor, the simulating cost may increase, especially for 3D problems, due to the need for a predictor–corrector computational procedure. Alternatively, based on the use of the 1D hybrid FA method (only the local spatial analytic solution is found) and applying the alternating direction implicit method (Peaceman and Rachford 1955) to increase the accuracy of the approximation for time derivative, there is another kind of FA method, namely the alternating direction scheme of the hybrid FA method (Lu et al. 1990; Lu and Shi 1990; Lu and Chen 1992; and Yang and Li 1992). In addition, in order to obviate the use of the finite difference approximation to the time derivative, Li et al. (1992) applied the Laplace transform technique to deal with the time derivative and obtained satisfactory results for the 1D solute transport equation. However, the application of the Laplace transformation is limited to linear differential equations and transposable boundary conditions. Moreover, calculation of the corresponding inverse Laplace transformation may be difficult, especially for multidimensional problems.

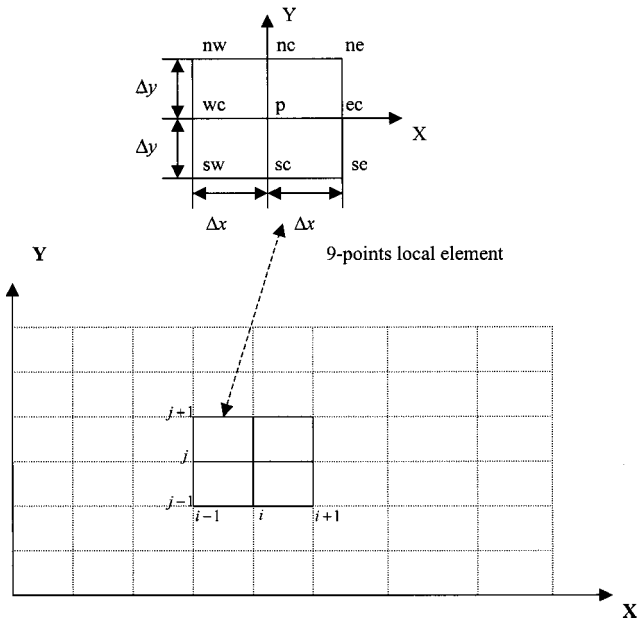
In this paper, a fractional steps scheme of the FA method with-

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**Fig. 1.** Nine-points local element for two-dimensional finite analytic method

out using finite difference approximation to time derivative is proposed to solve the multidimensional advection–diffusion equation by applying the method of fractional steps (Yanenko 1971; Tsai et al. 2001; Tsai et al. 2002), together with 1D FA method whose local analytic solution is found from both spatial and time domains. In order to examine this new type of FA method, four hypothetical examples, including 2D and 3D cases, are considered. Comparisons of simulated results by the traditional FA method, the optimal unsteady FA method, the alternating direction scheme of the hybrid FA method, and the present scheme are conducted.

### Brief Reviews of Former Finite Analytic Methods

#### Optimal Unsteady Finite Analytic Method

The 2D advection–diffusion equation can be written as

$$\frac{\partial \Phi}{\partial t} + u \frac{\partial \Phi}{\partial x} + v \frac{\partial \Phi}{\partial y} = \varepsilon_x \frac{\partial^2 \Phi}{\partial x^2} + \varepsilon_y \frac{\partial^2 \Phi}{\partial y^2} \quad (1)$$

where  $\Phi$ =concentration of contaminant or temperature;  $x$  and  $y$ =spatial coordinates;  $t$ =time;  $u$  and  $v$ =velocity components of flow in  $x$  and  $y$  directions, respectively; and  $\varepsilon_x$  and  $\varepsilon_y$ =diffusion coefficients. In Eq. (1),  $u$ ,  $v$ ,  $\varepsilon_x$ , and  $\varepsilon_y$  may be given as functions of  $x, y$ , and  $t$ .

In the FA method, the solution domain is subdivided into small element of  $2\Delta x$  by  $2\Delta y$  as shown in Fig. 1.  $\Delta x$  and  $\Delta y$  are grid sizes in  $x$  and  $y$  directions, respectively. Eq. (1) for each local element can be linearized and evaluated at time step  $n$  as

$$\frac{1}{(\varepsilon_x)_{i,j}^n} \left( \frac{\partial \Phi}{\partial t} \right)_{i,j}^n + 2A \frac{\partial \Phi^n}{\partial x} + 2BC \frac{\partial \Phi^n}{\partial y} = \frac{\partial^2 \Phi^n}{\partial x^2} + C \frac{\partial^2 \Phi^n}{\partial y^2} \quad (2)$$

where  $A=(u)_{i,j}^n/(2\varepsilon_x)_{i,j}^n$ ;  $B=(v)_{i,j}^n/(2\varepsilon_y)_{i,j}^n$ ; and  $C=(\varepsilon_x)_{i,j}^n/(\varepsilon_y)_{i,j}^n$ . The superscript  $n$  represents values evaluated at the  $(n)$ th time step. The subscript  $(i, j)$  represents values evaluated at the central node of rectangular local element as shown in Fig. 1.

The ease in finding an analytic solution to Eq. (2) is greatly increased greatly by replacing the time derivative with a finite difference approximation as

$$\left( \frac{\partial \Phi}{\partial t} \right)_{i,j}^n = \frac{1}{1-\omega} \left[ \frac{\Phi_{i,j}^n - \Phi_{i,j}^{n-1}}{\Delta t} - \omega \left( \frac{\partial \Phi}{\partial t} \right)_{i,j}^{n-1} \right] \quad (3)$$

where  $\omega$ =time-weighting factor and  $\Delta t$ =time step. In the traditional FA method, the time-weighting factor is equal to zero ( $\omega=0$ ), that is, a first-order finite difference approximation for time derivative. The optimal unsteady FA method (Tsai and Chen 1995) was presented with the introduction of an optimal time-weighting factor as

$$\omega = 0.5 \left[ \frac{\left( \frac{\partial \Phi}{\partial t} \right)_{i,j}^{n-1}}{\frac{\Phi_{i,j}^n - \Phi_{i,j}^{n-1}}{\Delta t}} \right]^{-0.28} \quad (4)$$

Substituting Eq. (3) into Eq. (2) and specifying four boundary conditions for a local element as shown in Fig. 1, an analytic solution to Eq. (2) could be found in each local element using the method of separation of variables. When this local analytic solution is evaluated at the central node  $(i, j)$  of the local element, an algebraic equation relating the evaluated nodal value to its eight neighboring nodal values and central nodal value at previous time step could be expressed as

$$\left[ 1 + \frac{a_p}{(1-\omega)\Delta t(\varepsilon_x)_{i,j}^n} \right] \Phi_{i,j}^n = a_{NW}\Phi_{i-1,j+1}^n + a_{SE}\Phi_{i+1,j-1}^n + a_{SW}\Phi_{i-1,j-1}^n + a_{WC}\Phi_{i-1,j}^n + a_{EC}\Phi_{i+1,j}^n + a_{NC}\Phi_{i,j+1}^n + a_{SC}\Phi_{i,j-1}^n + a_{NE}\Phi_{i+1,j+1}^n + \frac{a_{i,j}}{\Delta t(1-\omega)(\varepsilon_x)_{i,j}^n} \Phi_{i,j}^{n-1} + \frac{\omega}{(1-\omega)(\varepsilon_x)_{i,j}^n} \left( \frac{\partial \Phi}{\partial t} \right)_{i,j}^{n-1} \quad (5)$$

where the FA coefficients  $a_p, a_{NW}, \dots, a_{NE}$  could be obtained by Chen and Chen (1984) and Hwang et al. (1985). Eq. (5) could be applied for each unknown nodal point to construct a set of algebraic equations.

#### Alternating Direction Scheme of Hybrid Finite Analytic Method

The component of Eq. (1) in the  $x$  direction can be written as

$$\frac{\partial \Phi}{\partial t} + u \frac{\partial \Phi}{\partial x} = \varepsilon_x \frac{\partial^2 \Phi}{\partial x^2} \quad (6)$$

Like the traditional FA method as mentioned above, with the application of the first-order finite difference approximation to time derivative, Eq. (6) for a small element on both spatial and time domains as shown in Fig. 2 can be linearized and evaluated at time step  $n$  as

$$\frac{\partial^2 \Phi^n}{\partial x^2} = 2A_1 \frac{\partial \Phi^n}{\partial x} + s \quad (7)$$

where  $A_1=(u)_i^n/(2\varepsilon_x)_i^n$ , and  $s=(\Phi_i^n - \Phi_i^{n-1})/(\varepsilon_x)_i^n \Delta t$ .

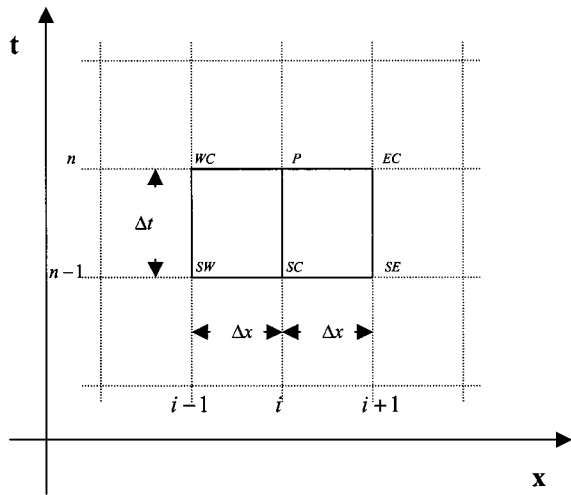


Fig. 2. Local element in one-dimensional finite analytic method

Eq. (7) is a linear ordinary differential equation that could be easily solved. With the local analytic solution, the FA algebraic equation at central point  $i$  in a local element as shown in Fig. 2 could be expressed as

$$\frac{\Phi_i^n - \Phi_i^{n-1}}{\Delta t} = \frac{(u)_i^n}{2\Delta x \sinh(A_1 \Delta x)} (e^{A_1 \Delta x} \Phi_{i-1}^n - 2 \cosh(A_1 \Delta x) \Phi_i^n + e^{-A_1 \Delta x} \Phi_{i+1}^n) \quad (8)$$

Eq. (8) is the so-called 1D hybrid FA method whose local analytic solution is only found from spatial domain as shown in Eq. (7).

Applying the idea of the alternating direction implicit method (Peaceman and Rachford 1955) together with the 1D hybrid FA method as shown in Eq. (8), an alternating direction scheme of the hybrid FA method has been proposed to solve the 2D advection–diffusion equation as follows:

$$\frac{\Phi_{i,j}^{n-1/2} - \Phi_{i,j}^{n-1}}{\Delta t/2} = L_x \Phi_{i,j}^{n-1/2} + L_y \Phi_{i,j}^n \quad (9)$$

$$\frac{\Phi_{i,j}^n - \Phi_{i,j}^{n-1/2}}{\Delta t/2} = L_x \Phi_{i,j}^{n-1/2} + L_y \Phi_{i,j}^n \quad (10)$$

in which

$$L_x \Phi_{i,j} = \frac{(u)_{i,j}^n}{2\Delta x \sinh(A_1^* \Delta x)} (e^{A_1^* \Delta x} \Phi_{i-1,j}^n - 2 \cosh(A_1^* \Delta x) \Phi_{i,j}^n + e^{-A_1^* \Delta x} \Phi_{i+1,j}^n) \quad (11)$$

$$L_y \Phi_{i,j} = \frac{(v)_{i,j}^n}{2\Delta y \sinh(B_1^* \Delta y)} (e^{B_1^* \Delta y} \Phi_{i,j-1}^n - 2 \cosh(B_1^* \Delta y) \Phi_{i,j}^n + e^{-B_1^* \Delta y} \Phi_{i,j+1}^n) \quad (12)$$

where  $A_1^* = (u)_{i,j}^n / (2\varepsilon_x)_{i,j}^n$ ; and  $B_1^* = (v)_{i,j}^n / (2\varepsilon_y)_{i,j}^n$ .

### Fractional Steps Scheme of Finite Analytic Method

The traditional FA method, the optimal unsteady FA method, and the alternating direction scheme of the hybrid FA method, as mentioned above, are all developed based on the use of the finite difference approximation to time derivative. However, in the dif-

ferent types of FA methods, only 1D FA method (not including the 1D hybrid FA method) does not need the use of the finite difference approximation to time derivative, and then obtains the local analytic solution from both time and spatial domains (Chen and Chen 1982). The 1D FA method could be straightforwardly applied to solve multidimensional problems in conjunction with the method of fractional steps (Yanenko 1971; Tsai et al. 2001, 2002)

Using the method of fractional steps, the 2D advection–diffusion equation as shown in Eq. (1) can be decoupled into a series of 1D advection–diffusion equations as

$$\frac{\partial \Phi}{\partial t} + u \frac{\partial \Phi}{\partial x} = \varepsilon_x \frac{\partial^2 \Phi}{\partial x^2} \quad (13)$$

and

$$\frac{\partial \Phi}{\partial t} + v \frac{\partial \Phi}{\partial y} = \varepsilon_y \frac{\partial^2 \Phi}{\partial y^2} \quad (14)$$

By approximating the flow velocity and diffusion coefficient as a constant over a small element as shown in Fig. 2, the linearized 1D advection–diffusion equation as shown in Eq. (13) can be expressed as

$$B_2 \frac{\partial \Phi}{\partial t} + 2A_2 \frac{\partial \Phi}{\partial x} = \frac{\partial^2 \Phi}{\partial x^2} \quad (15)$$

where  $A_2 = (u)_i^n / (2\varepsilon_x)_i^n$  and  $B_2 = 1 / (\varepsilon_x)_i^n$ .

Eq. (15) can be solved analytically in a small element by the method of separation of variables with the initial and boundary conditions are specified as

$$\Phi(x, 0) = a_x (e^{2A_2 x} - 1) + b_x x + c_x \quad (16)$$

$$\Phi(-\Delta x, t) = a_w + b_w t \quad (17)$$

$$\Phi(\Delta x, t) = a_E + b_E t \quad (18)$$

where the node  $i$  is taken as the origin. The coefficients in Eqs. (16)–(18) could be found in terms of the nodal values at the element boundaries as shown in Fig. 2

Evaluating the analytic solution for nodal point  $i$  an algebraic equation giving the nodal value  $\Phi_i^n$  as a function of its five neighboring nodal values shown in Fig. 2 can be expressed as

$$\Phi_i^n = b_{WC} \Phi_{i-1}^n + b_{EC} \Phi_{i+1}^n + b_{SW} \Phi_{i-1}^{n-1} + b_{SE} \Phi_{i+1}^{n-1} + b_{SC} \Phi_i^{n-1} \quad (19)$$

where the coefficients  $b_{WC}$ ,  $b_{EC}$ ,  $b_{SW}$ ,  $b_{SE}$ , and  $b_{SC}$  in Eq. (19) are functions of  $A_2$ ,  $B_2$ ,  $\Delta x$ , and  $\Delta t$  (Chen and Chen 1982) and are displayed in the Appendix. Eq. (19) is a 1D FA method whose local analytic solution is found from both time and spatial domains with the partial differential equation as given in Eq. (15) and initial and boundary conditions as shown in Eqs. (16)–(18).

The 1D FA method, i.e., Eq. (19), can be rewritten as

$$A_x \Phi_i^n = B_x \Phi_i^{n-1} \quad (20)$$

with introducing operators  $A_x$  and  $B_x$  as

$$A_x \Phi_i = -b_{WC} \Phi_{i-1} + \Phi_i - b_{EC} \Phi_{i+1} \quad (21)$$

and

$$B_x \Phi_i = b_{SW} \Phi_{i-1} + b_{SC} \Phi_i + b_{SE} \Phi_{i+1} \quad (22)$$

Thus, based on the technique of the fractional steps scheme as shown in Eqs. (13) and (14), together with the 1D FA method as shown in Eq. (21) for the  $x$  component and the one for the  $y$  component that can be easily found based on Eq. (20), a fractional steps scheme of the FA method is proposed to solve the 2D advection–diffusion equation as follows:

$$A_x \Phi_{i,j}^* = B_x \Phi_{i,j}^{n-1} \quad (23)$$

$$A_y \Phi_{i,j}^n = B_y \Phi_{i,j}^* \quad (24)$$

Here

$$A_x \Phi_{i,j} = -b_{WC} \Phi_{i-1,j} + \Phi_{i,j} - b_{EC} \Phi_{i+1,j} \quad (25)$$

$$B_x \Phi_{i,j} = b_{SW} \Phi_{i-1,j} + b_{SC} \Phi_{i,j} + b_{SE} \Phi_{i+1,j}$$

and

$$A_y \Phi_{i,j} = -b_{WC} \Phi_{i,j-1} + \Phi_{i,j} - b_{EC} \Phi_{i,j+1} \quad (26)$$

$$B_y \Phi_{i,j} = b_{SW} \Phi_{i,j-1} + b_{SC} \Phi_{i,j} + b_{SE} \Phi_{i,j+1}$$

where the superscript \* denotes intermediate value. The coefficients  $b_{WC}$ ,  $b_{EC}$ ,  $b_{SW}$ ,  $b_{SE}$ , and  $b_{SC}$  in Eq. (25) can be evaluated as shown in Eq. (19) with  $A_2 = (u)_{i,j}^n / (2\varepsilon_x)_{i,j}^n$ ; and  $B_2 = 1 / (\varepsilon_x)_{i,j}^n$ ; Similarly, the coefficients  $b_{WC}$ ,  $b_{EC}$ ,  $b_{SW}$ ,  $b_{SE}$ , and  $b_{SC}$  in Eq. (26) can be calculated as given in Eq. (19) with  $A_2 = (v)_{i,j}^n / (2\varepsilon_y)_{i,j}^n$ ;  $B_2 = 1 / (\varepsilon_y)_{i,j}^n$ ; and replacing  $\Delta x$  by  $\Delta y$ . The sketch of computational procedure for the fractional steps scheme of the FA method is depicted in Fig. 3.

## Demonstrations and Evaluations

### Advection and Diffusion of Point Source Contaminant

In order to examine the performances of the fractional steps scheme of the FA method, the advection and diffusion of a point source contaminant in a uniform flow is considered first. The problem is given by

$$\frac{\partial \Phi}{\partial t} + U \frac{\partial \Phi}{\partial x} = \varepsilon_x \frac{\partial^2 \Phi}{\partial x^2} + \varepsilon_y \frac{\partial^2 \Phi}{\partial y^2} \quad (27)$$

with boundary conditions of

$$\Phi(x, y, t) \rightarrow 0 \text{ as } |x| \rightarrow \pm \infty \text{ or } |y| \rightarrow \pm \infty \quad (28)$$

where  $U$  = constant flow velocity in the  $x$  direction. When the initial condition is a point source of mass  $M$  at  $x = x_0$  and  $y = y_0$ , the well-known exact solution is

$$\Phi(x, y, t) = \frac{M}{4\pi t(\varepsilon_x \varepsilon_y)^{1/2}} \exp \left\{ -\frac{[(x - x_0) - Ut]^2}{4\varepsilon_x t} - \frac{(y - y_0)^2}{4\varepsilon_y t} \right\} \quad (29)$$

To allow a numerical solution based on an initial peak concentration of unity, calculation begins at time  $t = t_0$  having a concentration distribution given by Eq. (29) with the point source of mass  $M = 4\pi t_0(\varepsilon_x \varepsilon_y)^{1/2}$ . In this numerical simulation, the following parameters are used:  $t_0 = 1,000$  s;  $U = 2$  m/s;  $\varepsilon_x = 3.2$  m<sup>2</sup>/s;  $\varepsilon_y = 1.6$  m<sup>2</sup>/s;  $\Delta x = \Delta y = 40$  m;  $\Delta t = 15$  s; and  $(x_0, y_0) = (80 \text{ m}, 2,000 \text{ m})$ .

Fig. 4 shows the contour plots of simulated results at time  $t = (t_0 + 600)$  s by the fractional steps scheme of FA (FSSFA)

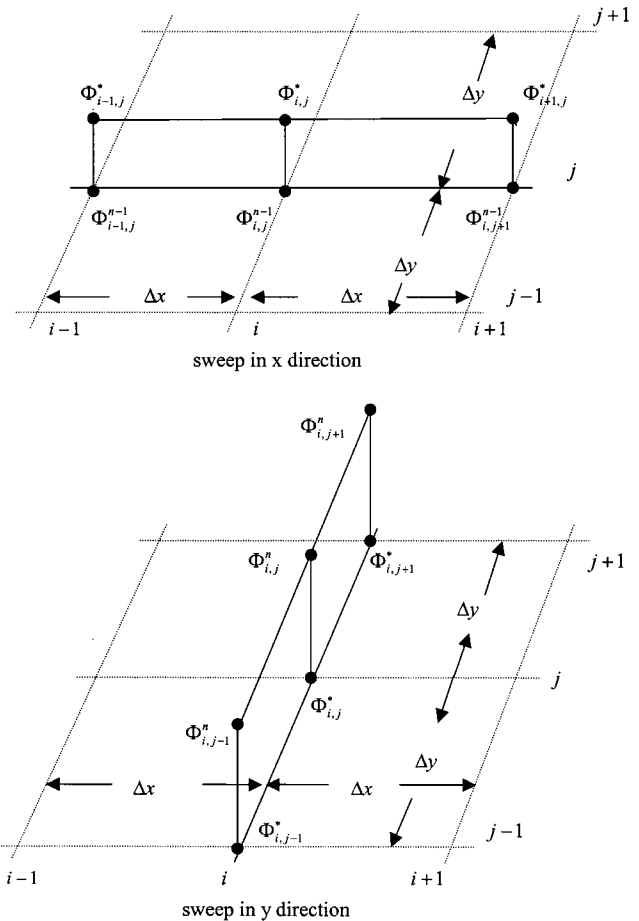


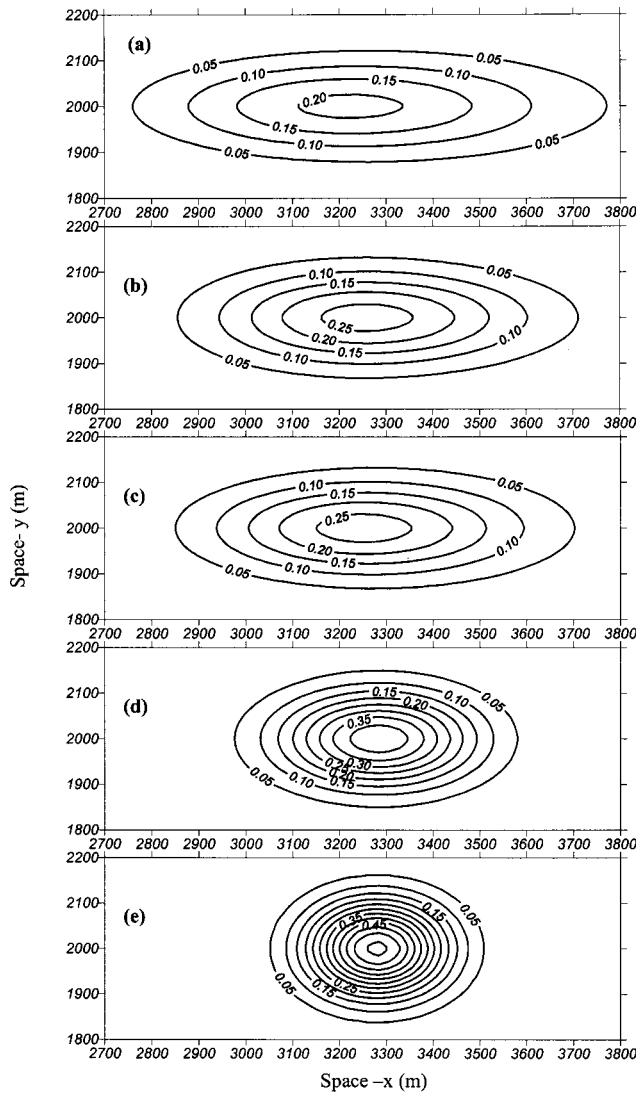
Fig. 3. Sketch of computational procedure for fractional steps scheme of finite analytic method

method, the alternating direction scheme of hybrid FA (ADSHFA) method, the optimal unsteady FA method, the traditional FA method, and the analytical solution. The computed results from those methods compared herein along the line  $y = 2,000$  m are displayed in Fig. 5. From Figs. 4 and 5, one can clearly find that the traditional FA method induces larger numerical diffusion than the optimal unsteady FA method in which an optimal time-weighting factor is introduced. The computational result by the alternating direction scheme of the hybrid FA method seems to agree with the one yielded by the optimal unsteady FA method. The fractional steps scheme of the FA method can greatly decrease numerical diffusion in comparison with the other three methods by evading the use of finite difference approximation to time derivative.

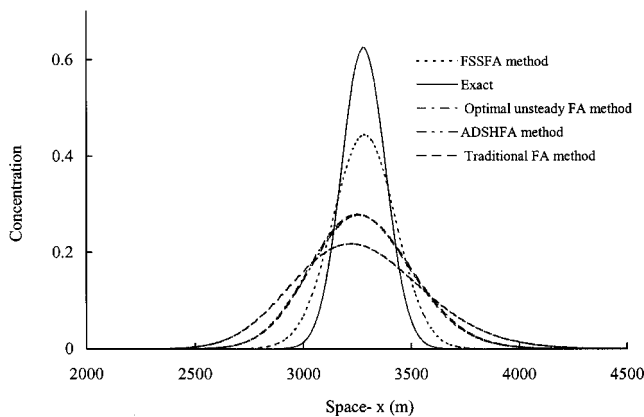
### Advection and Diffusion of Line Source Contaminant

This example simulates advection and diffusion of a line source contaminant in a uniform flow on semi-infinite domain as shown in Fig. 6. The governing equation is given by Eq. (27) with the boundary and initial conditions as follows:

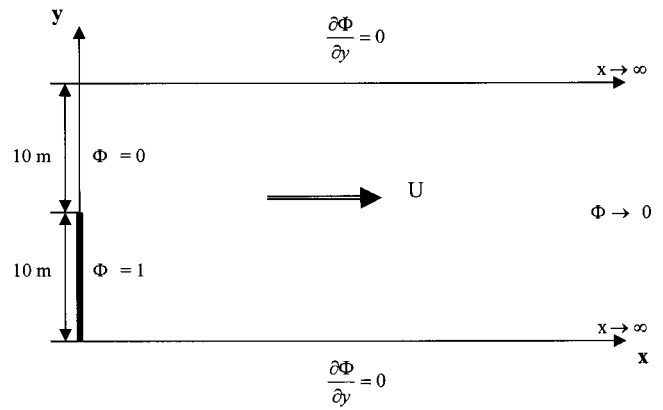
$$\begin{aligned} \Phi(0, y, t) &= 1 \\ 0 &\leq y \leq y_0 \end{aligned} \quad (30)$$



**Fig. 4.** Comparison of various schemes for advection and diffusion of point source contaminant: (a) traditional finite analytic method; (b) optimal unsteady finite analytic method; (c) alternating direction scheme of hybrid finite analytic method; (d) fractional steps scheme of finite analytic method; and (e) exact solution



**Fig. 5.** Comparison of various schemes for advection and diffusion of point source contaminant (along line  $y=2,000$  m)



**Fig. 6.** Domain and boundary conditions for calculation of advection and diffusion of line source contaminant

$$\Phi(0, y, t) = 0 \quad (31)$$

$$y_0 \leq y \leq y_1$$

$$\Phi(\infty, y, t) = \text{bounded} \quad (32)$$

$$0 \leq y \leq y_1$$

$$\left. \frac{\partial \Phi}{\partial y} \right|_{y=0} = 0 \quad (33)$$

$$x > 0$$

$$\left. \frac{\partial \Phi}{\partial y} \right|_{y=y_1} = 0 \quad (34)$$

$$x > 0$$

$$\Phi(x, y, 0) = 0 \quad (35)$$

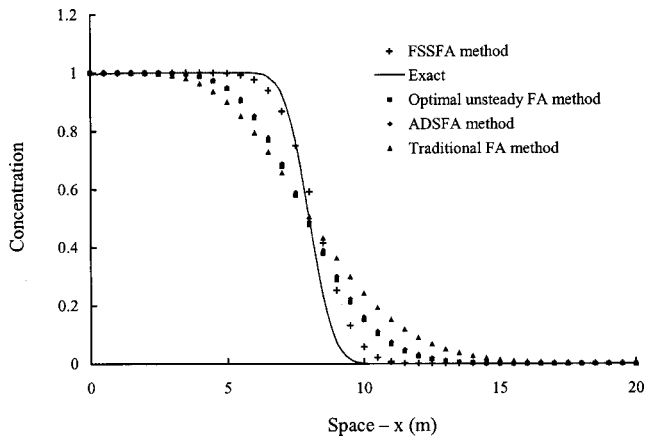
$$x > 0$$

$$0 \leq y \leq y_1$$

The exact solution was presented by Bruch and Street (1967). The FSSFA method, the ADSHFA method, the unsteady FA method, and the traditional FA method are used to simulate this problem. With  $y_1=20$  m;  $y_0=10$  m;  $U=0.1$  m/s;  $\Delta x=\Delta y=0.5$  m;  $\Delta t=4$  s;  $\varepsilon_x=0.003$  m<sup>2</sup>/s; and  $\varepsilon_y=0.001$  m<sup>2</sup>/s, the simulated results at  $t=80$  s and on the line  $y=5$  m are displayed in Fig. 7. It is clearly found that the fractional steps scheme of the FA method has the best results in comparison with the other three schemes. The traditional FA method produces larger numerical diffusion among those methods compared herein. The simulated results by the alternating direction scheme of the hybrid FA solution and the optimal unsteady FA method are comparable.

### Two-Dimensional Convective Transport Equation

A 2D nondimensional convective transport equation with a uniform flow is considered. The governing equation is



**Fig. 7.** Comparison of various schemes for advection and diffusion of line source contaminant (along line  $y=8$  m)

$$\frac{\partial \Phi}{\partial t} + \frac{\partial \Phi}{\partial x} + \frac{\partial \Phi}{\partial y} = D \left( \frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} \right) \quad (36)$$

where  $D$  represents the inverse of the Reynolds number. Under the initial condition

$$\Phi(x, y, 0) = \sin(\pi x) + \sin(\pi y) \quad (37)$$

and boundary conditions

$$\Phi(0, y, t) = (\sin(-\pi t) + \sin \pi(y - t)) \exp(-D\pi^2 t)$$

$$\Phi(1, y, t) = (\sin \pi(1 - t) + \sin \pi(y - t)) \exp(-D\pi^2 t)$$

$$\Phi(x, 0, t) = (\sin \pi(x - t) + \sin(-\pi t)) \exp(-D\pi^2 t)$$

$$\Phi(x, 1, t) = (\sin \pi(x - t) + \sin \pi(1 - t)) \exp(-D\pi^2 t) \quad (38)$$

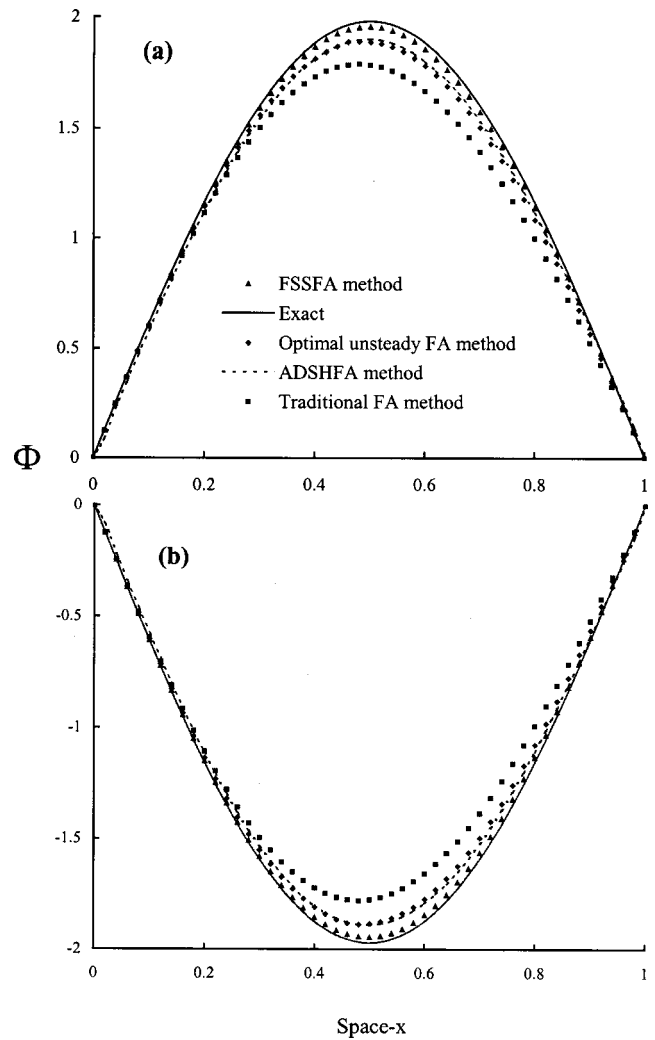
the exact solution to Eq. (36) can be expressed as

$$\Phi(x, y, t) = (\sin \pi(x - t) + \sin \pi(y - t)) \exp(-D\pi^2 t) \quad (39)$$

A uniform grid size of  $0.02 \times 0.02$ , time step of 0.025, and  $D = 0.0005$  are used for this simulation. The computed results along the line  $y=x$  by the FSSFA method, the ADSHFA method, the optimal unsteady FA method, and the traditional FA method are displayed in Fig. 8. The results show that the traditional FA method induces severe numerical diffusion. The alternating direction scheme of the FA method and the optimal unsteady FA method seem to provide comparable simulated results. The fractional steps scheme of the FA method, again, has the best results among the four methods considered.

### Three-Dimensional Diffusion in Shear Flow

In order to further investigate the capability of the fractional steps scheme of the FA method, a case for 3D diffusion in a shear flow is studied. 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 oceans, lakes, and estuaries. The governing equation for shear diffusion can be written as



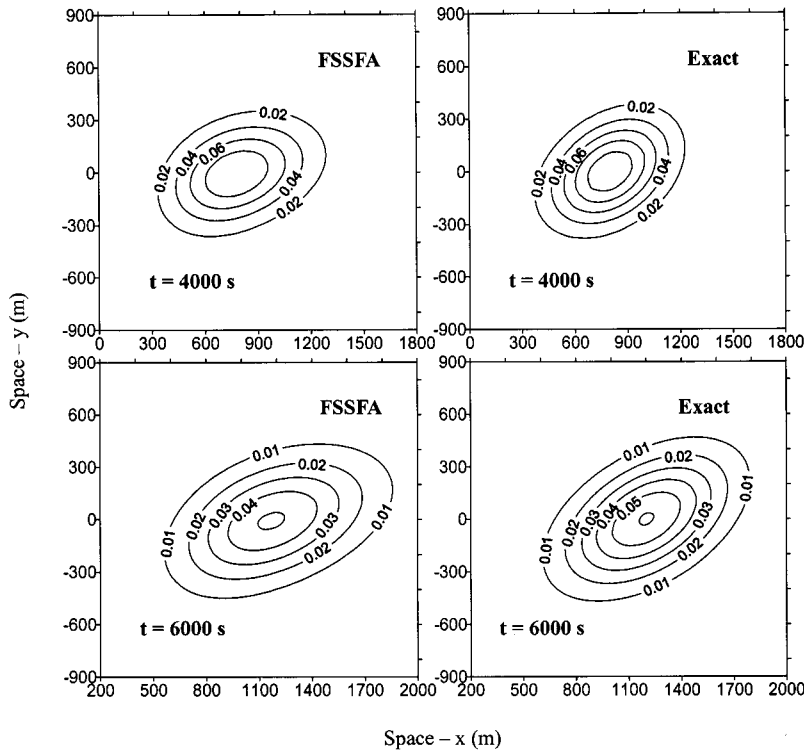
**Fig. 8.** Comparison of various schemes for the two-dimensional non-dimensional convective transport equation: (a)  $t=2$  and (b)  $t=3$

$$\frac{\partial \Phi}{\partial t} + (V_0 + \Omega_y y + \Omega_z z) \frac{\partial \Phi}{\partial x} = D_x \frac{\partial^2 \Phi}{\partial x^2} + D_y \frac{\partial^2 \Phi}{\partial y^2} + D_z \frac{\partial^2 \Phi}{\partial z^2} \quad (40)$$

where  $V_0$ =mean velocity in the  $x$  direction;  $\Omega_y$  and  $\Omega_z$  denote horizontal and vertical shear, respectively; and  $D_x$ ,  $D_y$ , and  $D_z$  represent 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 follows:

$$\begin{aligned} \Phi(x, y, z, t) = & \frac{M}{8\pi^{3/2}(D_x D_y D_z)^{1/2} t^{3/2} (1 + \beta^2 t^2)^{1/2}} \\ & \times \exp \left[ - \frac{(x - V_0 t - 0.5(\Omega_y y + \Omega_z z)t)^2}{4D_x t(1 + \beta^2 t^2)} \right. \\ & \left. + \frac{y^2}{4D_y t} + \frac{z^2}{4D_z t} \right] \end{aligned} \quad (41)$$

where



**Fig. 9.** Contour plots of diffusion in shear flow by fractional steps scheme of finite analytic on plane  $z=0$  at  $t=4,000$  and  $6,000$  s

$$\beta^2 = \frac{[(\Omega_y^2 D_y / D_x) + (\Omega_z^2 D_z / D_x)]}{12} \quad (42)$$

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

$$M = 8\pi^{3/2} (D_x D_y D_z)^{1/2} t_0^{3/2} (1 + \beta^2 t_0^2)^{1/2} \quad (43)$$

In the numerical simulation,  $t_0=1,000$  s;  $V_0=0.2$  m/s;  $\Omega_y=\Omega_z=0.0002$  1/s;  $D_x=D_y=D_z=5.0$  m<sup>2</sup>/s;  $\Delta t=100$  s; and grid space  $\Delta x=\Delta y=\Delta z=100$  m are used. Fig. 9 shows the contour plots of the fractional steps scheme of the FA method and the exact solution at  $t=4,000$  and  $6,000$  s on the plane  $z=0$ , respectively. From Fig. 9, one can observe that the fractional steps scheme of the FA method gives convincing simulated results.

## Conclusions

The FA method, unlike the finite difference method which applies the Taylor series expansion formulation or the finite element method which uses the weighted residual method with interpolation function and weighting function, is based on finding an analytic solution to a linear or linearized differential equation on a small subdomain of the problem domain. It is observed that replacing the time derivative with a first-order finite difference approximation in the traditional FA method may induce excessive numerical diffusion, especially for a large Péclet number. To improve the use of the first-order finite difference approximation to time derivative in the traditional FA method several alternatives, such as the applications of optimal time-weighting factor and the alternating direction implicit method, have been presented. In this paper, a new fractional steps scheme of the FA method is proposed, in which the local analytic solution is found

from both time and spatial domains. It is as expected that the traditional FA method induces the largest numerical diffusion among the four methods compared herein. The alternating direction scheme of the hybrid FA method and the optimal unsteady FA method seem to give comparably better results, while the proposed fractional steps scheme of the FA method gives the least numerical diffusion as compared with the other three methods due to avoiding the use of the finite difference approximation to the time derivative.

## Appendix. Coefficients of One-Dimensional Finite Analytic Method

$$b_{WC} = e^{A_2 \Delta x} S_1, \quad (44)$$

$$b_{EC} = e^{-A_2 \Delta x} S_1$$

$$b_{SW} = e^{A_2 \Delta x} S_2, \quad (45)$$

$$b_{SE} = e^{-A_2 \Delta x} S_2$$

$$b_{SC} = 4A_2 \Delta x \cosh(A_2 \Delta x) \coth(A_2 \Delta x) P_2 \quad (46)$$

$$S_1 = \frac{B_2 \Delta x^2}{\Delta t} (P_2 - Q_2) + Q_1 \quad (47)$$

$$S_2 = \frac{B_2 \Delta x^2}{\Delta t} (Q_2 - P_2) - 2A_2 \Delta x \coth(A_2 \Delta x) P_2 \quad (48)$$

$$P_2 = \sum_{m=1}^{\infty} \frac{(-1)^{m+1} \lambda_m \Delta x e^{-F_m \Delta t}}{[(A_2 \Delta x)^2 + (\lambda_m \Delta x)^2]^2} \quad (49)$$

$$F_m = \frac{A_2^2 + \lambda_m^2}{B_2} \quad (50)$$

$$\lambda_m = \frac{(2m-1)\pi}{2\Delta x} \quad (51)$$

$$Q_1 = \frac{1}{e^{A_2\Delta x} + e^{-A_2\Delta x}} \quad (52)$$

$$Q_2 = \frac{e^{A_2\Delta x} - e^{-A_2\Delta x}}{2A_2\Delta x(e^{A_2\Delta x} + e^{-A_2\Delta x})^2} \quad (53)$$

## Notation

The following symbols are used in this paper:

- $D$  = the inverse of Reynolds number;
- $D_x, D_y, D_z$  = eddy diffusivities in  $x, y,$  and  $z$  directions;
- $L_x, L_y$  = operators;
- $u, v, U$  = flow velocity component;
- $V_0$  = mean velocity in  $x$  direction;
- $\Delta t$  = time increment;
- $\Delta x, \Delta y, \Delta z$  = computational grid intervals in  $x, y,$  and  $z$  directions
- $\varepsilon_x, \varepsilon_y, \varepsilon_z$  = diffusion coefficients in  $x, y,$  and  $z$  directions;
- $\Phi$  = concentration; and
- $\Omega_y, \Omega_z$  = horizontal and vertical shear.

## Subscripts

- $i, j$  =  $x$  and  $y$  directional computational point index.

## Superscripts

- $n$  = time step index.

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