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INVESTIGATION OF USE OF REACH-BACK CHARACTERISTICS METHOD FOR 2D DISPERSION EQUATION

JINN-CHUANG YANG AND KUN-NAN CHEN

Department of Civil Engineering, National Chiao Tung University, Hsinchu, Taiwan 30050, R.O.C.

AND

HONG-YUAN LEE

Department of Civil Engineering, National Taiwan University, Taipei, Taiwan, R.O.C.

SUMMARY

The use of the Holly–Preissmann two-point scheme has been very popular for the calculation of the dispersion equation. The key to this scheme is to use the characteristics method incorporating the Hermite cubic interpolation technique to approximate the trajectory foot of the characteristics. This method can avoid the excessive numerical damping and oscillation associated with most finite difference schemes for advection computation. On the basis of the fundamental idea of the Holly–Preissmann two-point scheme, a new technique is introduced herein for the computation of the two-dimensional dispersion equation. This new scheme allows the characteristics projecting back several time steps to fall on the spatial or temporal axis, while the characteristics foot is still solved by the Holly–Preissmann two-point method. The diffusion portion of the dispersion equation is solved by the commonly used Crank–Nicholson method. The calculation for these two processes consisting of advection and diffusion is carried out separately but consecutively in one time step, a method known as the split operator algorithm. A hypothetical model was constructed to demonstrate the applicability of this new technique for the calculation of the pure advection and dispersion equation in two dimensions.

KEY WORDS Two dimension Dispersion Characteristics method

INTRODUCTION

A variety of numerical methods are available for the approximate solution of the dispersion equation and many are in use at the present time. However, no one method yet known is considered to be fully satisfactory. The primary difficulty arises from the combined hyperbolic (advection) and parabolic (diffusion) nature. To solve the dispersion problem in one- and two-dimensional flow by using numerical simulation, one has to be very careful to avoid possible numerical damping and oscillation problems. In order to tackle the numerical oscillation problem, several upwind-type finite difference methods have been proposed and investigated.[1–3] In addition, the upstream finite element method[4] was proposed and applied to solve the dispersion equation. Yeh[5] has also introduced a Lagrangian–Eulerian method with the use of a zoomable hidden fine-mesh approach which can give very convincing results in solving the advection–diffusion equation. However, each method has its own characteristics and limitations

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with respect to elimination of the numerical oscillation problem. Some of them may induce excessive numerical damping and may therefore mask the real physical diffusion processes. Some can only reduce the numerical oscillation problem under certain conditions of Courant number and Peclet number.

Among all these methods, it has been known that for the computation of pollutant dispersion along a river channel or coastal area, the Holly–Preissmann two-point method (H–P method) is one of the best and can give simulation results with few numerical oscillation and damping problems. The H–P method has also been extensively studied and applied to many hydraulic computation problems by many researchers.[6–12]

The H–P method is based on the fact that the higher-order interpolating polynomials are constructed from pairs of adjacent points on the spatial axis. In particular, for the case of transport in a coastal area where the transport phenomenon is dominated by advection rather than diffusion, with the use of the H–P method the numerical damping can be minimized.[6]

In fact, the H–P method is a kind of characteristics method, although only one characteristic is considered. When one looks through the unsteady flow problems solved by the characteristics method, one finds many investigators who have improved the characteristics method to give it various better and attractive features. Some extend the characteristics outwards in distance;[13–15] others extend the characteristics backwards in time.[16,17] Each extension has its accompanying improvements and merits. In this paper a similar concept of projecting the characteristics backwards in space and time with integration of the H–P method has been applied to solve the advection equation.

Two methods based on the fundamental concept of Holly and Preissmann's idea are introduced, which will be denoted as the Holly–Preissmann reach-back method (HPRB) and the Holly–Preissmann time-line interpolation method (HPTLI). The HPRB method allows the characteristics to project back several time steps beyond the present time level and fall on the spatial axis. The HPTLI method allows the characteristics to project several time steps beyond the present time level and fall on the temporal axis. In fact, the H–P method is a special case of the HPRB method where no reach-back characteristics are considered.

Stability analyses for the HPRB and HPTLI methods have been carried out for the one-dimensional advection equation by Yang and Hsu.[10,11] These authors have pointed out that the solution accuracy can be greatly improved by allowing the characteristics to project back beyond one time step with the use of either the spatial (HPPB) or the temporal interpolation (HPTLI) technique.

For the advection–diffusion (i.e. dispersion) problem the split operator algorithm is used to compute the advection and diffusion separately but consecutively in one time step. The advection portion will be computed by the HPRB or HPTLI method. For the diffusion portion the well-known Crank–Nicholson method is used. A hypothetical model is constructed for investigating the applicability of these new methods for the two-dimensional advection and dispersion equations through comparison with the original H–P method and the analytical solution.

GOVERNING EQUATIONS

The equation of 2D conservation of contaminant can be written as[6,18]

$$\frac{\partial(hC)}{\partial t}+\frac{\partial(huC)}{\partial x}+\frac{\partial(hvC)}{\partial y}=\frac{\partial}{\partial x}\left(h\varepsilon_{11}\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial x}\left(h\varepsilon_{12}\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial y}\left(h\varepsilon_{12}\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(h\varepsilon_{22}\frac{\partial C}{\partial y}\right), \quad (1)$$

in which x and y are horizontal Cartesian co-ordinates, t is time, $h(x, y, t)$ is the water depth, $C(x, y, t)$ is the depth-averaged contaminant concentration, $u(x, y, t)$ and $v(x, y, t)$ are the

depth-averaged velocities in the x- and y-directions respectively and $\varepsilon_{11}(x, y, t)$, $\varepsilon_{12}(x, y, t)$ and $\varepsilon_{22}(x, y, t)$ are components of the diffusion tensor ε. When the streamlines are aligned with the x- or y-axis, the term ε_{12} disappears.

The velocities and depths are assumed to be known quantities furnished by a previous mathematical or physical model study or even field measurement. Equation (1) can be simplified as

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}+v\frac{\partial C}{\partial y}=\frac{1}{h}\frac{\partial}{\partial x}\left(h\varepsilon_{11}\frac{\partial C}{\partial x}\right)+\frac{1}{h}\frac{\partial}{\partial x}\left(h\varepsilon_{12}\frac{\partial C}{\partial y}\right)+\frac{1}{h}\frac{\partial}{\partial y}\left(h\varepsilon_{12}\frac{\partial C}{\partial x}\right)+\frac{1}{h}\frac{\partial}{\partial y}\left(h\varepsilon_{22}\frac{\partial C}{\partial y}\right). \tag{2}$$

Equation (2) is a linear, second-order, parabolic partial differential equation. A variety of numerical methods are available for the solution of (2). In this paper the split operator strategy is applied to compute the advection and the diffusion separately but consecutively in one time step. The HPRB or HPTLI method is used to solve the advection portion. The diffusion portion is solved by the Crank–Nicholson method. The solution algorithms are described in the following sections.

REVIEW OF HOLLY–PREISSMANN METHOD

From (2) the two-dimensional advection portion can be written as

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}+v\frac{\partial C}{\partial y}=0. \tag{3}$$

Equation (3) can be recognized as a total derivative form

$$\frac{\mathrm{D}C}{\mathrm{D}t}=0 \tag{4}$$

along

$$\frac{\mathrm{d}x}{\mathrm{d}t}=u(x, y, t), \qquad \frac{\mathrm{d}y}{\mathrm{d}t}=v(x, y, t). \tag{5}$$

Integration of (4) and (5) yields

$$C_\eta=C_\xi \tag{6}$$

along

$$x_\eta-x_\xi=\int_{t_\xi}^{t_\eta}u(x, y, t)\,\mathrm{d}t, \tag{7}$$

$$y_\eta-y_\xi=\int_{t_\xi}^{t_\eta}v(x, y, t)\,\mathrm{d}t. \tag{8}$$

A schematic diagram of the characteristics trajectory is shown in Figure 1. C_η is the unknown concentration for grid point η at time level n which is to be solved. C_ξ is the concentration for point ξ at time level $n-1$ in which concentrations for all grid points are known.

Holly and Preissmann[2] used the concentration, its first derivatives and cross-derivatives at the neighbouring grid points to construct an interpolating polynomial to estimate C_ξ. It is clear from Figure 1 that this interpolating polynomial is constructed by the values of C, $Cx=\partial C/\partial x$, $Cy=\partial C/\partial y$ and $Cxy=\partial^2 C/\partial x\partial y$ at the four neighbouring nodes (i,j), $(i-1,j)$, $(i,j-1)$ and $(i-1,j-1)$. By following Holly and Preissmann's idea, C_ξ can be calculated by the relation

$$C_\xi(Rx, Ry)=\sum_{p=0}^{3}\sum_{q=0}^{3}a_{pq}(Rx)^p(Ry)^q, \tag{9}$$

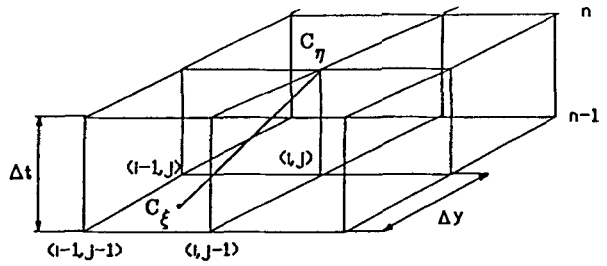

Figure 1. Schematic grid diagram for H–P method

where $Rx = u\,\Delta t/\Delta x$ and $Ry = v\,\Delta t/\Delta y$. Once the nodal values $C_\eta(C^n_{i,j})$ have thus been determined, the new nodal values of the derivatives, Cx^n, Cy^n and Cxy^n, must also be determined before the subsequent time step can be initiated. This is accomplished by differentiating (3) with respect to x and then y, yielding

$$\frac{\mathrm{D}Cx}{\mathrm{D}t} = -u_x Cx - v_x Cy, \tag{10}$$

$$\frac{\mathrm{D}Cy}{\mathrm{D}t} = -u_y Cx - v_y Cy, \tag{11}$$

in which D/Dt denotes the total derivative along the trajectory, $u_x = \partial u/\partial x$, $v_x = \partial v/\partial x$, $u_y = \partial u/\partial y$ and $v_y = \partial v/\partial y$.

The values of u_x, u_y, v_x and v_y can be obtained from the known velocity field; the system of equations (10) and (11) can be integrated from the foot of the trajectory (point ξ). The trapezoidal rule is used to integrate (10) and (11). In this manner Cx^n and Cy^n are therefore calculated for each node (i, j). Cxy^n can be solved by cross-differentiating (3):

$$\frac{\mathrm{D}Cxy}{\mathrm{D}t} = u_y Cxx - v_x Cyy - u_{xy} Cx - v_{xy} Cy - (u_x + v_y) Cxy. \tag{12}$$

The solution of this ordinary differential equation requires not only the cross-derivatives u_{xy} and v_{xy} but also the second derivatives Cxx and Cyy and cross-derivatives $(Cxy)_x$ and $(Cxy)_y$ for the interpolation of Cxy at point ξ. This closure problem is avoided by estimating Cxy at each node (i, j) by the divided difference just before each advection time step:

$$Cxy^n_{i,j} = \frac{1}{2}\left(\frac{Cx^n_{i,j+1} - Cx^n_{i,j-1}}{y_{j+1} - y_{j-1}}\right) + \frac{1}{2}\left(\frac{Cy^n_{i+1,j} - Cy^n_{i-1,j}}{x_{i+1} - x_{i-1}}\right). \tag{13}$$

The above procedures complete the computation of the advection portion in one time step.

DESCRIPTION OF NEW METHODS

The HPTLI method

The HPTLI method is to let the characteristics project back beyond the present time level to intercept on the time plane (i.e. x–t or y–t plane) between time levels t^{n-m} and t^{n-m-1} as shown in Figure 2, in which m denotes the reach-back number. The characteristics can fall on the x–t or y–t plane, and the justification is made on the basis of comparison of Rx and Ry. When Rx is greater

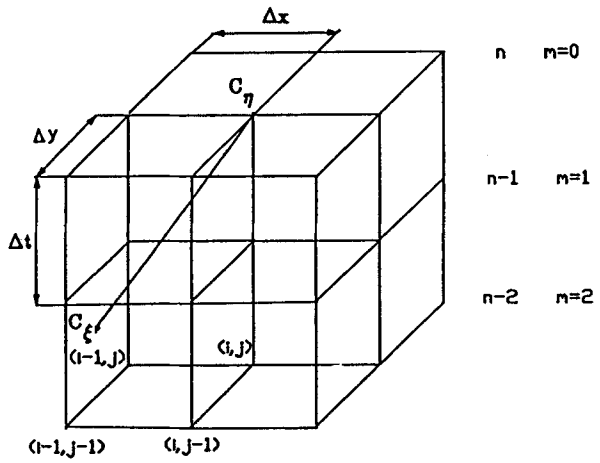

Figure 2. Schematic grid diagram for HPTLI method

than Ry, the characteristics fall on the y–t plane. When Ry is greater than Rx, the characteristics fall on the x–t plane. If Rx is equal to Ry, the characteristics fall on the intercepting line of the x–t and y–t planes between time levels t^{n-m} and t^{n-m-1}. The trajectory foot C_ξ can be evaluated by a cubic time-line interpolation polynomial. A similar technique has been described by Yang and Hsu[11] for calculation of the one-dimensional dispersion equation. For the 2D problem the interpolating polynomial will be a function of concentration C, temporal derivative Ct, spatial derivative Cx or Cy and cross-derivative $Cxt = \partial^2 C/\partial x\,\partial t$ or $Cyt = \partial^2 C/\partial y\,\partial t$. The selection of Cx, Cxt or Cy, Cyt is dependent on the values of Rx and Ry as stated previously. Similar to (9), C_ξ can be derived as

$$C_\xi(Rxt, Ryt) = \sum_{p=0}^{3}\sum_{q=0}^{3} b_{pq}(Rxt)^p(Ryt)^q, \tag{14}$$

in which Rxt and Ryt are interpolation parameters. The relation between Rxt, Ryt and Rx, Ry for the linear case can be summarized as follows.

1. If $Ry < Rx < 1$, then $Rxt = 1/Rx - m$ and $Ryt = Rx/mRy$, where m is the integer portion of $1/Rx$.
2. If $Rx < Ry < 1$, then $Rxt = Ry/mRx$ and $Ryt = 1/Ry - m$, where m is the integer portion of $1/Ry$.
3. If $Rx = Ry$, then one can select either the x–t or the y–t plane. If the x–t plane is used, then $Rxt = 1$ and $Ryt = 1/Ry - m$. On the other hand, if the $y - t$ plane is selected, then $Ryt = 1$ and $Rxt = 1/Rx - m$.

When point ξ is on the x–t plane, (14) can also be rewritten as

$$\begin{aligned} C_\xi(Rxt, Ryt) = {} & b_1 C_{i-1,j-1}^{n-m-1} + b_2 C_{i-1,j-1}^{n-m} + b_3 C_{i,j-1}^{n-m-1} + b_4 C_{i,j-1}^{n-m} \\ & + b_5 Cx_{i-1,j-1}^{n-m-1} + b_6 Cx_{i-1,j-1}^{n-m} + b_7 Cx_{i,j-1}^{n-m-1} + b_8 Cx_{i,j-1}^{n-m} \\ & + b_9 Ct_{i-1,j-1}^{n-m-1} + b_{10} Ct_{i-1,j-1}^{n-m} + b_{11} Cy_{i,j-1}^{n-m-1} + b_{12} Cy_{i,j-1}^{n-m} \\ & + b_{13} Cxt_{i-1,j-1}^{n-m-1} + b_{14} Cxt_{i-1,j-1}^{n-m} + b_{15} Cxt_{i,j-1}^{n-m-1} + b_{16} Cxt_{i,j-1}^{n-m}. \end{aligned} \tag{15}$$

When point ξ is on the y–t plane, a relation for C_ξ similar to (15) can be derived. The difference will only be the independent variables and the coefficients.

Once the nodal values C_η ($C^n_{i,j}$) have thus been determined, the new nodal values of the derivatives, Ct^n, Cx^n, Cy^n and Cxt^n or Cyt^n, must also be determined. This is accomplished by differentiating (4) with respect to x, y and t. When the characteristics fall on the x–t plane, one has to solve two further equations:

$$\frac{\mathrm{D}Cx}{\mathrm{D}t} = -u_x Cx - v_x Cy, \tag{16}$$

$$\frac{\mathrm{D}Ct}{\mathrm{D}t} = -u_t Cx - v_t Cy, \tag{17}$$

where Cx and Ct can be estimated by equations similar to (14) and (15). Cy and Cxt^n are evaluated by

$$Cy^n_{i,j} = \frac{C^n_{i,j+1} - C^n_{i,j-1}}{y_{j+1} - y_{j-1}}, \tag{18}$$

$$Cxt^n_{i,j} = \frac{Ct^n_{i+1,j} - Ct^n_{i-1,j}}{x_{i+1} - x_{i-1}}. \tag{19}$$

Similarly, when the characteristics fall on the y–t plane, two more equations are needed.

$$\frac{\mathrm{D}Cy}{\mathrm{D}t} = -u_y Cx - v_y Cy, \tag{20}$$

$$\frac{\mathrm{D}Ct}{\mathrm{D}t} = -u_t Cx - v_t Cy, \tag{21}$$

where Cy and Ct can also be estimated by equations similar to (14) and (15). Cx and Cyt can be evaluated by the discrete forms

$$Cx^n_{i,j} = \frac{C^n_{i+1,j} - C^n_{i-1,j}}{x_{i+1} - x_{i-1}}, \tag{22}$$

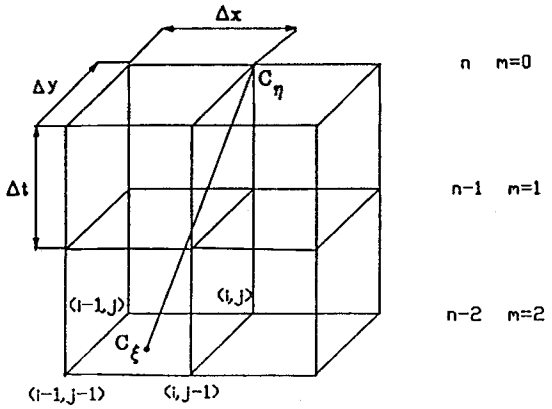

Figure 3. Schematic grid diagram for HPRB method

$$Cyt^n_{i,j}=\frac{Ct^n_{i,j+1}-Ct^n_{i,j-1}}{y_{j+1}-y_{j-1}}. \tag{23}$$

Equations (14)–(23) complete the calculation of the advection portion.

The HPRB method

The HPRB method is to let the characteristics project back beyond the present time level for the space domain interpolation. A schematic diagram of the characteristics trajectory is shown in Figure 3. When the reach-back number $m=1$, the HPRB method is identical to the original H–P method.

The interpolation polynomial is similar to the H–P technique. On the basis of (9), the following relation for C_ξ can be obtained:

$$\begin{aligned}C_\xi(Rx, Ry)=&a_1 C^{n-m}_{i-k-1,j-r-1}+a_2 C^{n-m}_{i-k-1,j-r}+a_3 C^{n-m}_{i-k,j-r-1}\\&+a_4 C^{n-m}_{i-k,j-r}+a_5 Cx^{n-m}_{i-k-1,j-r-1}+a_6 Cx^{n-m}_{i-k-1,j-r}\\&+a_7 Cx^{n-m}_{i-k,j-r-1}+a_8 Cx^{n-m}_{i-k,j-r}+a_9 Cy^{n-m}_{i-k-1,j-r-1}\\&+a_{10} Cy^{n-m}_{i-k-1,j-r}+a_{11} Cy^{n-m}_{i-k,j-r-1}+a_{12} Cy^{n-m}_{i-k,j-r}\\&+a_{13} Cxy^{n-m}_{i-k-1,j-r-1}+a_{14} Cxy^{n-m}_{i-k-1,j-r}\\&+a_{15} Cxy^{n-m}_{i-k,j-r-1}+a_{16} Cxy^{n-m}_{i-k,j-r},\end{aligned} \tag{24}$$

where Rx and Ry are the decimal portions of mRx and mRy respectively, k is the integer portion of mRx and r is the integer portion of mRy. If $m=1$, then $k, r=0$ and this technique is exactly the H–P method.

The procedures for the transport of Cx, Cy and Cxy along the trajectory are identical to those performed for the H–P method.[6]

SOLUTION FOR DISPERSION EQUATION

The dispersion equation (1) can be rewritten as

$$\frac{DC}{Dt}=\frac{1}{h}\frac{\partial}{\partial x}\left(h\varepsilon_{11}\frac{\partial C}{\partial x}\right)+\frac{1}{h}\frac{\partial}{\partial x}\left(h\varepsilon_{12}\frac{\partial C}{\partial y}\right)+\frac{1}{h}\frac{\partial}{\partial y}\left(h\varepsilon_{12}\frac{\partial C}{\partial x}\right)+\frac{1}{h}\frac{\partial}{\partial y}\left(h\varepsilon_{22}\frac{\partial C}{\partial y}\right) \tag{25}$$

along

$$\frac{dx}{dt}=u, \qquad \frac{dy}{dt}=v.$$

Equation (25) can be solved by decomposition into pure advection and pure diffusion. It has been described previously that the advection can be solved by the HPRB or HPTLI method. The diffusion will be computed by the Crank–Nicholson method. The solution algorithms are as follows.

When HPRB method used for advection portion

Once the new advected concentration values $C^n_{i,j}$ at each node have been obtained as described in the previous section, this new concentration field must be allowed to diffuse for the same time period of advection. However, in the advection scheme two additional unknowns Cx and Cy have been added; they must also be diffused to be consistent. This is accomplished by differentiating (3)

with respect to x and y to obtain dispersion equations for Cx and Cy. By using the symbol ψ for the dependent variables C, Cx and Cy, the three dispersion equations for C, Cx and Cy can be written as a single expression

$$h\frac{D\psi}{Dt}=\frac{\partial}{\partial z}\left(h\varepsilon\frac{\partial\psi}{\partial z}\right)+\frac{\partial}{\partial z}\left(h\varepsilon_{12}\frac{\partial\psi}{\partial w}\right), \tag{26}$$

in which $z=x$ or y, $w=y$ or x and $\varepsilon=\varepsilon_{11}$ or ε_{22}.

The problem then becomes one of solving (26) along each line $y=$constant to allow x-diffusion of the advected ψ-values, and solving (26) along each line $x=$constant to allow y-diffusion of the x-diffused ψ-values. This must be done independently for $\psi=C$, $\psi=Cx$ and $\psi=Cy$. Using the Crank–Nicholson method (26) is discretized as

$$\begin{aligned}h_i\frac{\psi_i^n-\psi_i^a}{\Delta t}=&\frac{2\theta}{z_{i+1}-z_{i-1}}\left(\frac{h_i^+\varepsilon_i^+(\psi_{i+1}^n-\psi_i^n)}{z_{i+1}-z_i}-\frac{h_i^-\varepsilon_i^-(\psi_i^n-\psi_{i-1}^n)}{z_i-z_{i-1}}\right)\\&+\frac{2(1-\theta)}{z_{i+1}-z_{i-1}}\left(\frac{h_i^+\varepsilon_i^+(\psi_{i+1}^{n-1}-\psi_i^{n-1})}{z_{i+1}-z_i}-\frac{h_i^-\varepsilon_i^-(\psi_i^{n-1}-\psi_{i-1}^{n-1})}{z_i-z_{i-1}}\right)\\&+\frac{2}{z_{i+1}-z_{i-1}}\left[h_i^+(\varepsilon_{12})_i^+\left(\frac{\partial\psi}{\partial w}\right)_i^+-h_i^-(\varepsilon_{12})_i^-\left(\frac{\partial\psi}{\partial w}\right)_i^-\right],\end{aligned} \tag{27}$$

in which ψ_i^a has been obtained by using the HPRB method for advection computation, Δt is the time step, θ is a weighting factor i is the index of computational points along z, i.e. x or y, $h_i^+=(h_i+h_{i+1})/2$, similarly for ε_i^+ and $(\partial\psi/\partial w)_i^+$, and $h_i^-=(h_i+h_{i-1})/2$, similarly for ε_i^- and $(\partial\psi/\partial w)_i^-$. If the flow direction coincides with the x- or y-axis, then $\varepsilon_{12}=0$ and the last term of (27) disappears.

The evaluation of cross-derivatives $\partial\psi/\partial w$ can best be explained with reference to Table I, which shows that for the diffusion of the concentration, $\psi=C$, the cross-term $\partial\psi/\partial w$ is just Cx or Cy. Since Cx and Cy are part of the advection solution, they are known at all nodes at the end of the advection step and thus the last term of (27) can be solved explicitly. When $\psi=Cx$ or Cy, Cxy appear, the cross derivatives can be evaluated by using the divided difference approximation of (13). The remaining two terms Cxx and Cyy can be estimated by the following divided difference procedure at the end of the advection step:

$$Cyy_{i,j}=\left(\frac{C_{i,j+1}-C_{i,j}}{y_{i+1}-y_i}-\frac{C_{i,j}-C_{i,j-1}}{y_i-y_{i-1}}\right)\frac{1}{z_{i+1}-z_{i-1}}. \tag{28}$$

Equation (27) can be solved by the tridiagonal matrix (double-sweep) method. The solutions for C, Cx and Cy along any given line can be carried out in parallel using the same influence coefficients, since only the free term changes from one case to another.

Table I

Calculation direction (z)	Perpendicular direction (w)	$\partial\psi/\partial w$		
		$\psi=C$	$\psi=Cx$	$\psi=Cy$
x	y	Cy	Cxy	Cyy
y	x	Cx	Cxx	Cxy

Table II

Calculation direction (z)	Perpendicular direction (w)	$\partial\psi/\partial w$			
		$\psi=C$	$\psi=Cx$	$\psi=Cy$	$\psi=Ct$
x	y	Cy	Cxy	Cyy	Cyt
y	x	Cx	Cxx	Cxy	Cxt

When HPTLI method used for advection portion

When the HPTLI method is used to compute the advection portion, (27) has to be rewritten as

$$h_i\frac{\psi_i^n-\psi_i^a}{\Delta t}=\frac{2\theta}{z_{i+1}-z_{i-1}}\left(\frac{h_i^+\varepsilon_i^+(\psi_{i+1}^n-\psi_i^n)}{z_{i+1}-z_i}-\frac{h_i^-\varepsilon_i^-(\psi_i^n-\psi_{i-1}^n)}{z_i-z_{i-1}}\right)$$
$$+\frac{2(1-\theta)}{z_{i+1}-z_{i-1}}\left(\frac{h_i^+\varepsilon_i^+(\psi_{i+1}^{n-m}-\psi_i^{n-m})}{z_{i+1}-z_i}-\frac{h_i^-\varepsilon_i^-(\psi_i^{n-m}-\psi_{i-1}^{n-m})}{z_i-z_{i-1}}\right)$$
$$+\frac{2}{z_{i+1}-z_{i-1}}\left[h_i^+(\varepsilon_{12})_i^+\left(\frac{\partial\psi}{\partial w}\right)_i^+-h_i^-(\varepsilon_{12})_i^-\left(\frac{\partial\psi}{\partial w}\right)_i^-\right], \tag{29}$$

in which ψ_i^a has been obtained during the advection computation and ψ^{n-m} denotes the ψ-value at time level $n-m$.

The computation of $\partial\psi/\partial w$ can be explained with reference to Table II. On the x–t plane, $\psi=C$, the cross-term $\partial\psi/\partial w$ is just Cx or Cy. Cx appearing in the last term of (27) can be evaluated explicitly. Cy can be treated by using the discrete form of (18). $\psi=Ct$ can be evaluated by using the discrete form of (19) and (23). For $\psi=Cx$ the cross-term $\partial\psi/\partial w$ is Cxy or Cxx. Cxy can be estimated by using the same type of divided difference approximation as (13). Cxx can be evaluated by using the same type of approximation as (28). The computation of $\partial\psi/\partial w$ on the y–t plane is the same as that on the x–t plane described above.

DEMONSTRATION AND EVALUATION

Calculation of pure advection

The pure advection of a Gaussian concentration distribution for various Courant numbers Cr with constant Δx and Δy has been computed. The distribution of mean position $x=2200$ m, $y=2200$ m and standard deviation $\sigma_x=\sigma_y=264$ m is defined on a regular grid $\Delta x=\Delta y=200$ m. The velocities u and v are assumed to be 0·5 m s^{-1} and therefore the term ε_{12} disappears in (3). In such a situation the analytical solution exists. The weighting factor $\theta=0{\cdot}5$ is fixed for all test cases. For the downstream boundary condition it is assumed that C and its derivatives are equal to zero. Cases with Courant numbers $Rx=Ry=Cr=0{\cdot}1$, 0·25, 0·5 and 0·75 for time steps $\Delta t=40$, 100, 200 and 300 s are tested. The initial distribution is transported for time $T=9600$ s. Another scheme may be needed to set up the initial condition when one applies the HPRB or HPTLI method for computing the advection portion. For the cases studied herein the original H–P method is used to establish the initial condition. In the following comparison figures the analytical solution is denoted Exact, the solution from the HPTLI method is denoted HPTLI and the solution from the HPRB method is denoted HPRB.

Figures 4(a)–4(d) show the simulated concentration distributions along one flow direction for various Courant numbers. In each figure, four simulations for reach-back numbers $m=1$, 2, 3 and 4 were performed. It is obvious that the results get closer to the exact solution as the reach-back number increases. In Figure 4(b) the simulation result with $m=4$ is identical to the exact solution. This occurs because the characteristics fall exactly on the grid node. Similarly, for the case of $Cr=0{\cdot}5$ the characteristics will fall on the grid node when $m=2$ is used. This again can be observed in Figure 4(c). The same result has also been obtained for the computation of the 1D dispersion equation by Yang and Hsu.[11]

From Figures 4(b) and 4(c) for $Cr=0{\cdot}25$ and $0{\cdot}5$ one can see that the HPTLI method gives very good results which are almost consistent with the exact solution. However, when Cr is too small,

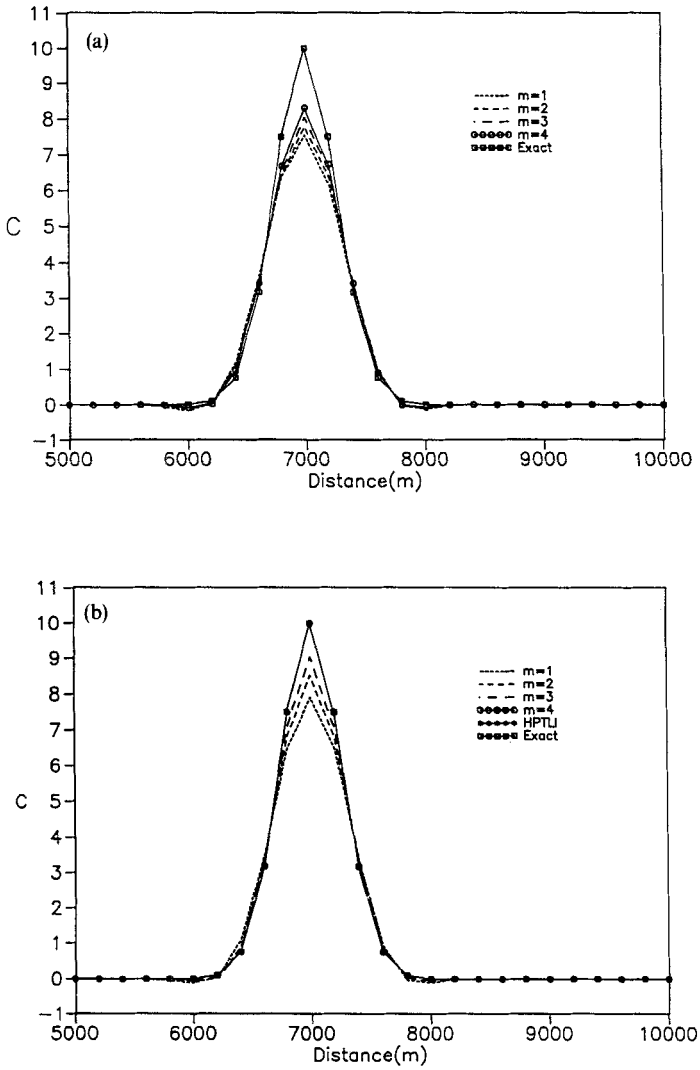

Figure 4. Comparison of analytical and numerical solutions for advection equation: (a) $Cr=0{\cdot}1$; (b) $Cr=0{\cdot}25$; (c) $Cr=0{\cdot}50$; (d) $Cr=0{\cdot}75$

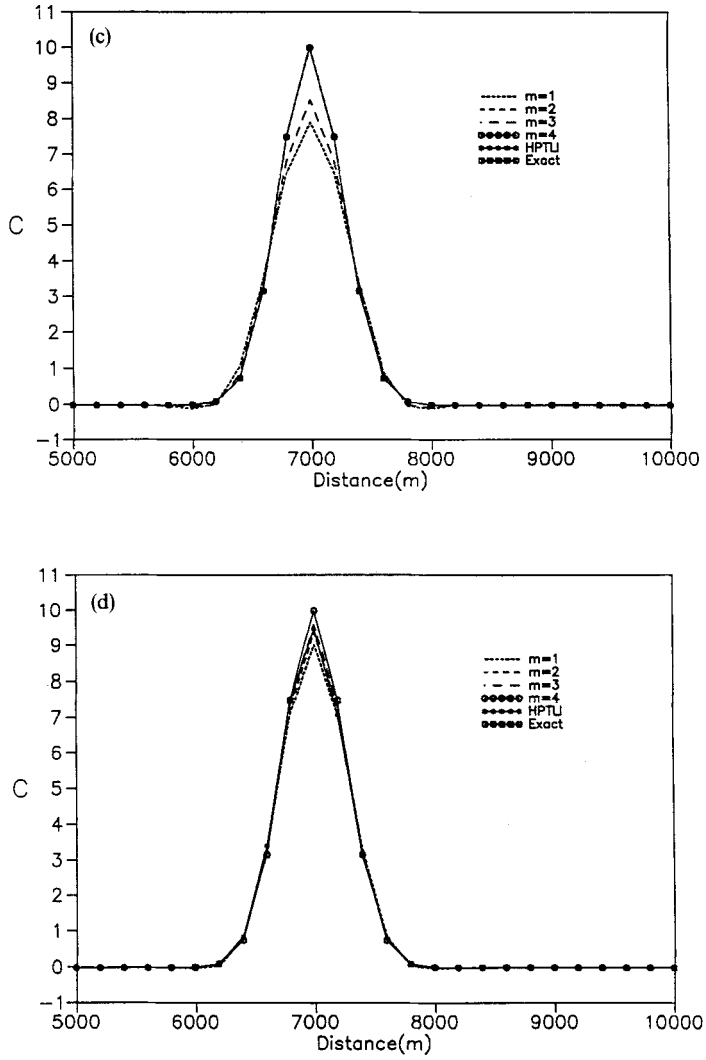

Figure 4. (Continued)

e.g. $Cr=0{\cdot}1$, the large value of reach-back number required may create difficulties in setting up the initial condition. Therefore no results computed by the HPTLI method for the case of $Cr=0{\cdot}1$ are shown herein. In addition, the programme coding will become more complex and require a large memory. Therefore, when Cr is too small, say less than 0·25, the HPTLI method will not be appropriate for the advection computation.

Calculation of dispersion equation

The advection–diffusion of a hypothetical Gaussian distribution under different velocity fields has been tested. The mass of the contaminant is assumed to be 36 100 units. The distribution of mean position $x=2200$ m, $y=2200$ m and standard deviation $\sigma_x=\sigma_y=300$ m is defined on

regular grid $\Delta x = \Delta y = 200$ m. For the downstream boundary condition it is again assumed that the concentration and its derivatives are equal to zero. Diffusivities $\varepsilon_{11} = \varepsilon_{22} = 0{\cdot}1$ m^2 s^{-1} are used for this case.

The results along one flow direction for all the test cases with various Courant numbers are shown in Figures 5(a)–5(d). Again, the same conclusions as for the calculation of 1D advection and 1D advection–diffusion problems described by Yang and Hsu[10,11] are observed. The reach-back number m plays a significant role in the solution accuracy. A better solution can be obtained with a larger value of m when the HPRB method is used to compute the advection portion. It can also be observed that the results computed by the HPTLI method are quite convincing.

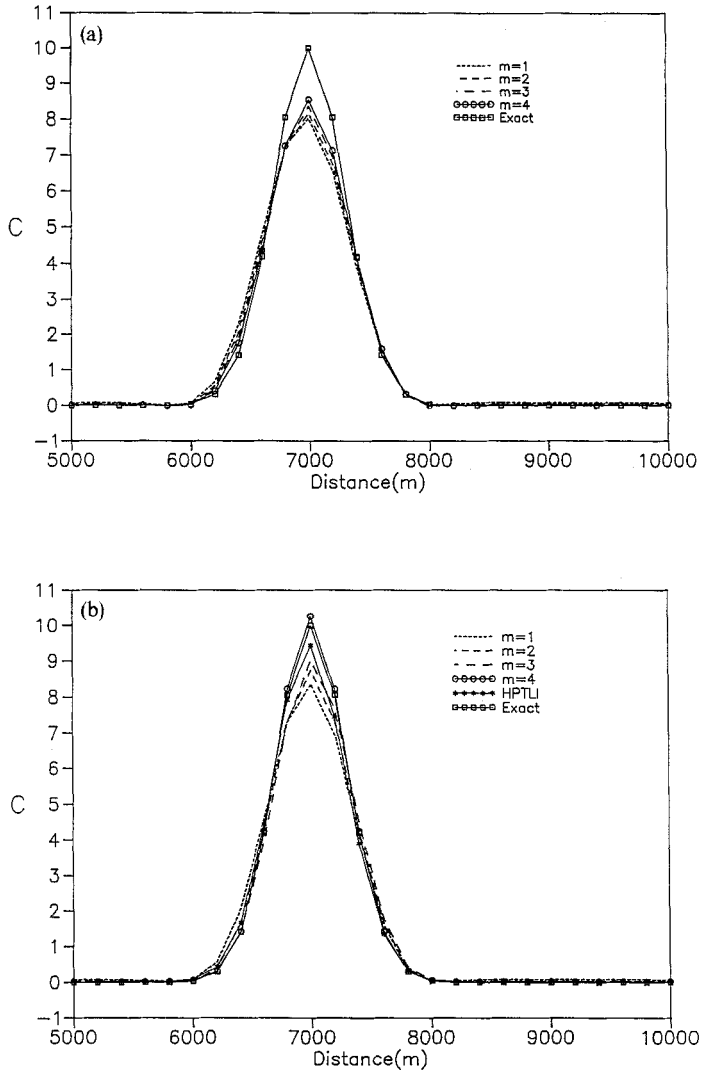

Figure 5. Comparison of analytical and numerical solutions for dispersion equation: (a) $Cr = 0{\cdot}1$; (b) $Cr = 0{\cdot}25$; (c) $Cr = 0{\cdot}50$; (d) $Cr = 0{\cdot}75$

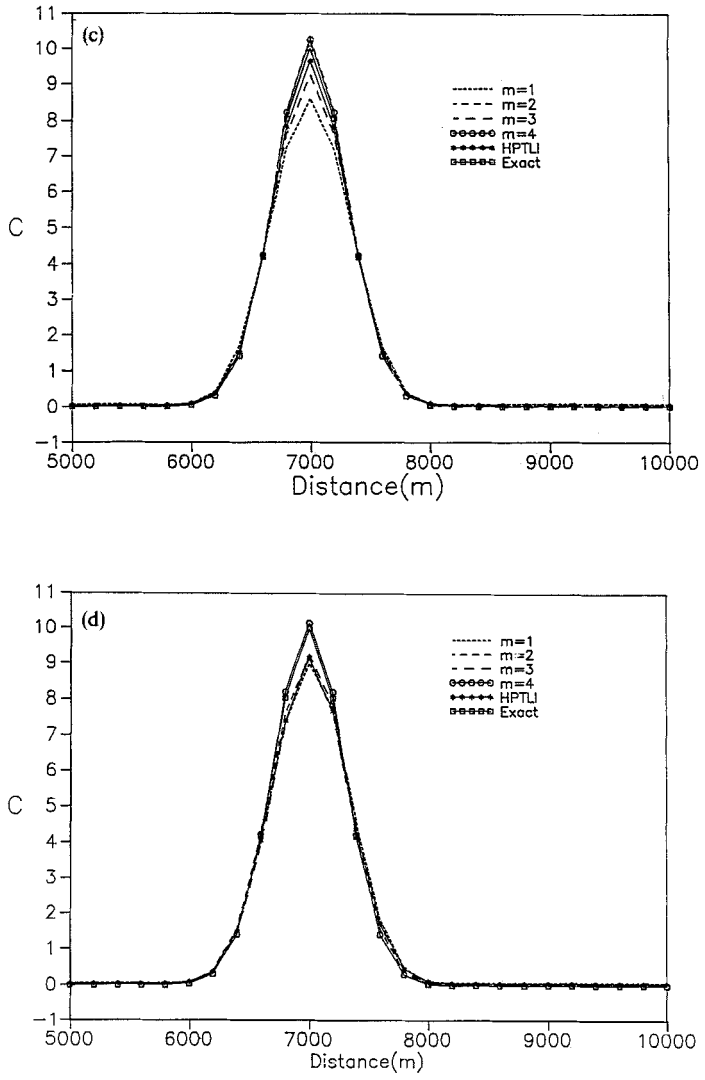

Figure 5. (Continued)

CONCLUSIONS

On the basis of the main framework of the Holly–Preissmann two-point method, a new interpolation technique incorporating consideration of the reach-back characteristics has been introduced for 2D advection–diffusion computation. From the demonstrated cases, whether for the computation of the pure advection or the advection–diffusion problem, one can conclude that the better simulation results can always be obtained with an increase of reach-back number m when the HPRB method is used for the advection computation. Furthermore, as long as the Courant number is not too small, the solution from the HPTLI method is also very convincing.

APPENDIX: NOTATION

$a_1, \ldots, a_{16}$	HPRB method concentration interpolation coefficients
$b_1, \ldots, b_{16}$	HPTLI (x–t plane) concentration interpolation coefficients
C	concentration
Ct	$\partial c/\partial t$
Cx	$\partial C/\partial x$
Cxt	$\partial^2 C/\partial x \partial t$
Cxx	$\partial^2 C/\partial x^2$
Cxy	$\partial^2 C/\partial x \partial y$
Cy	$\partial C/\partial y$
Cyy	$\partial^2 C/\partial y^2$
Cyt	$\partial^2 C/\partial y \partial t$
h	water depth
m	reach-back number
Rx	$u\Delta t/\Delta x$
Ry	$v\Delta t/\Delta y$
Rxt	if $Rx<Ry<1$, $Rxt=Ry/mRx$; if $Ry<Rx<1$, $Rxt=1/Rx-m$
Ryt	if $Ry<Rx<1$, $Ryt=Rx/mRy$; if $Rx<Ry<1$, $Ryt=1/Ry-m$
t	time
u	x-direction velocity
u_t	$\partial u/\partial t$
u_x	$\partial u/\partial x$
u_y	$\partial u/\partial y$
u_{xy}	$\partial^2 u/\partial x \partial y$
v	y-direction velocity
v_t	$\partial v/\partial t$
v_x	$\partial v/\partial x$
v_y	$\partial v/\partial y$
v_{xy}	$\partial^2 v/\partial x \partial y$
Δx	x-direction space increment
Δy	y-direction space increment
Δt	time increment
θ	weighting factor
ψ	dependent variables
η	characteristics head position
ξ	characteristics foot position
ε	diffusivity tensor

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