Journal of Hydroscience and Hydraulic Engineering
Vol. 11, No. 2, January, 1994, 49-56

NUMERICAL SIMULATION OF ADVECTIVE-DIFFUSION MASS TRANSPORT

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SYNOPSIS

Accurate solutions for the partial differential equation describing advective and diffusive transport of mass have been the focus of many investigations in recent years. Most of the solution procedures developed during these investigations have been based on the implementation of a split-operator approach. In a split-operator approach, the advection and diffusion processes are treated independently of one another. Presented in this paper is a solution technique based on a combined operator approach where the advection and diffusion processes are treated concurrently. The implementation of the solution algorithm is simple yet it provides an accurate prediction of the mass transport. Finally, comparisons with alternative schemes are presented in the paper.

INTRODUCTION

Solution of the partial differential equations describing advective and diffusive transport of mass in one and two-dimensions requires, in general, the adoption of numerical techniques. These procedures are adopted for reasons of adaptability to realistic flow characteristics. However, implementation of numerical solution techniques introduces the possibility of numerical diffusion; in some cases the magnitude of this numerical diffusion may be greater than the physical diffusion processes being modelled. The problem of controlling this numerical diffusion has been the focus of many previous studies which have lead to a number of alternative approaches.

One approach is by the use of the split-operator algorithm whereby the advective and diffusive term are solved separately. Holly and Preissman (3) obtained a high accuracy in the prediction of mass transport using a fourth order scheme in one and two-dimension with a Hermite cubic interpolating polynomial between the two points. However, the method uses not only the concentration but also the spatial derivative of the concentration as a dependent variable. Komatsu et al. (6) reported on the use of a six-point scheme as an alternative approach where the only dependent variable was the concentration. This was an extension of the eight-point method presented previously by Holly and Komatsu (4) who solved the far extreme points by using linear extrapolation. The accuracy of the method is affected in dealing with the estimation of the boundary conditions. The accuracy of the six point scheme was improved by Komatsu et al. (5), through the addition of an artificial diffusion term to compensate for the numerical diffusion. However, determination of the coefficients for this artificial diffusion is difficult, especially for non-constant flow characteristics.

Another approach to the prediction of the advective and diffusive transport of mass is through

solution of the differential equation with the advective and diffusive terms being solved concurrently. This means that the computed pollutant concentration at the next time step (n+1), accounts for the contribution due to both the advetion and diffusion processes. In this paper, an algorithm based on this approach is presented. To eliminate the possibility of numerical oscillation due to the use of a centered scheme for the advection term, weighting coefficients are introduced to the pollutant concentration in the time stepping. The method is similar concept to the technique proposed by Stone and Brian (7) but differs in the numerical algorithm used. Stone and Brian (7) assigned weighting coefficients in both the temporal and spatial direction. This complicated the algorithm especially in the determination of the coefficient values. The proposed solution technique presented here introduce weighting coefficients only in the temporal direction which simplifies the algorithm. Also, the algorithm offers a simple and accurate prediction for the one-dimensional transport of a conservative pollutant constituent.

POLLUTANT MASS TRANSPORT

Theory

The advective and diffusive transport of the mass of a pollutant constituent in a one–dimensional flow regime can be described by a partial differential equation which can be developed from a consideration of the conservation of the pollutant constituent mass. Fisher et al. (2) presents a detailed development of this equation, which for one dimensional flow is

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} = D\frac{\partial 2C}{\partial x2} \qquad (1)$$

where C(x,t) = cross–sectional average concentration of pollutant, U(x,t) = the cross sectional average velocity, D = diffusion coefficient and, x and t are the spatial and temporal locations. The diffusion coefficient, D as explained by Fischer et al. (2) accounts for mixing arising from molecular, turbulent, and effects due to differential advection. There are several assumption involved in the development of the Eq. 1; Chatwin (1) outlined these assumptions as follows:

i) The velocity field is statistically constant;
ii) Buoyancy effects are neglected;
iii) The cross-sectional area is invariant in space and time; and
iv) Complete mixing of the pollutant over the cross-section has taken place.

PROPOSED NUMERICAL SCHEME

Finite Difference Approximation

The proposed numerical solution technique described herein is based on the use of a finite difference approximation which uses the spatial-temporal grid illustrated in Fig. 1.

Using this grid, a finite difference approximation to Eq. 1 can be developed as

$$\frac{C_m^{n+1} - C_m^n}{\Delta t} + \frac{U}{2\Delta x}\left[\theta\left(C_{j+1}^{n+1} - C_{j-1}^{n+1}\right) + (1-\theta)\left(C_{j+1}^{n} - C_{j-1}^{n}\right)\right] =$$
$$\frac{D}{\Delta x^2}\left[\theta\left(C_{j+1}^{n+1} + C_{j-1}^{n+1} - 2C_j^{n+1}\right) + (1-\theta)\left(C_{j+1}^{n} - C_{j-1}^{n} - 2C_j^{n}\right)\right] \qquad (2)$$

where θ = temporal weighting coefficient and C_m = the weighted average concentration at a time level which is given by

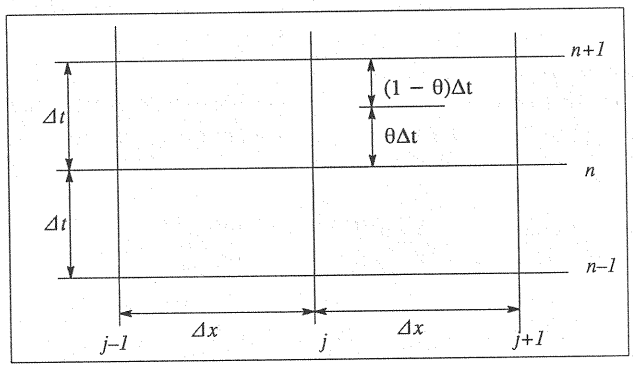

Fig. 1 Finite difference grids

$$C_m = \varepsilon_1 C_{j-1} + \varepsilon_2 C_j + \varepsilon_3 C_{j+1} \tag{3}$$

subject to the constraint that

$$\varepsilon_1 + \varepsilon_2 + \varepsilon_3 = 1 \tag{4}$$

Values for the arbitrary weighting coefficients $\varepsilon_1, \varepsilon_2, \varepsilon_3$ are obtained by mathematical manipulation to obtain the best accuracy from the numerical algorithm. These coefficients are functions of Courant number (C_r), diffusion coefficient (D), and the temporal weighting coefficient (θ), but not on the concentration itself. Thus, for a given velocity field and a known diffusion coefficient one can easily calculate the values of these arbitrary coefficients. Details of this calculation are presented more fully in a latter section.

Substitution of Eq. 3 into Eq. 2 results, after rearrangement of the terms, in

$$\left(\varepsilon_1 - \frac{\theta C_r}{2} - \theta S_x\right) C_{j-1}^{n+1} + (\varepsilon_2 + 2S_x\theta)\, C_j^{n+1} + \left(\varepsilon_3 + \frac{\theta C_r}{2} - S_x\theta\right) C_{j+1}^{n+1} =$$
$$\left(\varepsilon_1 + \frac{C_r}{2} - \frac{\theta C_r}{2} + S_x - S_x\theta\right) C_{j-1}^{n} + (\varepsilon_2 - 2S_x + 2S_x\theta) C_j^{n} +$$
$$\left(\varepsilon_3 - \frac{C_r}{2} + \frac{\theta C_r}{2} + S_x - S_x\theta\right) C_{j+1}^{n} \tag{5}$$

where C_r = the Courant number which is defined by

$$C_r = \frac{U\Delta t}{\Delta x} \tag{6}$$

and S_x = diffusion parameter which is defined by

$$S_x = \frac{D\Delta t}{\Delta x^2} \tag{7}$$

Application of Eq. 5 along a spatial domain results in a set of finite difference equations which are banded about centre diagonal. The bandwidth of this set of equations is three which enables their solution using simple tridiagonal matrix manipulation techniques.

Truncation Error

The magnitude of any potential numerical diffusion may be considered by assessing the consistency of the finite difference scheme with respect to the original partial differential equation when a Taylor's series expansion is applied. A Taylor's series about the node (j,n) in the temporal and spatial directions may be written as

$$[C]_j^{n+1} = C_j^n + \frac{\Delta t}{1!}\left\{\frac{\partial C}{\partial t}\right\}_j^n + \frac{\Delta t^2}{2!}\left\{\frac{\partial^2 C}{\partial t^2}\right\}_j^n + \frac{\Delta t^3}{3!}\left\{\frac{\partial^3 C}{\partial t^3}\right\}_j^n + \ldots \quad (8)$$

and

$$[C]_{j+1}^n = C_j^n + \frac{\Delta x}{1!}\left\{\frac{\partial C}{\partial x}\right\}_j^n + \frac{\Delta x^2}{2!}\left\{\frac{\partial^2 C}{\partial x^2}\right\}_j^n + \frac{\Delta x^3}{3!}\left\{\frac{\partial^3 C}{\partial x^3}\right\}_j^n + \ldots \quad (9)$$

Similar functions may be developed for other nodes.

Through the application of the appropriate Taylor's series in Eq. 5, the consitency and the leading term of the truncation error may be determined as

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} - D\frac{\partial^2 C}{\partial x^2} = \left[\varepsilon_3 - \varepsilon_1 + C_r(\theta - 0.5)\right] C_r \frac{\Delta x^2 \partial^2 C}{\Delta t\, \partial x^2} + \left[C_r S_x (1-\theta) + (\varepsilon_1 - \varepsilon_3 - C_r\theta)\left(S_x + \frac{C_r^2}{2}\right) + \left(\varepsilon_1 + \varepsilon_3 - \frac{1}{3}\right)\frac{C_r}{2} + \frac{C_r^3}{6}\right] \frac{\Delta x^3 \partial^3 C}{\Delta t\, \partial x^3} \quad (10)$$

In order to obtain the best accuracy for the numerical algorithm, each term of the right hand side of Eq. 10 must be equal to zero. It follows that

$$\varepsilon_3 - \varepsilon_1 + Cr(\theta - 0.5) = 0 \quad (11)$$

$$C_r S_X (1-\theta) + (\varepsilon_1 - \varepsilon_3 - C_r\theta)\left(S_x + \frac{C_r^2}{2}\right) + \left(\varepsilon_1 + \varepsilon_3 - \frac{1}{3}\right)\frac{C_r}{2} + \frac{C_r^2}{6} = 0 \quad (12)$$

Since the coefficients ε_1, ε_2, and ε_3 are arbitrary, their values can be assumed to satisfy the conditions given by Eqs. 11 and 12. Eq. 11 is satisfied by assuming that ε_1 is equal to ε_3 and that the temporal weighting coefficient θ is equal to 0.5. Knowing the values of C_r, and S_x the coefficient ε_2 can then be solved using Eq. 12. Satisfying Eqs. 11 and 12 results in the proposed finite difference approximation having a fourth order consistency with the partial differential equation.

NUMERICAL TESTS OF PROPOSED TECHNIQUE

A series of tests of the predicted pollutant mass transportation obtained using the proposed solution technique and those previously presented by Holly and Preissmann (3) and Stone and Brian (7) were undertaken. All tests were carried out on a 13km. hypothetical channel of unit width; spatial increments along the channel were constant at 200m. Flow characteristics within the channel were constant at 0.5m/s. A Gaussian pollutant mass as shown in Fig. 2 was introduced to the channel. The peak value of inflow concentration was equal to 10 units.

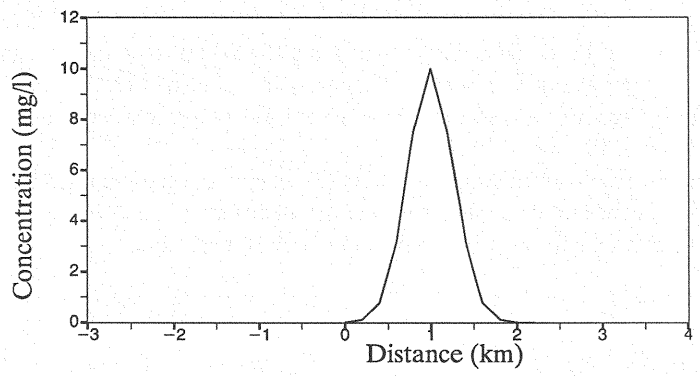

Fig.2 Initial concentration profile

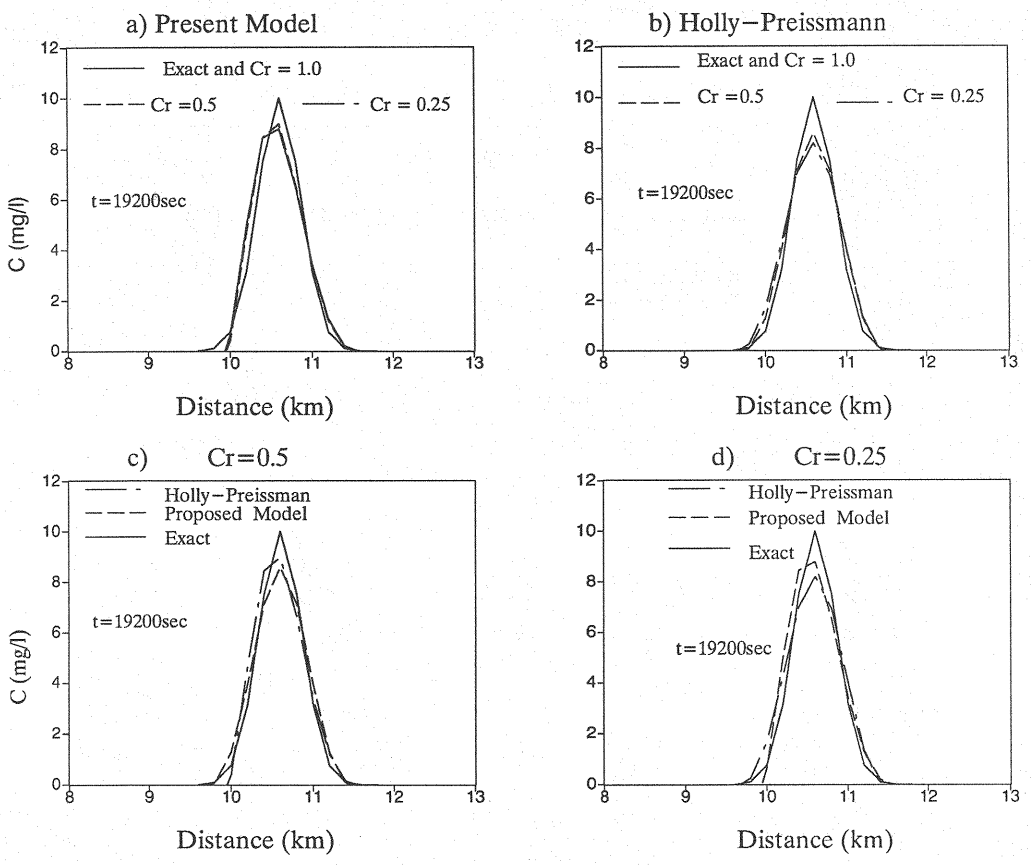

Fig. 3 Comparison of results for purely advection problem

Shown in Fig. 3 are the predicted pollutant concentration obtained for the pure advection problem. It is noted that a greater attenuation in the peak is observed for lower values of the Courant number, both for the proposed numerical model and Holly-Preissman Scheme. For a Courant number equal to 0.25, the amplitude error obtained from the proposed model is 12% after 19200 seconds. It was found that the scheme became unstable when the weighting coefficient θ was less than 0.5 and that the concentration peak could be preserved for θ approximeately 0.47 at the expense of a visible wiggle in the tail portion of

the curve. It was also found that the ideal value of θ was equal to 0.5.

Similar tests were made for the combined advection and diffusion transport of pollutant mass. Results for these tests are shown in Fig.4. The error in the peak at a time of 19200 seconds for the proposed scheme and Holly-Preissman (3) scheme are 4 percent and 7.6 percent respectively when the diffusion coefficient was equal to 1 m^2/s.

Shown in Fig. 5 are the results from Stone and Brian (7) scheme and the proposed numerical model. As far as the peak of concentration, there is no significant difference between the two schemes. However, the Stone and Brian scheme shows significant numerical dispersion.

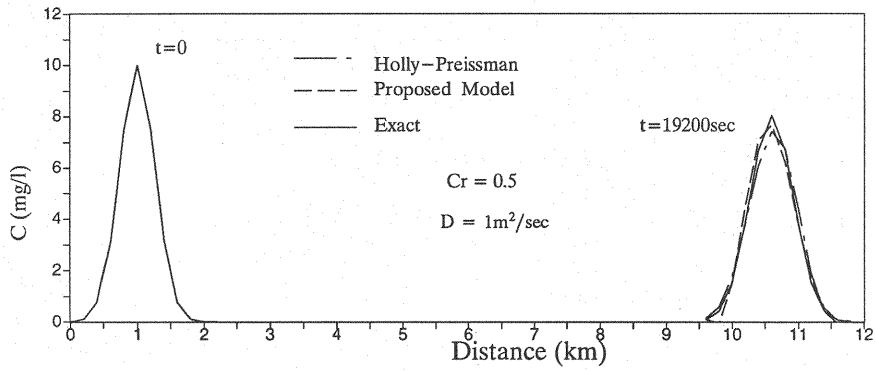

Fig. 4 Test results of present model and Holly—Preissman's scheme

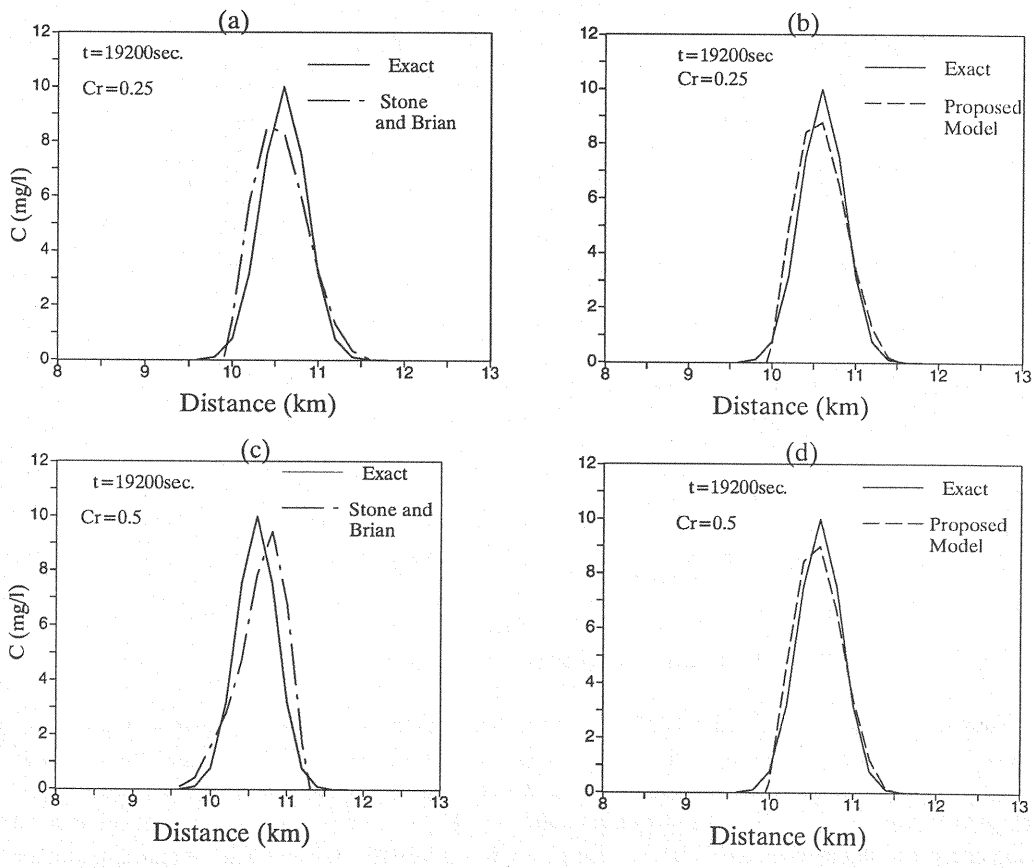

Fig. 5 Comparison between present model and Stone and Brian scheme

CONCLUSION

The proposed numerical scheme using a combined–operator approach for solution of the partial differential equation describing the advection and diffusion provides a simple yet accurate solution algorithm for water quality modeling in open channel flows. The proposed numerical scheme provides a fourth order consistency with the partial differential equation. By introducing the weighting coefficients in the temporal direction on the pollutant concentration, the numerical scheme could give high accuracy in the prediction of pollutant constituent. The amplitude and phase error in the estimation of the pollutant concentration can be greatly reduced.

ACKNOWLEDGEMENT

The authors wish to acknowledge the generousity of AIDAB for the financial support of this project and to the School of Civil Engineering for providing the computer facilities.

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APPENDIX - NOTATION

The following symbols defined below are used in this paper:

$C(x,t)$	=	cross-sectional average pollutant concentation;
C_r	=	Courant number;
D	=	diffusion coefficient;
i,j	=	grid index point;
n	=	time index;
S_x	=	diffusion parameter;
t	=	time coordinate;
$U(x,t)$	=	cross-sectional average velocity;

x	=	coordinate along x-axis;
y	=	coordinate along y-axis;
Δ	=	prefix for incremental quantity;
$\varepsilon_1, \varepsilon_2, \varepsilon_3$	=	coefficients; and
θ	=	temporal weighting coefficient.

(Received March 8, 1993; revised May 12, 1993)