INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN FLUIDS, VOL. 9, 235–244 (1989)

SHORT COMMUNICATION

PROCESS SPLITTING OF THE BOUNDARY CONDITIONS FOR THE ADVECTION–DISPERSION EQUATION

KOLAWOLE O. AIYESIMOJU AND RODNEY J. SOBEY

Department of Civil Engineering, University of California, Berkeley, CA 94720, U.S.A.

SUMMARY

Rational strategies are considered for the specification of the intermediate boundary condition at an inflow boundary where process splitting (fractional steps) is adopted in solving the advection–dispersion equation. Three lowest-order methods are initially considered and evaluation is based on comparisons with an analytical solution. For flow and dispersion parameter ranges typical of rivers and estuaries, the given boundary condition for the complete advection–dispersion equation at the end of the complete time step provides a satisfactory estimate of the intermediate boundary value. This was further confirmed by the development and evaluation of two higher-order methods. These required non-centred discrete approximations for spatial derivatives, which offset any special advantages from the higher truncation error order.

KEY WORDS Process splitting Advection–dispersion equation Boundary conditions

INTRODUCTION

For solving the one-dimensional advection–dispersion equation

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

where C is the concentration of some solute, u is the flow velocity, D is the dispersion coefficient, t is the time and x is the spatial position, the fractional step algorithm[1–3] has achieved reasonable precision and economy without recourse to higher-order approximations. It involves splitting equation (1) into its component processes of advection and dispersion respectively as follows:

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}=0, \tag{2a}$$

$$\frac{\partial C}{\partial t}=D\frac{\partial^2 C}{\partial x^2}. \tag{2b}$$

The complete problem is replaced by a succession of advection and dispersion steps, appropriate solution algorithms being utilized for the separate steps.

The major criticism of all splitting techniques[4] is that the known boundary conditions correspond to the complete differential equation and not to the split equations. This problem has received considerable attention in the context of initial value problems in two space dimensions; for example, for hyperbolic systems[5,6] and parabolic systems.[1] Leveque and Oliger[7] considered

0271–2091/89/020235–10$05.00

Received 30 December 1987
Revised 5 May 1988

boundary conditions for time-split methods for hyperbolic systems which describe transport at two disparate speeds, such as the one-dimensional long-wave equations.

These approaches all implicitly assume that higher-order estimates of the intermediate boundary condition are consistent with higher-order accuracy. In the specific context of transient mass transport response of rivers and estuaries, where advection is overwhelmingly the dominant process but with dispersion dominant over relatively short periods of time (e.g. at slack water[8]), it will be shown that the given boundary condition at the end of the complete advection–dispersion time step provides a satisfactory estimate of the intermediate boundary value despite the fact that it is a lowest-order estimate. It in fact outperforms a higher-order method.

The numerical context of this solution is the fractional step algorithm of Sobey,[3] which solves the advection step using a moving co-ordinate system. The concentration at a node remains constant during the advection step but the node location changes, generally resulting in a non-uniform grid. The dispersion step adopts the Asymmetric Dispersion Algorithm,[9] a finite difference algorithm that accommodates grid asymmetry to optimum precision at lowest order.

INFLOW AND OUTFLOW BOUNDARIES

The following discussion will be restricted to a left-hand boundary, as equivalent considerations for a right-hand boundary follow directly and do not require separate discussion. Let the spatial position of node j at time $k\Delta t$ be designated x_j^k and the numerical estimate of the solution at that position and time be designated C_j^k. Subsequently, the analytical solution to the complete advection–dispersion equation for node j at time $k\Delta t$ will be designated A_j^k, where C and A are comparable only at complete time steps. The boundary node at each half time step will be designated as $j=0$. Let the given boundary conditions to the unsplit problem at time $k\Delta t$ be $\Psi(k\Delta t)$, which is designated as Ψ^k. The given boundary conditions are then

$$C_0^n = \Psi^n \qquad \text{and} \qquad C_0^{n+1} = \Psi^{n+1} \tag{3}$$

at complete time steps where equation (1) and equations (2) correspond.

Process splitting requires also that $C_0^{n+1/2}$ (Figures 1 and 2) be specified and this is the essential problem. The geometry at left-hand inflow and outflow boundaries is illustrated in Figures 1 and 2 respectively. For an inflow boundary the advection step characteristic path to node $x_0^{n+1/2}$ comes from outside the solution domain and $C_0^{n+1/2}$ remains unknown. For an outflow boundary,

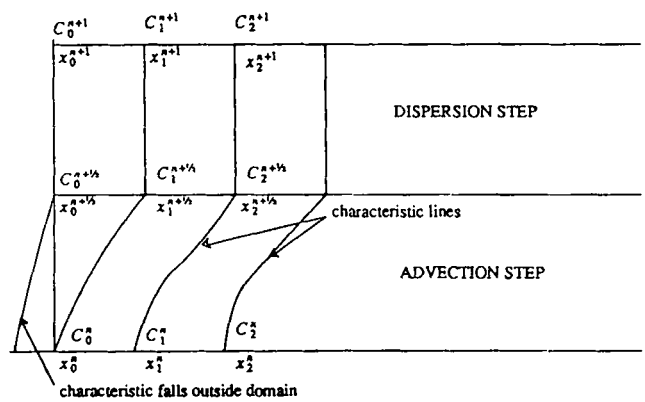

Figure 1. Process splitting at left inflow boundary

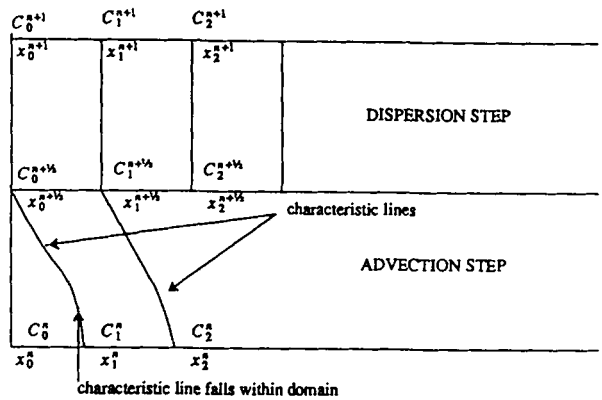

Figure 2. Process splitting at left outflow boundary

however, the advection step characteristic path to node $x_0^{n+1/2}$ comes from within the solution field. The intermediate numerical boundary condition is available from the solution of the advection step (Figure 2) as

$$C_0^{n+1/2} = C_1^n. \tag{4}$$

TAYLOR SERIES ESTIMATES OF INTERMEDIATE INFLOW BOUNDARY VALUES

Rational extrapolation in time about known boundary values C_0^n and C_0^{n+1} are based on Taylor series expansions, giving

$$C_0^{n+1/2} = C_0^n + \Delta t \frac{\partial C}{\partial t}\Big]_0^n + \frac{\Delta t^2}{2}\frac{\partial^2 C}{\partial t^2}\Big]_0^n + O(\Delta t^3), \tag{5}$$

$$C_0^{n+1/2} = C_0^{n+1} - \Delta t \frac{\partial C}{\partial t}\Big]_0^{n+1} + \frac{\Delta t^2}{2}\frac{\partial^2 C}{\partial t^2}\Big]_0^{n+1} + O(\Delta t^3). \tag{6}$$

A number of first- and higher-order approaches have been systematically adopted from equations (5) and (6) for further analysis. *Method A* is the obvious initial estimate, namely the boundary condition to the complete equation at time $(n+\frac{1}{2})\Delta t$:

$$C_0^{n+1/2} = \Psi^{n+1/2}. \tag{7}$$

This is the average of equations (5) and (6) to infinite order. *Method B* truncates equation (5) after the initial term, defining the $O(\Delta t)$ estimate:

$$C_0^{n+1/2} = \Psi^n. \tag{8}$$

Method C is the analogous $O(\Delta t)$ estimate from equation (6):

$$C_0^{n+1/2} = \Psi^{n+1}. \tag{9}$$

Initial analysis will consider these three lowest-order methods.

GLOBAL ANALYSIS

As a consequence of the moving co-ordinate system adopted for the advection step and the varying number of nodes with time, standard methods of stability analysis are inappropriate. Global analysis will be based on numerical experiments.

The numerical experiments were conducted in a dimensionless framework, in terms of Δx and Δt as the space and time scales. Equation (1) becomes

$$\frac{\partial C}{\partial t'} + u' \frac{\partial C}{\partial x'} = D' \frac{\partial^2 C}{\partial x'^2}, \tag{10}$$

where $x' = x/\Delta x$, $t' = t/\Delta t$, $u' = u\Delta t/\Delta x$ (flow parameter) and $D' = D\Delta t/\Delta x^2$ (dispersion parameter). Dropping superscripts, equation (10) reverts to equation (1) with u and D being flow and dispersion parameters respectively; t is now the number of time steps and x is the number of space steps.

The initial conditions (see Figure 3) are a Gaussian hump with a unit peak at $x = 0$ and an initial half-width of B, i.e. $C(\pm B, 0) = 0{\cdot}5$. The analytical solution is

$$C(x, t) = \left(\frac{t}{t_0} + 1\right)^{-1/2} \exp\left(\frac{-(x-ut)^2}{4D(t+t_0)}\right), \tag{11}$$

where $t_0 = B^2/4D \ln 2$. The extreme concentration gradients imposed here are typical of those conditions that maximize numerical difficulties in field applications of the advection–dispersion equation in the river and estuary context.

An integral measure of the performance of a method over the complete solution field is the normalized mean square error

$$E = \frac{1}{N} \sum_n \left[\frac{1}{L} \sum_j ((C_j^n - A_j^n)/A_{\max}^n)^2 \right]^{1/2}, \tag{12}$$

where $L(n)$ is the total number of spatial nodes at time n and N is the total number of time steps in the numerical experiment. $A_{\max}^n$ is the maximum concentration after n time steps, obtained from the analytical solution as $A_{\max}^n = (n/t_0 + 1)^{-1/2}$.

Typically, flow parameters u are of order 1 and dispersion parameters D are of order 0·01 in rivers and estuaries. Numerical experiments were conducted for u ranging from 0 to 3 and D

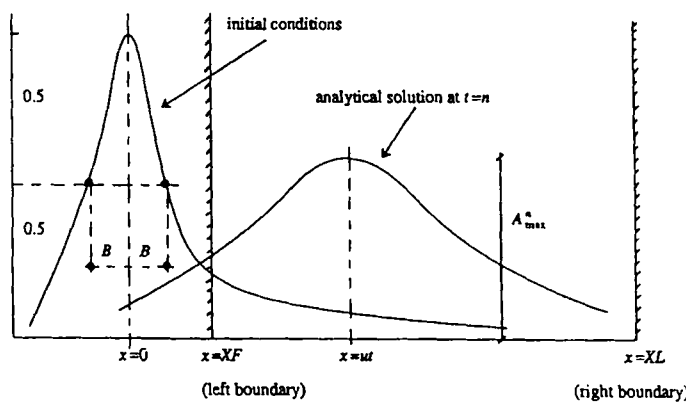

Figure 3. Boundary condition test problem

ranging from 10^{-5} to 10. For these experiments, N was 15 and $L(0)$ was 56. With an initial half-width B of 1·0 (almost beyond the resolution capability of the grid), the experiments for the most part represent the propagation of an initially steep concentration peak across the left-hand boundary and into the solution domain. The computed mean square errors E for methods A, B and C are presented in Figures 4(a), 4(b) and 4(c) respectively as contour plots.

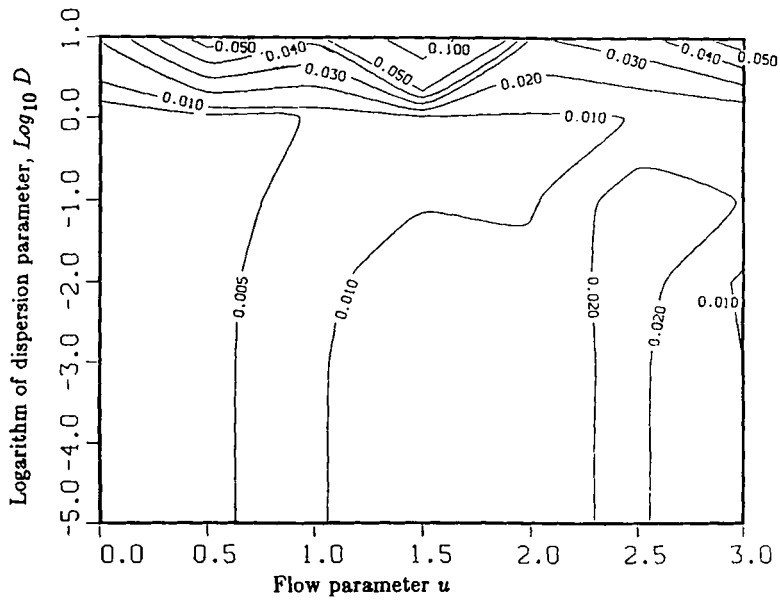

Figure 4(a). Normalized mean square error for method A

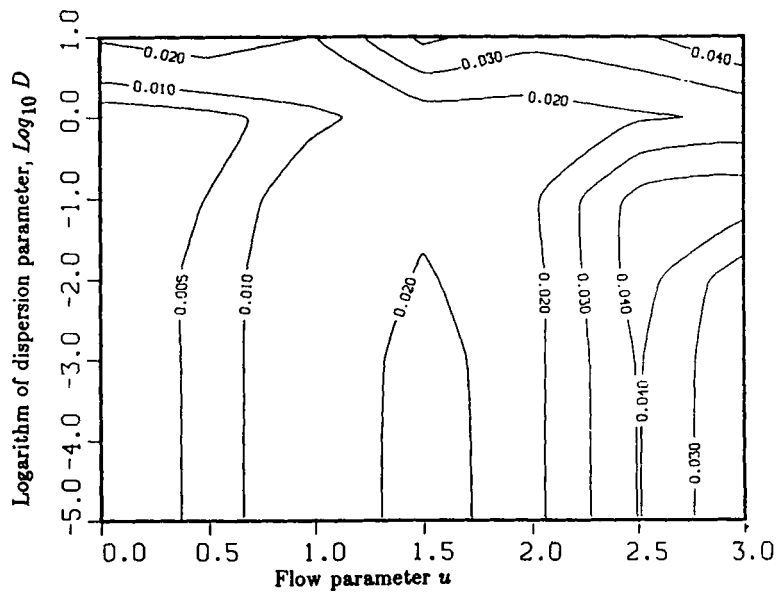

Figure 4(b). Normalized mean square error for method B

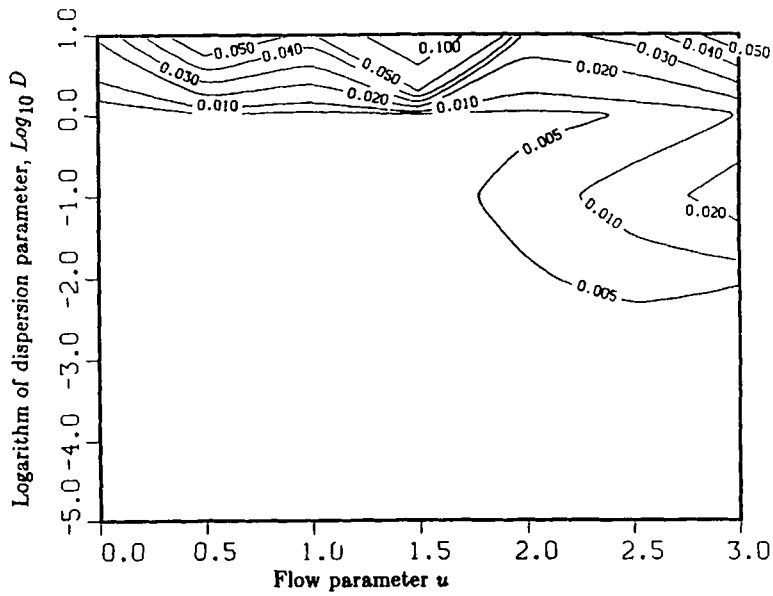

Figure 4(c). Normalized mean square error for method C

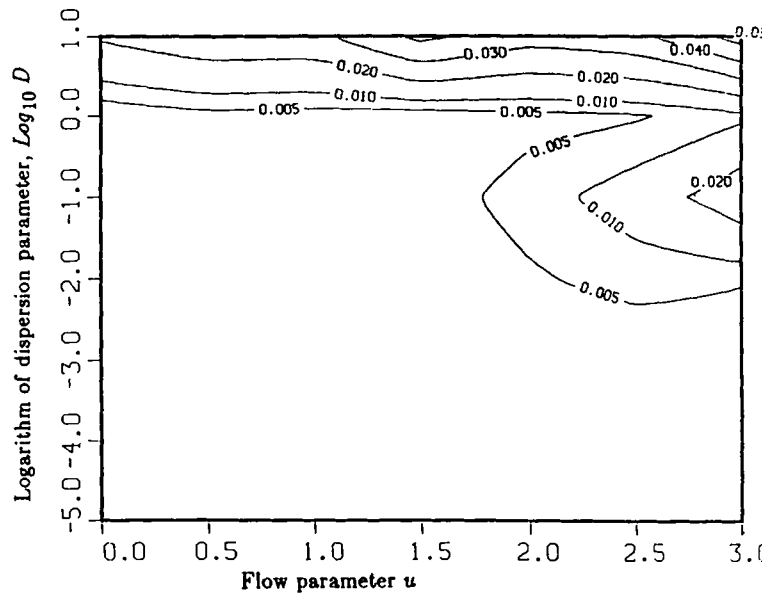

Figure 4(d). Normalized mean square error for 'exact' method

There are two significant sources of error in these computations; one is due to the intermediate boundary value specification and the other to the numerical approximation to the dispersion step. To isolate the errors due to the intermediate boundary value specification, Figure 4(d) shows the mean square errors for the 'exact' intermediate boundary value. At the beginning of each complete time step, before advection, the analytical concentration distribution is known (equation (11)). At

a left-hand inflow boundary (see Figure 3) the exact specification for $C_0^{n+1/2}$ is $C(XF-u, n)$, the concentration at $x=XF-u$ being advected during the advection step to $x=XF$. This 'exact' method for the advection step provides a truly exact solution only if there is no error in the dispersion step computation. Residual errors are attributable almost entirely to this dispersion step. Of course this 'exact' method is not available in practice, where there would be no knowledge of the concentration distribution outside the boundaries.

Comparison of Figures 4(a), 4(b) and 4(c) demonstrates the generally superior performance of method C over methods A and B, where the dispersion parameter is less than 1. The mean square errors are very small for all the methods for flow parameters less than 2 ($E<0{\cdot}02$ for method A, $E<0{\cdot}03$ for method B and $E<0{\cdot}01$ for method C). The agreement between method C and the 'exact' method is nearly perfect. The relative success of method C is clearly attributable to the major role played by advection in this parameter range. There is a local maximum of the mean square error (still $<0{\cdot}03$) at $u=3{\cdot}0$ and $D=10^{-1}$ for both method C and the 'exact' method, which is not due to the intermediate boundary specification method. In the original analysis of the fractional step algorithm (Figure 4 of Sobey[3]), plots of integrated square error also show a local peak of the error at dispersion parameters between 1 and 10 and this quite naturally is repeated in the present analysis.

For dispersion parameters in excess of 1, the results deteriorate for all the methods, including the 'exact' method. The asymmetric dispersion algorithm[9] was not designed for such large dispersion parameters, which rarely occur in rivers or estuaries. In the advection-dominated context of rivers and estuaries, method C is satisfactory throughout the parameter range and would clearly be chosen over methods A and B.

The mean square error provides a global measure of the performance of the various intermediate boundary value estimators, but reveals little of response extremes. The maximum and minimum normalized differences (i.e. the largest positive and largest negative differences) between the computed solution C_j^n and the analytical solution A_j^n over all nodes and all time steps are

$$E_{\max}=\max_n\left\{\max_j\left\{\frac{C_j^n-A_j^n}{A_{\max}^n}\right\}\right\} \quad \text{and} \quad E_{\min}=\min_n\left\{\min_j\left\{\frac{C_j^n-A_j^n}{A_{\max}^n}\right\}\right\}. \tag{13}$$

For dispersion parameters less than 1 and flow parameters less than 2, values of $E_{\max}$ and $E_{\min}$ generally confirm[10] the superiority of method C and its closeness to the 'exact' method. In addition, the maximum error bounds for method C remain acceptably small (approximately $-0{\cdot}04$ to $0{\cdot}03$). Outside this parameter range the maximum error bounds increase substantially. Within active parameter ranges for river and estuarine situations, however, these results confirm that method C provides an appropriate estimate of the intermediate boundary value.

HIGHER-ORDER ESTIMATES

The above analysis provides compelling evidence to recommend the adoption of method C without further consideration. Further confirmation, however, is provided by higher-order approximations from equations (5) and (6) respectively.

Method D is based on equation (5). The Taylor series expansion for $C_0^{n+1/2}$ about C_0^n traverses the region of the solution domain governed not by the full advection–dispersion equation but by the advection equation (equation (2a)), which implies that

$$\frac{\partial C}{\partial t}\Big]_0^n=-u\frac{\partial C}{\partial x}\Big]_0^n.$$

In addition, where u is constant (a convenient but not a necessary assumption),

$$\left.\frac{\partial^2 C}{\partial t^2}\right]_0^n = u^2 \left.\frac{\partial^2 C}{\partial x^2}\right]_0^n.$$

Substituting for

$$\left.\frac{\partial C}{\partial t}\right]_0^n \quad \text{and} \quad \left.\frac{\partial^2 C}{\partial t^2}\right]_0^n$$

in equation (5) gives

$$C_0^{n+1/2} = C_0^n - u\Delta t \left.\frac{\partial C}{\partial x}\right]_0^n + \frac{u^2\Delta t^2}{2} \left.\frac{\partial^2 C}{\partial x^2}\right]_0^n + O(\Delta t^3). \tag{14}$$

A discrete approximation to the second derivative at the left-hand boundary will require at least three spatial nodes: the boundary node 0 and the next two internal nodes 1 and 2. It is convenient to use these same three nodes to approximate the first derivative. These non-centred approximations are[10]

$$\left.\frac{\partial C}{\partial x}\right]_0^n = \frac{1}{\Delta r}\left\{\frac{-(3+A)}{2(1+A)} C_0^n + \frac{2}{1-A^2} C_1^n - \frac{1+A}{2(1-A)} C_2^n\right\}, \tag{15}$$

$$\left.\frac{\partial^2 C}{\partial x^2}\right]_0^n = \frac{1}{\Delta r^2}\left\{\frac{1}{1+A} C_0^n - \frac{2}{1-A^2} C_1^n + \frac{1}{1-A} C_2^n\right\}, \tag{16}$$

where $A = (x_1^n - x_0^n - \Delta r)/\Delta r$ and $\Delta r = (x_2^n - x_0^n)/2$. Equations (15) and (16) can be used in equation (14) to establish the predictive equation for method D:

$$C_0^{n+1/2} = C_0^n - \frac{u\Delta t}{\Delta r}\left\{\frac{-(3+A)}{2(1+A)} C_0^n + \frac{2}{1-A^2} C_1^n - \frac{1+A}{2(1-A)} C_2^n\right\} + \frac{1}{2}\left(\frac{u\Delta t}{\Delta r}\right)^2 \left\{\frac{1}{1+A} C_0^n - \frac{2}{1-A^2} C_1^n + \frac{1}{1-A} C_2^n\right\}. \tag{17}$$

This is the asymmetric equivalent of the well known downwinding algorithm.

Similarly for *Method E*, equation (6) is rearranged as

$$C_0^{n+1/2} = C_0^{n+1} - \Delta t\left\{\frac{1}{2}\left.\frac{\partial C}{\partial t}\right]_0^{n+1} + \frac{1}{2}\left.\frac{\partial C}{\partial t}\right]_0^{n+1/2}\right\} + O(\Delta t^3). \tag{18}$$

Equation (2b) is the governing equation in this solution region, giving

$$C_0^{n+1/2} = C_0^{n+1} - \frac{D\Delta t}{2}\left\{\left.\frac{\partial^2 C}{\partial x^2}\right]_0^{n+1} + \left.\frac{\partial^2 C}{\partial x^2}\right]_0^{n+1/2}\right\} + O(\Delta t^3). \tag{19}$$

Substituting for $\partial^2 C/\partial x^2$ from equation (16) gives method E as

$$C_0^{n+1/2} = C_0^{n+1} - \frac{D\Delta t}{2\Delta r^2}\left\{\frac{1}{1+A}(C_0^{n+1/2} + C_0^{n+1}) - \frac{2}{1-A^2}(C_1^{n+1/2} + C_1^{n+1}) + \frac{1}{1-A}(C_2^{n+1/2} + C_2^{n+1})\right\}. \tag{20}$$

Evaluation of these higher-order estimates for the intermediate boundary condition is again based on the global mean square error. Figures 5(a) and 5(b) show the flow–dispersion

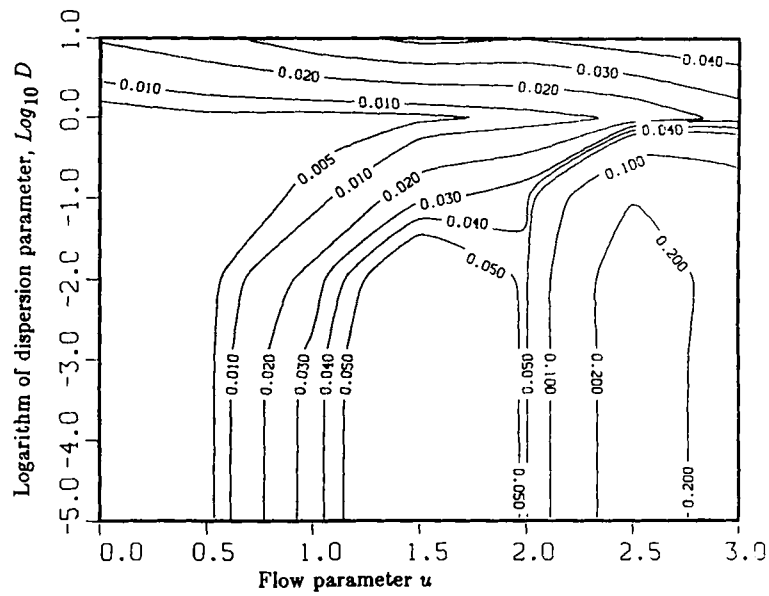

Figure 5(a). Normalized mean square error for method D

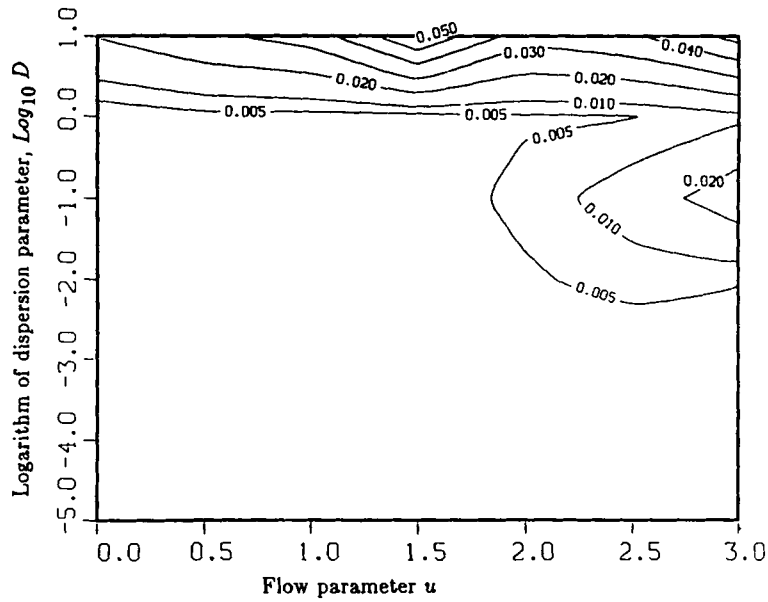

Figure 5(b). Normalized mean square error for method E.

dependency for methods D and E respectively. Method D in particular performs quite poorly in comparison with the 'exact' method, mean square errors exceeding 0·05 in the river and estuarine parameter range ($u<2$, $D<1$). Method D is in fact significantly less satisfactory than any of the $O(\Delta t)$ estimators in Figures 4(a)–4(c). This is not surprising, however, given the very substantial distortions that are a direct consequence of downwinding. Figure 5(b) on the other hand is almost

identical to Figures 4(c) and 4(d). As expected perhaps because of its close relationship to method C, the performance of method E is excellent, but the non-centred discrete approximations have almost exactly offset any advantage from the higher truncation error order. There is no measurable improvement over method C.

CONCLUSIONS

Three lowest-order approximations (methods A, B and C) for specifying the intermediate boundary value in the fractional step solution of the advection–dispersion equation were initially evaluated. Method A adopts the known boundary condition to the complete equation at the intermediate time. Methods B and C are $O(\Delta t)$ estimates from the known boundary conditions at times $n\Delta t$ and $(n+1)\Delta t$ respectively.

The performance of method C was excellent for flow parameters less than about 2 and dispersion parameters less than about 1, the range of typical river and estuarine flows for which the fractional step algorithm was designed.

Methods D and E investigated the potential of higher-order approximations. Their performance was, however, disappointing as they required estimates of spatial derivatives at the boundary. The consequent non-centred discrete approximations offset any potential advantage from the higher truncation error order. For method D in particular the downwinding errors became dominant. Method E was almost identical to method C, which because of its simplicity and accuracy remains the recommended approach for typical river and estuarine systems.

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