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A HIGHER-ORDER EULERIAN SCHEME FOR COUPLED ADVECTION–DIFFUSION TRANSPORT

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SUMMARY

A new accurate high-order numerical method is presented for the coupled transport of a passive scalar (concentration) by advection and diffusion.

Following the method of characteristics, the pure advection problem is first investigated. Interpolation of the concentration and its first derivative at the foot of the characteristic is carried out with a fifth-degree polynomial. The latter is constructed by using as information the concentration and its first and second derivatives at computational points on current time level t in Eulerian co-ordinates. The first derivative involved in the polynomial is transported by advection along the characteristic towards time level $t+\Delta t$ in the same way as is the concentration itself. Second derivatives are obtained at the new time level $t+\Delta t$ by solving a system of linear equations defined only by the concentrations and their derivatives at grid nodes, with the assumption that the third-order derivatives are continuous. The approximation of the method is of sixth order.

The results are extended to coupled transport by advection and diffusion. Diffusion of the concentration takes place in parallel with advection along the characteristic. The applicability and precision of the method are demonstrated for the case of a Gaussian initial distribution of concentrations as well as for the case of a steep advancing concentration front. The results of the simulations are compared with analytical solutions and some existing methods.

KEY WORDS Advection Diffusion Concentration Coupled solution Polynomial

1. INTRODUCTION

To solve the equation of advection–diffusion transport accurately is very important in various areas such as ground-water flow and suspended sediment and pollutant transport.

When transport processes of suspended load and pollution in rivers, canals and coastal waters are considered, advection is the dominant transport process. It is very easy to introduce numerical attenuation, and often in the numerical solution artificial diffusion is added to the physical diffusion. In order to reduce numerical difficulties, a number of numerical methods that couple finite differences or finite elements (for the diffusive term) with a method of characteristics (for the advective term) are in use involving the operator-splitting algorithms (see e.g. References 1–4).

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The solution techniques of the operator-splitting approach encounter criticism because advection and diffusion transport, which are two simultaneous physical processes,[3] are artificially separated and simulated alternately within one discrete time step. Benqué *et al.*[1] mention that the model time step should be limited in order that these two alternate processes converge to the physically meaningful result.

In the above analyses we can see that the fractional step approach has been frequently applied because it has special features whereby the difficulties of the numerical solution due to advection and diffusion are successively overcome in one small interval time. This feature leads us to select some suitable operator in an alternate process. For this reason, a coupling approach to advection–diffusion transport, whereby the coupled solution can be obtained within one time step, has not become popular because of the absence of a numerical method (operator) appropriate to the simultaneous solution of the advective and diffusive terms. Almost all of the proposed coupling approaches suffer from loss of precision. Stone and Brian[5] described a coupling approximation that deals with the advection and diffusion terms through a six-point implicit scheme, but this scheme exhibits numerical damping and dispersion. Holly and Preissmann[6] proposed a numerical method in which both the advection and diffusion are approximated by a fourth-order Hermitian polynomial. This scheme may deform the physical wave (concentration profile) in the diffusion situation because the fourth-order Hermitian polynomial gives inconsistent numerical second derivatives at grid nodes.[7] Another coupling approach[8] combines the fourth-order Hermitian polynomial with the centred finite difference at Eulerian grid nodes, but it does not avoid numerical dispersion.

The present paper describes the construction of a higher-order numerical scheme for coupled transport by advection and diffusion. The principle of the coupled solution of the problem is that the calculation of both advective and diffusive terms is of the same accuracy. The advective term, which is a key problem in numerical calculations, has priority of consideration. The paper begins with a study of the pure advection problem. A sixth-order polynomial for interpolation of the concentration at the foot of a characteristic is constructed between two adjacent computational nodes using the concentration and its first and second derivatives. All three are considered as dependent variables. The concentration is advected along the characteristic from its foot to time level $(n+1)\Delta t$. Diffusion is computed in parallel with advection along the characteristic, the diffusive term being approached explicitly at the foot of the characteristic on the current time level with the aid of the second and third derivatives of concentration at the nodes. The latter are interpolated by fourth- and third-degree polynomials respectively. At the end of the time step level a coupled solution is obtained. The results of calculations of the propagation of an initially Gaussian distribution of concentration and of an initially sharp concentration front are given, as well as the amplitude and phase portraits of the proposed method.

2. 1D GOVERNING EQUATION OF ADVECTION–DIFFUSION

Consider the one-dimensional equation governing advection–diffusion:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D_x \frac{\partial^2 C}{\partial x^2}, \tag{1}$$

where $C(x, t)$ is the concentration, $u(x, t)$ is the flow velocity, D_x is the constant diffusion coefficient in the x-direction, x is the positive direction of flow and t is time. The second term on the left-hand side of equation (1) represents advection, whereby the concentration profile is transported without damping; the term on the right-hand side represents diffusion. The relative intensity of these two terms, which can be represented by the Peclet number Pe,[9] determines the

character of the equation. If the velocity is high, *Pe* is large, so that advection is the dominant transport factor, equation (1) is nearly hyperbolic and the numerical difficulties are considerable. If *Pe* is small, the equation is nearly parabolic and diffusion transport is dominant. In real life the velocity can change with time and so can the features of the equation.

2.1. Eulerian pure advection calculation

2.1.1. Description of the method

Formal solution and approach

In the case of pure advection, with the assumption of a constant velocity u_0, the equation of a characteristic curve is

$$dx/dt = u_0. \tag{2}$$

We can obtain a formal solution along this curve by integrating equation (1):

$$C_P = C_A \quad \text{or} \quad C(x, t+\Delta t) = C(x - u_0 \Delta t, t). \tag{3}$$

Within one time step the particle of fluid moves from point A to point P, the 'new' concentration at point P being the same as that at point A. Thus it is very important to find the current value of the concentration at A (see Figure 1).

There exist many methods which can be used to find this concentration.[10–13] Unfortunately, all of these methods use a linear interpolation which introduces smoothing, i.e. artificial diffusion. It is well known that the linear interpolation used to find the concentration at A is not critically satisfactory. Holly and Preissmann[6] proposed an interpolation for the concentration by using a third-degree Hermitian polynomial. The method was widely accepted by various workers.[1–4, 8, 14] Belleudy and Sauvaget[14] extended this scheme using implicit time line interpolation. Komatsu *et al.*[15] developed Holly and Preissmann's method by using the information at six grid nodes to construct a higher-order polynomial. Fryxell *et al.*[16] described a method of the Godunov type. These methods have not fully avoided the difficulties revealed by Yang,[7] namely that third-degree spline functions exhibit severe numerical attenuation when used for the advection problem.

Define a grid as shown in Figure 1,

$$\Delta x_j = x_j - x_{j-1}, \quad j = 1, 2, \ldots, N-1,$$

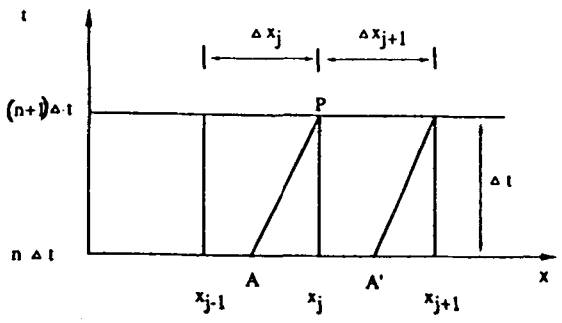

Figure 1. Grid definition

and an irregular grid space step ratio

$$\lambda_j=\frac{\Delta x_j}{\Delta x_j+\Delta x_{j+1}}, \qquad \mu_j=1-\lambda_j. \tag{4}$$

Let the Courant number be

$$Cr=u_0\Delta t/\Delta x_j$$

and

$$Cr=\frac{x_j-x_A}{x_j-x_{j-1}}<1,$$

i.e. the point A is located between points $j-1$ and j at current time level $n\Delta t$. The concentrations at all grid nodes at this time level are known:

$$C^n_{j-1}, \quad C^n_j, \quad C^n_{j+1}, \quad j=1, 2, \ldots, N.$$

We propose to find the concentration at A using a fifth-degree polynomial in terms of the Courant number:

$$C_A(Cr)=\sum_{i=1}^{6} A_i Cr^{6-i}. \tag{5}$$

If one wishes to use only two adjacent grid nodes so that the method becomes more convenient for variable intervals, six coefficients A_i ($i=1, 2, \ldots, 6$) have to be found subject to the following conditions:

$$\begin{aligned} C_A(1)&=C^n_{j-1}, & C_A(0)&=C^n_j,\\ \partial C_A(1)/\partial x&=CX^n_{j-1}, & \partial C_A(0)/\partial x&=CX^n_j,\\ \partial^2 C_A(1)/\partial x^2&=CM^n_{j-1}, & \partial^2 C_A(0)/\partial x^2&=CM^n_j, \end{aligned} \tag{6}$$

where CX_j and CM_j are the first and second derivatives respectively of the concentration C_j at current time level $n\Delta t$. After performing the necessary algebra, the expressions for the six coefficients A_i defined by these known values can be obtained[7] and the polynomial (5) can be written as a function of the Courant condition and these known values:

$$C_A(Cr)=a_1C^n_{j-1}+a_2C^n_j+a_3CX^n_{j-1}+a_4CX^n_j+a_5CM^n_{j-1}+a_6CM^n_j, \tag{7}$$

where the a_i, which are different from the A_i, are given by

$$\begin{aligned} a_1&=6Cr^5-15Cr^4+10Cr^3, & a_2&=1-a_1,\\ a_3&=(3Cr^5-7Cr^4+4Cr^3)\Delta x_j, & a_4&=(3Cr^5-8Cr^4+6Cr^3-Cr)\Delta x_j,\\ a_5&=(Cr^5-2Cr^4+Cr^3)\Delta x_j^2/2, & a_6&=(-Cr^5+3Cr^4-3Cr^3+Cr^2)\Delta x_j^2/2. \end{aligned}$$

For the pure advection calculation the concentration at time level $(n+1)\Delta t$,

$$C^{n+1}_j=C_P=C_A(Cr),$$

can be determined explicitly from equation (7). The calculation cannot be performed, however, if the first and second derivatives are not known. Thus it will in turn be necessary to know these derivatives at time level $(n+1)\Delta t$ for further computation.

Estimation of first derivatives

The simple advection (for a constant velocity) of the first derivative can be found by differentiation of equation (1) while neglecting the diffusive term. Along the same characteristic

$$dx/dt = u_0.$$

For the concentration the formal solution for the first derivative at the point P can be obtained:

$$CX_P = CX_A. \tag{8}$$

The interpolation of the first derivative CX_A at time level $n\Delta t$ should be compatible with that applied to the concentration. It can be approximated by differentiating polynomial (5) with respect to x:

$$CX_A(Cr) = \frac{-1}{\Delta x} \sum_{i=1}^{5} (6-i) A_i Cr^{5-i}. \tag{9}$$

Substituting the known A_i into the fourth-degree polynomial (9), one obtains

$$CX_A(Cr) = b_1 C_{j-1}^n + b_2 C_j^n + b_3 CX_{j-1}^n + b_4 CX_j^n + b_5 CM_{j-1}^n + b_6 CM_j^n, \tag{10}$$

where

$$b_1 = (-30Cr^4 + 60Cr^3 - 30Cr^2)(1/\Delta x_j), \qquad b_2 = -b_1,$$
$$b_3 = (-15Cr^4 + 28Cr^3 - 12Cr^2), \qquad b_4 = (-15Cr^4 + 32Cr^3 - 18Cr^2 + 1),$$
$$b_5 = (-5Cr^4 + 8Cr^3 - 3Cr^2)(\Delta x_j/2), \qquad b_6 = (5Cr^4 - 12Cr^3 + 9Cr^2 - Cr)(\Delta x_j/2).$$

Again all first derivatives at time level $(n+1)\Delta t$ at nodes $j = 1, 2, \ldots, N$ can be evaluated from equation (9), i.e.

$$CX_j^{n+1} = CX_A(Cr). \tag{11}$$

Evaluation of second derivatives

By adding the second derivatives in polynomial (5), the order of accuracy of the numerical solution can be increased without increase of the number of nodes. The second derivatives have then to be defined at time level $(n+1)\Delta t$ for further solution. Advection of the second derivative as an extension of Holly and Preissmann's method[6] is not adopted here because it produces residual terms in the variable velocity field, the discretization of which in turn introduces numerical errors.

In order to define the second derivatives, the hypothesis of the continuity of the third derivative of polynomial (5) at computational grid nodes is used. Thus the value of the third derivative on the left-hand side of the point j ($x_A \to x_j$), which is given by the polynomial defined over the interval $(j-1, j)$, is taken to be equal to the third derivative on the right-hand side of j ($x_{A'} \to x_j^+$), given by the polynomial defined over the interval $(j, j+1)$:

$$\lim_{x_A \to x_j^-} \left(\frac{\partial^3 C_A(Cr)}{\partial x^3} \right) = \lim_{x_{A'} \to x_j^+} \left(\frac{\partial^3 C_A(Cr)}{\partial x^3} \right). \tag{12}$$

The third derivative obtained by differentiation of polynomial (5) with respect to x can be written at any grid:

$$\frac{\partial^3 C_A(Cr)}{\partial x^3} = \sum_{i=1}^{3} (6-i)(5-i)(4-i) A_i Cr^{3-i} \left(\frac{\partial Cr}{\partial x} \right)^3. \tag{13}$$

Note that

$$\frac{\partial Cr}{\partial x}=\frac{-1}{\Delta x_j}, \qquad \frac{\partial^i Cr}{\partial x^i}=0 \quad \text{for } i=2,3$$

and that

$$\lim_{x_A \to x_j^-} Cr=0, \qquad \lim_{x_{A'} \to x_j^+} Cr=1.$$

Substituting the known coefficients A_i into (13), together with hypothesis (12), a linear equation in CM_j is defined for time step $n\Delta t$:

$$\mu_j CM_{j-1}^n - 3CM_j^n + \lambda_j CM_{j+1}^n = d_j^n, \tag{14}$$

where

$$d_j^n=\frac{-20}{\mu_j^2}\left(\frac{\mu_j^3 C_{j-1}^n-(\mu_j^3+\lambda_j^3)C_j^n+\lambda_j^3 C_{j+1}^n}{\Delta x_j^2}\right)-\frac{2}{\mu_j}\left(\frac{4\mu_j^2 CX_{j-1}^n+(\mu_j^2-\lambda_j^2)CX_j^n-4\lambda_j^2 CX_{j+1}^n}{\Delta x_j}\right). \tag{15}$$

For N computational grid nodes one can write $N-2$ linear equations (14) for N unknown variables CM_j ($j=1, 2, \ldots, N$). The system (14) should be closed by two boundary conditions. For this reason the second derivatives at two boundary points $j=1, N$ should be known:

$$CM_{1,N}=\left(\frac{\partial^2 C}{\partial x^2}\right)_{j=1,N}=CXX_{1,N}. \tag{16}$$

For a uniform grid $\Delta x_j=\Delta x_{j+1}=\Delta x$, λ_j and $\mu_j=\frac{1}{2}$, so that the system (14), (15) together with the boundary condition (16) can be written

$$[A]\overrightarrow{CM}=\vec{D}, \tag{17}$$

$$[A]=\begin{bmatrix} -3 & 0 & & & & \\ \frac{1}{2} & -3 & \frac{1}{2} & & \mathbb{0} & \\ & & \frac{1}{2} & -3 & \frac{1}{2} & \\ & \mathbb{0} & & & & \\ & & & 0 & -3 \end{bmatrix}, \qquad \overrightarrow{CM}=\begin{bmatrix} CM_1^n \\ CM_2^n \\ \vdots \\ CM_{N-1}^n \\ CM_N^n \end{bmatrix}, \qquad \vec{D}=\begin{bmatrix} d_1^n \\ d_2^n \\ \vdots \\ d_{N-1}^n \\ d_N^n \end{bmatrix},$$

where $d_{1,N}^n=-3CXX_{1,N}$ and the d_j^n ($j=2, 3, \ldots, N-1$) are computed by

$$d_j^n=-10\left(\frac{C_{j-1}^n-2C_j^n+C_j^n}{\Delta x^2}\right)-4\left(\frac{CX_{j+1}^n-CX_{j-1}^n}{\Delta x}\right).$$

2.1.2. Linear error analysis of the method. Following Leendertse,[17] two convergence factors R_1 and R_2 between the numerical solution of the linear system and the analytical solution are

investigated:

$$R_1 = \frac{\text{amplitude of numerical solution}}{\text{amplitude of analytical solution}},$$
$$R_2 = \frac{\text{speed of numerical solution}}{\text{speed of analytical solution}}. \tag{18}$$

For convergence it is necessary that $R_1 \to 1$ and $R_2 \to 1$ when $(\Delta x, \Delta t) \to 0$ for a determined relationship between Δx and Δt.

In the numerical scheme presented here, the linear advection differential equation is approximated by equations (7) and (10) through two dependent variables C and CX and by an additional algebraic system of equations (14). Following Neumann's stability analysis,[18] the convergence factors R_1 and R_2 can be found by the method of Fourier series. They are functions of the Courant number Cr and of the relative wavelength $L/\Delta x$ (L is the wavelength of the single Fourier component, Δx is the grid space step). Since the details of the analysis have already been documented,[7] only final results are given here.

In Figures 2–4 are shown the two convergence factors R_1 and R_2 (the so-called 'amplitude portrait' and 'phase portrait') and the relative amplitude error (in per cent). The numerical scheme is stable for $Cr < 1$. It gives the exact solution for $Cr = 0$ or $Cr = 1$ independently of the ratio $L/\Delta x$. For $Cr < 1$ the scheme introduces a negligibly small artificial damping. The largest relative amplitude error given by the scheme is 0·25% for $L/\Delta x > 3$ and $Cr = 0{\cdot}5$. After expansion in Taylor series one can demonstrate that the system (7)–(10) approximates the advection differential equation with sixth-order accuracy provided that the linear system (14) exactly evaluates the second derivatives at grid nodes. Thus the amplitude error introduced by the scheme disappears quickly as the grid space step Δx decreases.

2.2. *Coupled advection–diffusion problem*

It was demonstrated in the previous subsection that a fifth-degree polynomial results in sixth-order-accurate approximation for pure advection. This result can be extended to a coupled advection–diffusion problem. Equation (1) can be written as a total derivative along the characteristic defined by (2):

$$\frac{DC}{Dt} = D_x \frac{\partial^2 C}{\partial x^2}, \tag{19}$$

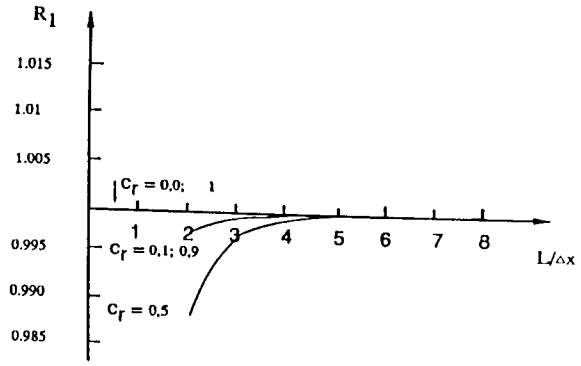

Figure 2. R_1 (amplitude portrait) for pure advection problem

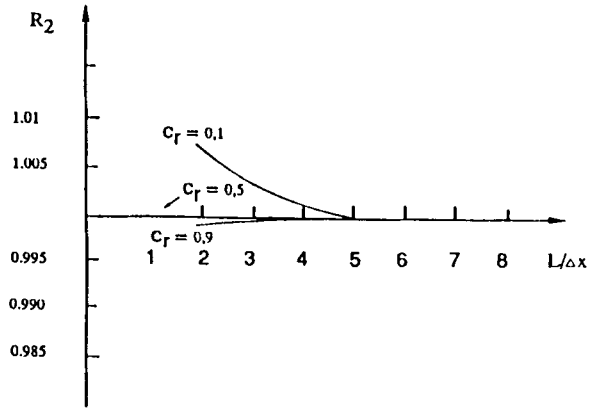

Figure 3. R_2 (phase portrait) for pure advection problem

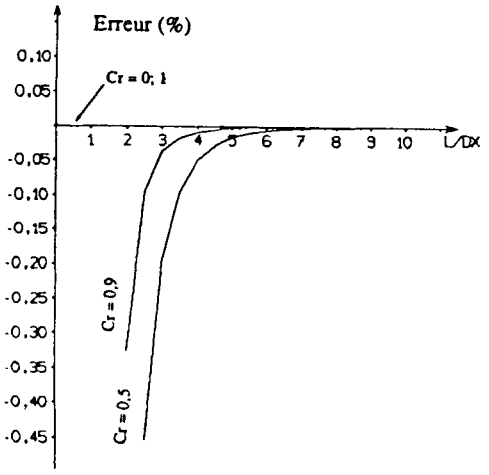

Figure 4. Relative amplitude error for pure advection problem

where

$$\frac{\mathrm{D}}{\mathrm{D}t}=\frac{\partial}{\partial t}+u\frac{\partial}{\partial x}.$$

The numerical approximation is carried out by replacing the two terms on the left-hand side term of equation (1) by (19) and applying discretizations along the characteristic (see Figure 1):

$$\frac{\mathrm{D}C}{\mathrm{D}t}=\frac{C_j^{n+1}-C_{\mathrm{A}}^n}{\Delta t}, \tag{20}$$

$$D_x\frac{\partial^2 C}{\partial x^2}=D_x CXX_{\mathrm{A}}^n. \tag{21}$$

From equations (19)–(21) one obtains a difference equation for the primary dependent variable C:

$$C_j^{n+1}=C_{\mathrm{A}}^n+D_x\Delta t CXX_{\mathrm{A}}^n. \tag{22}$$

With the assumption that the velocity u and the diffusion coefficient D_x are constant, the approximation of the first derivative CX is obtained by differentiation of equation (1) with respect to space:

$$CX_j^{n+1} = CX_A^n + D_x \Delta t CXXX_A^n. \tag{23}$$

C_A, CX_A, CXX_A and $CXXX_A$ in equations (22) and (23) are respectively the values of the concentration and the first, second and third derivatives of concentration at the foot of the characteristic. With zero diffusion coefficient one can find the solution for pure advection in (22) and (23).

The difficulty of using equations (22) and (23) as a basis for the method lies in obtaining an accurate evaluation of C_A and CX_A, which are needed for the advection calculation, and of CXX_A and $CXXX_A$, necessary for diffusion. It is important to select a polynomial that can give accurate solutions for both processes at the same time. Use of a third-degree Hermitian polynomial as in the Holly–Preissmann[6] method gives acceptable solutions for the advection calculation but not necessarily for diffusion. When a third-degree polynomial is used, interpolation of the second derivative is implemented by a linear function and the third derivative is constant.[7]

For this reason, equations (22) and (23) are associated with the fifth-degree polynomial introduced above. The second derivative at the foot of the characteristic is then expressed as third-degree polynomial in terms of the Courant number Cr:

$$CXX_A(Cr) = c_1 C_{j-1}^n + c_2 C_{j-1}^n + c_3 CX_{j-1}^n + c_4 CX_j^n + c_5 CM_{j-1}^n + c_6 CM_j^n, \tag{24}$$

where

$$c_1 = (120Cr^3 - 180Cr^2 + 60Cr)(1/\Delta x_j^2), \qquad c_2 = -c_1,$$
$$c_3 = (60Cr^3 - 84Cr^2 + 24Cr)\Delta x_j, \qquad c_4 = (60Cr^3 - 96Cr^2 + 24Cr)\Delta x_j,$$
$$c_5 = (10Cr^3 - 12Cr^2 + 3Cr)\Delta x_j^2, \qquad c_6 = (-10Cr^3 + 18Cr^2 - 9Cr + 1)\Delta x_j^2.$$

In turn, the third derivative of concentration is expressed as a second-degree polynomial compatible with (24). Note that the accuracy of the second derivatives given by (24) is limited because the values CM_j are evaluated using the linear system (14).

2.3. Demonstrative computation

The numerical method described previously has been tested to demonstrate its merit by application to three specific situations: pure advection, advection–diffusion and pure diffusion in the uniform channel flow problem with constant velocity and uniform grid $\lambda_j = \mu_j = \frac{1}{2}$. All computations were carried out by three different methods: analytical, Holly–Preissman[6] and that proposed here.

2.3.1. Pure advection problem. This problem of pure advection without diffusion of an initially Gaussian concentration (i.e. equation (1) with $D_x = 0$) has an exact solution

$$C(x, t) = \exp\left(\frac{-(x-\bar{x})^2}{2\sigma_0^2}\right), \tag{25}$$

where $\bar{x}=x_0+u_0t$, when the initial and boundary conditions are

$$C(x,0)=\exp\left(\frac{-(x-x_0)^2}{2\sigma_0^2}\right), \tag{26}$$

$$C(0,t)=0. \tag{27}$$

Let the physical and grid parameters be $D_x=0$, $\Delta t=50$ s, $\Delta x_j=100$ m, $Cr=0{\cdot}5$ and $Pe=u_0\Delta x_j/D_x\to\infty$. The numerical results shown in Figure 5 for $t=10\,000$ s (i.e. after 200 time steps) were obtained by the system (7), (10) and (14) with the compatible boundary conditions (26) and (27) imposed as follows:

$$CX(x,0)=\partial C(x,0)/\partial x, \qquad CX(0,t)=0,$$

$$CM(0,t)=0, \qquad CM(L,t)=0.$$

Two computations were carried out, one with initial standard deviation $\sigma_0=264$ m (Figure 5(a)), the other with $\sigma_0=100$ m (Figure 5(b)). The standard deviation not only determines the shape of the Gaussian distribution but is also a criterion for testing a numerical method. The

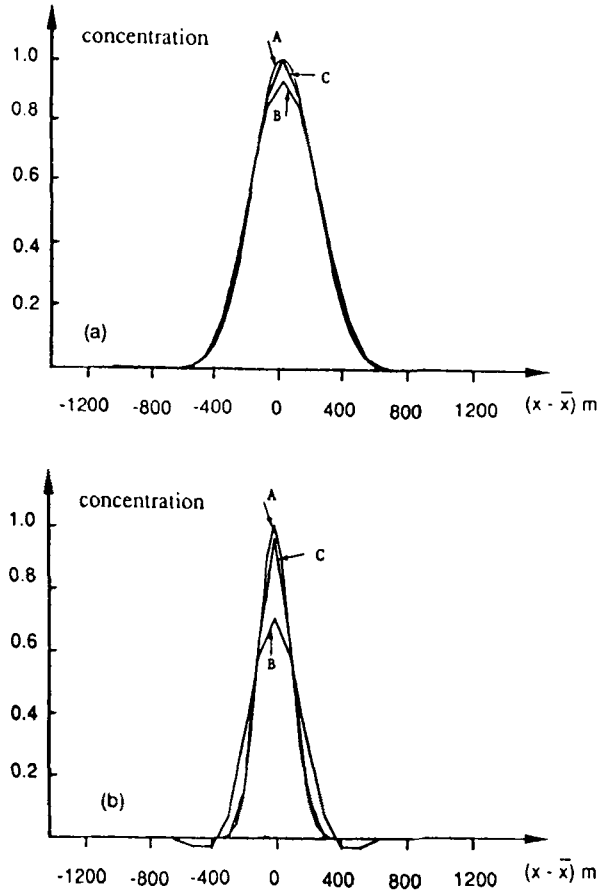

Figure 5. Results of pure advection problem for $t=10\,000$ s, $\Delta x=100$ m, $\Delta t=50$ s, $Cr=0{\cdot}5$ and $Pe=\infty$: (a) $\sigma_0=264$ m; (b) $\sigma_0=100$ m; A, analytical solution; B, Holly–Preissmann scheme; C, proposed scheme

smaller its value, the sharper is the distribution and the more difficult are the computations. The results of computations with $\sigma_0 = 100$ m show the accuracy of the proposed method for sharp variations of concentration. The method is not sensitive to the number of time steps, the results being very close after 100 and 200 time cycles. We also note that the proposed method does not introduce negative concentrations, unlike many numerical schemes in advection–diffusion problems.

The initial and boundary conditions for the first and second derivatives in equations (7), (10) and (14) should be imposed. These values are not available in practical problems. It is thus important to test the sensitivity of the method to errors in the initial and boundary estimates of the derivatives.

The second derivatives are computed at the end of each time level by solving the linear system (14) defined by the concentration and its first derivative. Consequently, the initial estimate of the second derivative does not influence the results, but the initial specification of the first derivative affects the evaluation of the second derivative at the next time level. Figure 6 shows the results after 200 time steps in a situation similar to Figure 5(a), except that the following initial condition for the first derivative, which is not compatible with (26), is imposed:

$$CX(x, 0) = 0.$$

The small degree of damping in the figure, in which the phase error is always zero, indicates that the method is slightly more sensitive to the initial estimation of the first derivative than is the two-point fourth-order method,[6] but the peak concentration is good.

In order to show the influence of the boundary condition estimates of the second derivative being inconsistent with the imposed boundary concentration, a small cosine perturbation of the boundary estimate is imposed:

$$CXX(0, t) = -\frac{4\pi^2}{T}\cos\left(\frac{2\pi t}{T}\right), \quad t > 0. \tag{28}$$

The numerical results for the system (7)–(10) are presented in Figure 7. The comparison of the numerical calculation with the exact solution shows no detectable difference in peak concentration for a small boundary perturbation $T = 50\Delta t$ or for a larger perturbation $T = 10\Delta t$. The peak concentration is not found to be affected after 100 time steps, but oscillations appear at the

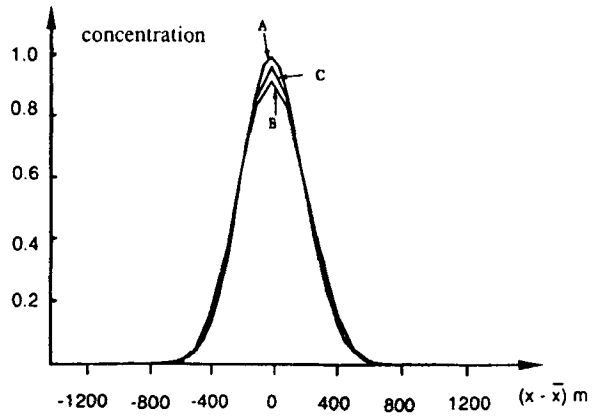

Figure 6. Results of pure advection problem for $t = 10\,000$ s, $\Delta x = 100$ m, $\Delta t = 50$ s, $Cr = 0{\cdot}5$ and $CX(x, 0) = 0$: A, analytical solution; B, Holly–Preissmann scheme; C, proposed scheme

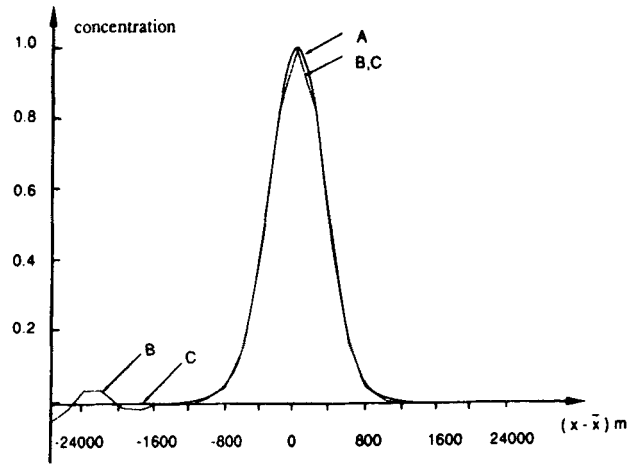

Figure 7. Results of pure advection problem for $t=1000$ s, $\Delta x=200$ m, $\Delta t=100$ s, $Cr=0{\cdot}48$ and $Pe=\infty$: A, analytical solution; B, proposed scheme using $T=10\,\Delta t$; C, proposed scheme using $T=50\,\Delta t$

beginning of the range. Consequently, if the second derivatives at boundaries are unknown, zero values can be imposed as a remedy.

2.3.2. Advection–diffusion problem. Two test problems are presented: the transport of an initially Gaussian concentration and the transport of a sharp concentration front.

In the first problem the exact Gaussian solution of the advection–diffusion equation (1) for conditions (26) and (27) is

$$C(x,t)=\frac{\sigma_0}{\sigma}\exp\left(\frac{-(x-\bar{x})^2}{2\sigma_0^2}\right), \tag{29}$$

where $\sigma^2=\sigma_0^2+2D_x t$. For the numerical solution a Courant number of 0·5 was selected with $\Delta t=96$ s and $\Delta x_j=200$ m, at which stability analysis shows that the largest numerical damping will hinder the advection calculation. The transition from strongly dominant diffusion with a Peclet number $Pe=10$ to strongly dominant advection with $Pe=40$ is presented. The results for $t=9600$ s are shown in Figure 8(a), in which the insignificant dissipative and dispersion errors due to the advection and diffusion calculations have appeared for $\sigma_0=264$ m. Figure 8(b) shows the results obtained by Holly and Preissmann's interpolation for the same situation. The proposed method performs as well as in the pure diffusion problem. It is superior to the standard Crank–Nicholson scheme and minimizes amplitude and phase errors (results not shown).

The second problem is the propagation of a discontinuous concentration front having an exact solution for equation (1),

$$C(x,t)=\frac{1}{2}\left[\operatorname{erfc}\left(\frac{x-u_0 t}{2\sqrt{(D_x t)}}\right)+\exp\left(\frac{u_0 x}{D_x}\right)\operatorname{erfc}\left(\frac{x+u_0 t}{2\sqrt{(D_x t)}}\right)\right], \tag{30}$$

for initial and boundary conditions

$$C(x,0)=0, \quad 0<x<\infty,$$

$$C(0,t)=1, \quad t>0.$$

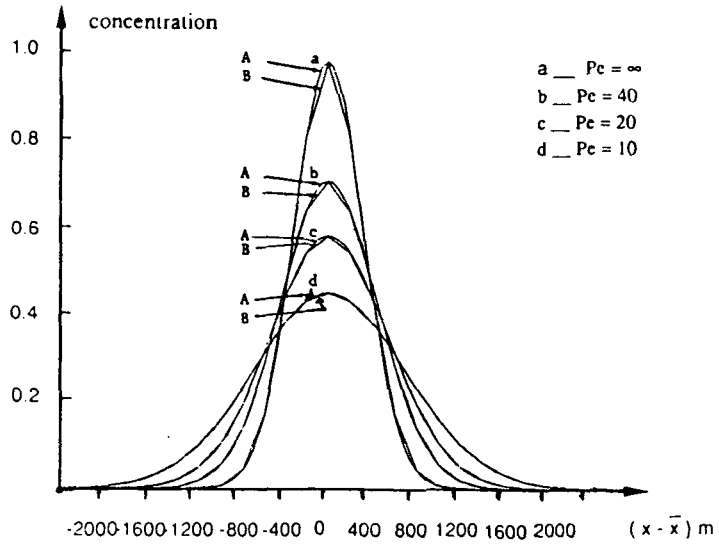

Figure 8(a). Results of advection–diffusion problem for $t = 9600$ s, $\Delta x = 200$ m, $\Delta t = 96$ s and $Cr = 0{\cdot}48$: A, analytical solution; B, proposed scheme

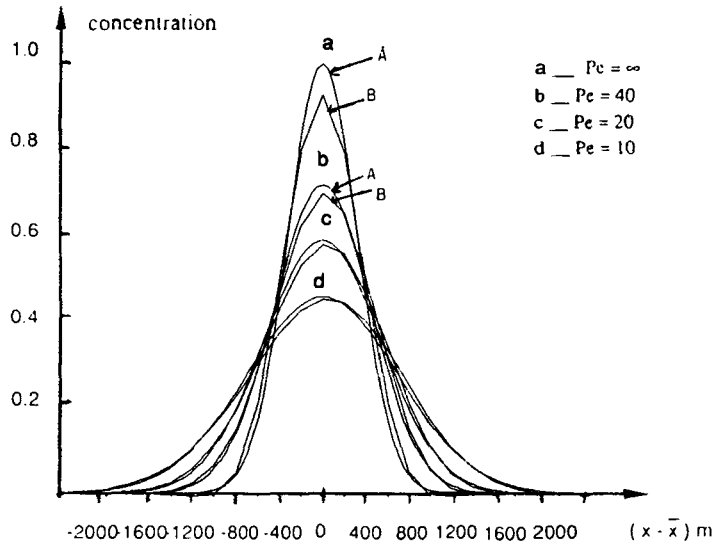

Figure 8(b). Results of advection–diffusion problem for $t = 9600$ s, $\Delta x = 200$ m, $\Delta t = 96$ s and $Cr = 0{\cdot}48$: A, analytical solution; B, Holly–Preissmann cubic polynomial

This problem is inappropriate as a demonstration of the merit of the method when diffusion is dominant. Indeed, in such a situation the discontinuous concentration is 'smoothed' and the inaccuracies of the method are hidden. For this reason, advection-dominated transport is used to test the method.

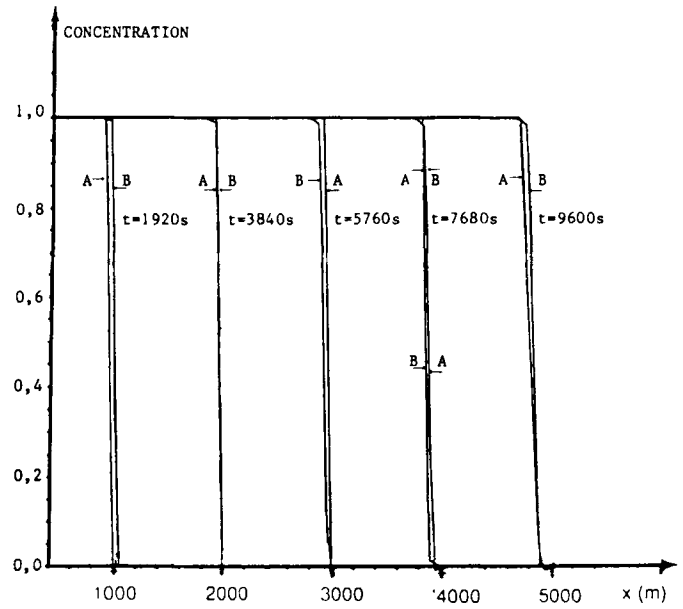

Figure 9. Results of advection–diffusion problem for $Pe = \infty$, $Cr = 0{\cdot}96$ and $\Delta x = 50$ m: A, analytical solution; B, proposed scheme

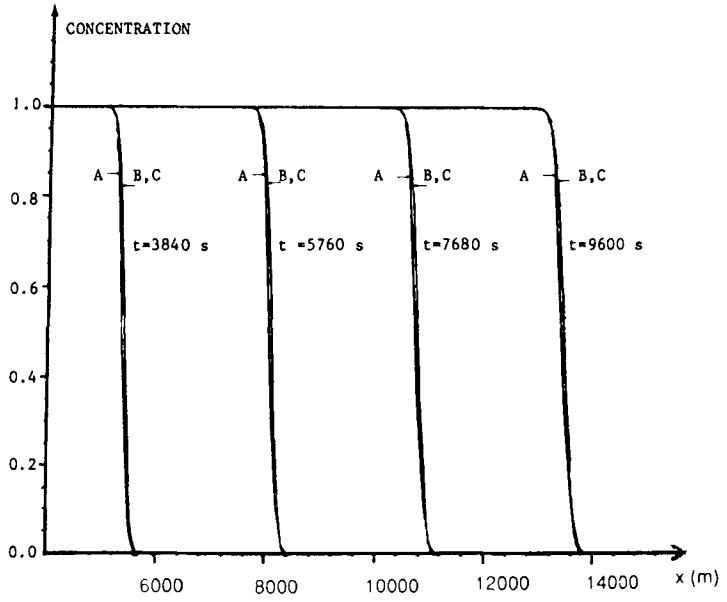

Figure 10. Results of advection–diffusion problem for $Pe = 70$, $Cr = 0{\cdot}96$ and $\Delta x = 50$ m: A, analytical solution; B, proposed scheme; C, Holly–Toda three-point diffusion

The results for $t = 9600$ s, in which $u_0 = 0{\cdot}5$ and $1{\cdot}5$ m s^{-1}, $\Delta x_j = 50$ m and $\Delta t = 96$ s are taken for pure advection ($Pe \to \infty$) and for diffusion with strongly dominant advection ($Pe = 70$) respectively, are shown in Figures 9 and 10. In the case of pure advection ($Pe \to \infty$) the analytical solution is a step function with the jump introduced over one grid point. It can be seen that no numerical oscillations are present at the upstream discontinuous point, and the undershoot phenomenon (or numerical 'dip') at the downstream discontinuous point certainly does not exist here.

3. CONCLUSIONS

For the numerical solution of the advection–diffusion transport problem in which advection is dominant, a number of numerical procedures use the method of characteristics coupled with interpolation at the foot of the characteristic in order to minimize numerical errors due to schematization of the advection term. Lower-order interpolation polynomials cannot lead to satisfactory results: linear interpolation is definitely criticizable, and third-degree spline functions and Hermitian polynomials can prove unsatisfactory in certain circumstances. This paper presents a new method of sixth-order accuracy for one-dimensional transport problems, based on an interpolation polynomial of fifth degree. The method is superior to the two-point fourth-order scheme in terms of the accuracy of the uncoupled and coupled solutions of advection–diffusion problems.

The fifth-degree polynomial is constructed using the values of the concentration and its first and second derivatives at all grid nodes instead of just the concentration values as in conventional methods. The method requires one more equation to be solved than in the two-point fourth-order method. The second derivatives are found by solving a linear tridiagonal system by means of the double-sweep method. Continuity of the third-order derivatives is assumed. The computing time is not greatly increased but the accuracy of the method is higher.

The method is in principle constructed at two computational nodes in order to be easily implemented in practical problems. The three points involved in the linear equation for the second derivative do not affect the operation of the method, because the linear system is solved at the end of each time level independently of the solution for the concentration and its first derivative.

APPENDIX: NOTATIONS

A_i	polynomial coefficients
a_i	concentration interpolation coefficients
b_i	first-derivative interpolation coefficients
c_i	second-derivative interpolation coefficients
$C(x, t)$	concentration
CX	concentration first derivative
CXX	concentration second derivative
$CXXX$	concentration third derivative
C_j^n	grid node concentration
CX_j^n	first derivative of the grid node concentration
CM_j^n	second derivative of the grid node concentration
C_A	interpolating concentration
C_P	unknown concentration
Cr	Courant number
D_x	constant diffusion coefficient in the x-direction

i	1, 2, 3, 4, 5, 6
j	number of distance step
n	number of time step
u_0	constant velocity
x	distance co-ordinate
Δx	distance step
t	time co-ordinate
Δt	time step
R_1	amplitude factor
R_2	phase factor
σ_0	initial standard deviation
σ	standard deviation depending on time
T	time period
L	wavelength

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