INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN FLUIDS, VOL. 15, 1259–1275 (1992)

A FLUX-BASED MODIFIED METHOD OF CHARACTERISTICS

PATRICK J. ROACHE

Ecodynamics Research Associates, Inc., PO Box 9229, Albuquerque, NM 87119-9229, U.S.A.

SUMMARY

A flux-based modified method of characteristics (MMOC) methodology in 1D is described which has the following properties: unconditional stability (though explicit), exact answers for integer *CFL* (Courant) numbers, completely conservative (locally and globally) and able to utilize various flux limiters and various characteristic- (trajectory-) tracking algorithms. The use of characteristics based on cell-wise constant characteristic velocities results in considerable code simplification, and Van Leer's MUSCL is an accurate and cost-effective flux limiter. For $CFL>1$ the flux limiter is applied only to the non-integer part of *CFL*, whereas the integer part is exact for constant velocities; therefore accuracy improves with larger *CFL*. It is not a cheap algorithm, although explicit, because the operation count per time step increases with the integer part of *CFL*, but it is much more accurate than the commonly used implicit upstream differencing. This flux-based MMOC method is well suited for groundwater flow calculations in which large local Courant numbers arise owing to grid clustering.

KEY WORDS Characteristics Conservation Flux limiters

INTRODUCTION

In the reservoir simulation communities (both hydrocarbon and water), especially for two-phase flows, implicit upstream differencing is still a commonly used method for treating advection terms, as in the discretization of the constant coefficient model equation

$$\partial f/\partial t = -u\,\partial f/\partial x \tag{1}$$

for $u>0$ by

$$f(i, n+1) = f(i, n) - CFL(f(i, n+1) - f(i-1, n+1)), \tag{2}$$

where *CFL* is the Courant number (or Courant–Friedrichs–Lewy number)

$$CFL = u\Delta t/\Delta x. \tag{3}$$

This widespread use of implicit upstream differencing occurs in spite of the well-known and serious accuracy problems associated with the implicit artificial viscosity of the method. Explicit upstream differencing

$$f(i, n+1) = f(i, n) - CFL(f(i, n) - f(i-1, n)), \tag{4}$$

is bad enough, with a simple Taylor series analysis[1] indicating the transient artificial viscosity

0271–2091/92/231259–17$13.50

Received 12 September 1991
Revised 8 April 1992

coefficient

$$\alpha_e(\text{explicit upstream}) = (u\Delta x/2)(1 - CFL), \tag{5}$$

but the implicit upstream method gives

$$\alpha_i(\text{implicit upstream}) = (u\Delta x/2)(1 + CFL). \tag{6}$$

We note immediately that at least the explicit upstream method for the constant coefficient model equation gives the exact answer for $CFL = 1$, i.e. $f(i, n+1) = f(i-1, n)$, whereas the implicit upstream differencing method never does. More significantly, the artificial viscosity of the implicit upstream method gets very bad for $CFL \gg 1$, which is, after all, the only condition which justifies its use compared to explicit upstream differencing. Comparing $CFL = 0{\cdot}5$ for explicit and $CFL = 5$ (considered low) for implicit, this simple analysis indicates $(1+5)/(1-0{\cdot}5) = 12$ times the artificial viscosity. (Also note that explicit upstream differencing has the transportive property,[1] whereas implicit upstream differencing, and indeed all other implicit methods, do not.)

NON-FLUX-BASED MMOC DERIVATIONS OF DIFFERENCE METHODS

Recently, many authors (see e.g. References 2–19) have been developing and applying the modified method of characteristics (MMOC) and related methods ('Eulerian–Lagrangian' methods, etc.) to these problems in both a finite difference and a finite element framework. (For the history and scholarly comparisons of these various characteristics-based methods, see Reference 2 or 3 and the recent review of 'semi-Lagrangian' methods by Staniforth and Côté.[20]) The MMOC approach takes a Lagrangian viewpoint, or particle tracking, for advection. Basically, the evolutionary equation is a discrete analogue of the substantial derivative equation $D(f)/Dt = 0$, expressed as

$$f(i, n+1) = f\# = f(x\#, n). \tag{7}$$

The location $x\#$ at the 'foot' of the characteristic is found by ray-tracing the velocity field backwards from $(x(i), n+1)$ to time level n. Then the value $f\# = f(x\#, n)$ is found by interpolation in the 'core' cell or 'core element'[3] containing the foot of the characteristic.

Consider constant $u > 0$ and $CFL < 1$; then $x\#$ lies between $x(i-1)$ and $x(i)$ as in Figure 1. If $f\# = f(x\#)$ is evaluated by linear interpolation between $x(i-1)$ and $x(i)$, with CFL being the interpolation parameter, the result is just explicit upstream differencing, equation (2). If quadratic interpolation between $x(i-1)$, $x(i)$ and $x(i+1)$ is used, the result is just Leith's method or (for the single constant u-equation) the Lax–Wendroff method,

$$f(i, n+1) = f(i, n) - (CFL/2)(f(i+1, n) - f(i-1, n)) + (CFL^2/2)(f(i+1, n) - 2f(i, n) + f(i-1, n)). \tag{8}$$

See e.g. Reference 1. (Although equation (8) is specific to both u and Δx constant, quadratic interpolation still gives the generalization of Lax–Wendroff for variable Δx.)

We see again what often happens in CFD, that distinctions in 'methods' such as finite difference versus finite element versus finite volume, or in this case finite difference versus method of characteristics, are often distinctions not in the numerical 'method' at all but rather in the 'methodology' used to derive the numerical method; see e.g. Reference 21. However, the methodology can be very significant. For example, the usual methodology of finite differences is based on Taylor series expansions which presume the existence of ever higher derivatives, whereas the MMOC approach only requires interpolation accuracy, which is satisfied with the weaker

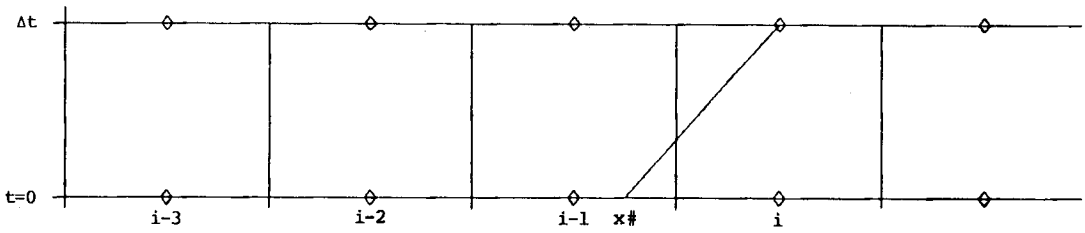

Figure 1. Non-flux-based MMOC derivation of difference equations for $CFL<1$

Lipschitz condition. More importantly, the Taylor series approach alone would never suggest (we maintain) the extension of the explicit method for $CFL>1$, which is obvious from the MMOC viewpoint, as shown in Figure 2 for $2<CFL<3$, namely linear interpolation for $f(x\#)$ between $i-3$ and $i-2$ for upstream and quadratic interpolation for $f(x\#)$ between $i-3$, $i-2$ and $i-1$ for Lax–Wendroff.

The original interpretation of the CFL stability limit $CFL<1$ for explicit methods (as given by CFL themselves[22]) was based on characteristics theory and terminology, namely that the discrete domain of influence must include the continuum domain of influence, which reduces to requiring that the explicit upstream method must interpolate for $f(x\#)$, not extrapolate. (Note that this is so well known by now that it seems intuitively obvious, but it was not, since CFL required good mathematics to prove it.) The same interpretation holds for MMOC, but since the interpolation interval is changed for $CFL>1$, there is no stability limitation, i.e. this explicit method is unconditionally stable.[3,20,23] (Is *this* intuitively obvious?) For u constant and Δx constant this MMOC viewpoint results in a simply shifted finite difference algorithm and one obtains the exact solution not just for the condition $CFL=1$ but for $CFL=$any integer, the exact solution being $f(i, n+1)=f(i-CFL, n)$.

When the backward-tracked characteristic extends beyond the spatial domain of the problem, say to the left of $x(1)$, the interpolation is now done over the possibly time-dependent boundary conditions, between $f(x(1), n+1), f(x(1), n), f(x(1), n-1)$, etc. Since these may be known in some continuum (possibly analytic) basis, these may be more accurate evaluations (not requiring spatial discretization), so the influence of boundaries can be more accurate than with the 'interior' discretizations.[24]

TWO PROBLEMS WITH NON-FLUX-BASED MMOC

There are two problems with this standard finite difference non-flux-based MMOC methodology, namely non-conservation and 'wiggles'. When applied to the variable coefficient problem (varying u), the method is not conservative. Several authors note this[5–9,13,14,20] and find for their problems that the error is tolerable. (The ELLAM method of Celia *et al.*[2] is globally conservative, at least for the constant coefficient problem.) The wiggles[1] are of course easily cured by two-point linear interpolation, i.e. upstream differencing, but the accuracy suffers. We want to use higher-order interpolation, i.e. Lax–Wendroff differencing, but this is subject to bad oscillations for steep fronts, so we also want to use a non-linear flux limiter such as FCT (flux-corrected transport),[25–28] TVD (total-variation-diminishing methods, see e.g. References 29–36), ENO (essentially non-oscillatory),[37,38] PPM (piecewise parabolic method):[39] or UL (ULTIMATE limiter),[40] but these are not readily applied to the non-conservation (substantial derivative) form of the governing equations.

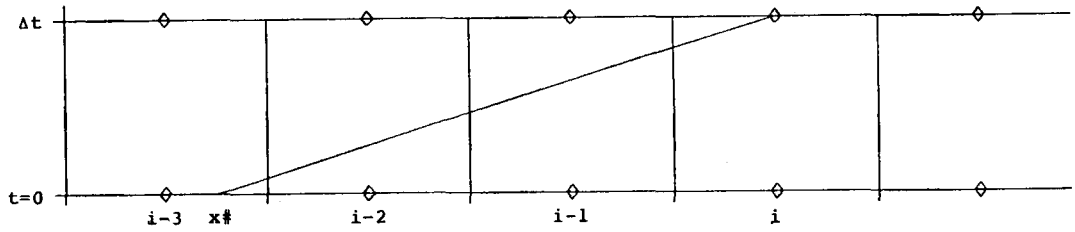

Figure 2. Non-flux-based MMOC derivation of difference equations for $CFL>1$

Fortunately, both these problems are solved by adoption of a flux-based MMOC methodology (FB-MMOC), which we now describe. (See Reference 41 for an earlier description and preliminary results.)

FLUX-BASED MMOC DERIVATIONS OF DIFFERENCE METHODS

Adopting now a finite volume viewpoint, as shown in Figure 3 for $CFL<1$, we focus on the evaluation of fluxes into and out of the control volume consisting of cell i. We know that conservation is guaranteed (independently of accuracy) if the flux into the cell at i over the left face (at '$i-\frac{1}{2}$') is algebraically identical to the flux out of the cell at $i-1$ over the same face. Also, the face fluxes are all that we need to apply the now highly developed machinery of flux limiters to control the wiggles.

For $CFL<1$ as shown in Figure 3, the integrated flux across the left face of cell i is given by $f\#_L U_L \Delta t$, where U_L is the fluxing velocity at the left face, perhaps interpolated to $\Delta t/2$ between time levels n and $n+1$, and $f\#_L$ is the value of f interpolated to the foot of the characteristic that passes through the centre (at $\Delta t/2$) of the left face. (Note the underlying assumption of linear variation, i.e. second-order accuracy.) Similarly for the flux through the right face with fluxing velocity U_R. The corresponding flux-based time-stepping formula is

$$f(i, n+1)=f(i, n)-\Delta t(U_R f\#_R - U_L f\#_L/\Delta x. \tag{9}$$

In this finite volume viewpoint, the fs are spatial control volume averages, rather than nodal values, whereas the $Uf\#$ terms are time averages. The flux-based time-stepping derivation requires lower-order interpolation to generate the same difference methods as the non-flux-based MMOC, i.e. linear interpolation for flux quantities $f\#$ now yields the Lax–Wendroff method and piecewise constant (upstream-biased) 'interpolation' yields the explicit upstream differencing method.

ERRONEOUS FLUX-BASED MMOC METHODOLOGY FOR $CFL>1$

The obvious next step is to extend this derivation for the flux-based MMOC to $CFL>1$, as in the non-flux-based MMOC. However, there is a key point involved in evaluating the face fluxes. A naive and disastrous methodology consists simply of using the MMOC to track back the time-centred face flux quantities, $f\#_L$ at $x(i-\frac{1}{2}, n+\frac{1}{2})$ and $f\#_R$ at $x(i+\frac{1}{2}, n+\frac{1}{2})$, as shown in Figure 4(a), and again apply the flux-based time-stepping formula, equation (9).

The inadequacy of this approach is demonstrated by the counter-example (provided by Dr. K. Salari) shown in Figure 4(b). Considering $CFL\gg 1$ and a step function profile which is

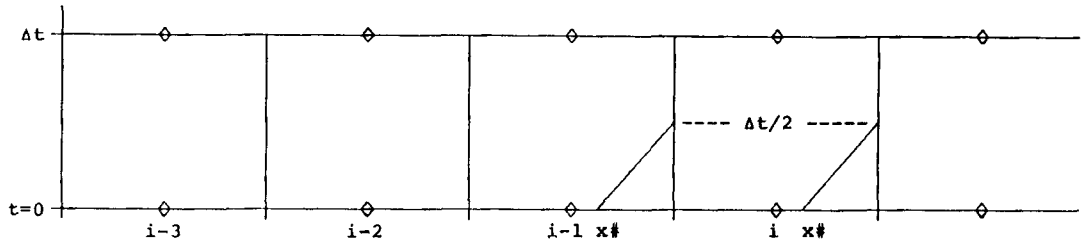

Figure 3. Flux-based MMOC derivation of difference equations for $CFL<1$

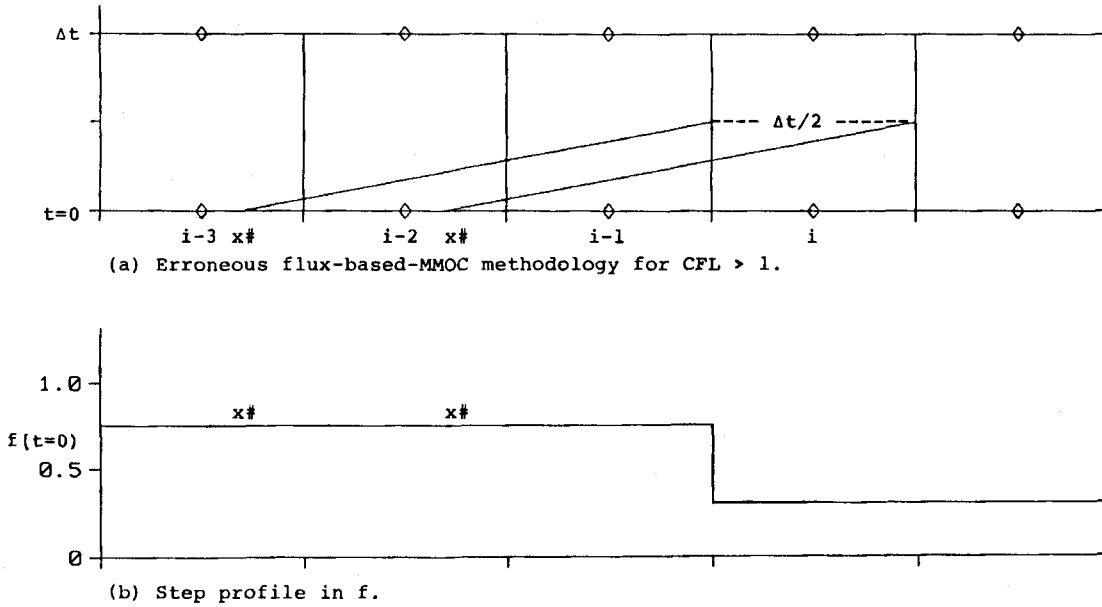

Figure 4. Flux-based MMOC derivation of difference equations for $CFL>1$

advected to the right, it is clear that the fluxes into and out of the cell at i to the right of the step profile are identical and hence the application of equation (9) at i calculates no change!

CORRECT FLUX-BASED MMOC METHODOLOGY FOR $CFL>1$

The key point is to evaluate the sum of flux contributions over all intermediate cells, as in the work of Russell[42] and the ELLAM method of Celia *et al.*[2] Basically, from a finite volume viewpoint (or perhaps finite element in time? or McCormick and Cai's[43] 'finite volume element'?) we need to evaluate the integral of flux across the cell face over time. In the naive FB-MMOC above we attempted a trapezoidal rule integration

$$\int_t^{t+\Delta t} f(i-\tfrac{1}{2}, t)\, U\, \mathrm{d}T = f\#\ U(n+\tfrac{1}{2})\,\Delta t + O(\Delta x^2, \Delta t^2). \tag{10}$$

Although centred in time and therefore 'second-order-accurate', the method can fail for $CFL>1$ when the midpoint value may not be a good representation of the average.

The correct methodology is to approximate the integral by piecewise constant increments from each upstream cell, located by characteristic tracking:

$$\int_t^{t+\Delta t} f(i-\tfrac{1}{2}, t)\, U\, dT = f(i-1, n)\, \tau(i-1)\, Uc(i-1) + f(i-2, n)\, \tau(i-2)\, Uc(i-2) + f(i-3, n)\, \tau(i-3)\, Uc(i-3) + \ldots + f\#_L(\Delta t - t_{bot})\, Uc(\#). \quad (11)$$

The notation is clumsy, but the methodology is easily described geometrically, as in Figure 5. The notation is simplified if we start the time step at $t=0$. (For a general method of trajectory tracking, the characteristic lines in Figure 5 could be curved.) The unmarked solid characteristic lines indicate characteristics tracked forwards from the edges of upstream computational cells. The characteristic line marked by triangles is tracked backwards from the end of the time step Δt. The dashed characteristic line is tracked backwards from $t\#$, the centre of the last (partial) cell time interval. The τs are partial time increments. The Ucs are the fluxing velocities at the cell face, (possibly) interpolated to time level tc. The tcs are time levels at the centre of the partial time increments. The time level t_{bot} is determined by the intersection of the leading-face characteristic from cell $i-iCFL$ to the face at $i-\frac{1}{2}$. The index value $i-iCFL$ is the i-index of the 'core cell' for the face at $i-\frac{1}{2}$, i.e. the most upstream cell whose leading-face characteristic reaches the cell face $i-\frac{1}{2}$ (at which we are evaluating the flux). The characteristic tracked forwards from the trailing face of cell $i-iCFL$ is above $t+\Delta t$ at the location $i-\frac{1}{2}$.

This flux-based MMOC methodology incorporates many possible methods, with differences primarily involved with the following four evaluations.

The fluxing velocities at the interfaces

These are the terms $Uc(i-ii)$, where ii runs from 1 to $iCFL$. A more suggestive notation for $Uc(i-ii)$ is $U(i-\frac{1}{2}, tc(i-ii))$, where $tc(i-ii)$ is the centre of the partial time interval corresponding to the characteristic boundaries tracked from both edges (trailing and leading) of cell ii.

For an independently determined velocity field, as in the case of passive scalar (contaminant or radionuclide) transport, the obvious choice consistent with second-order accuracy is linear

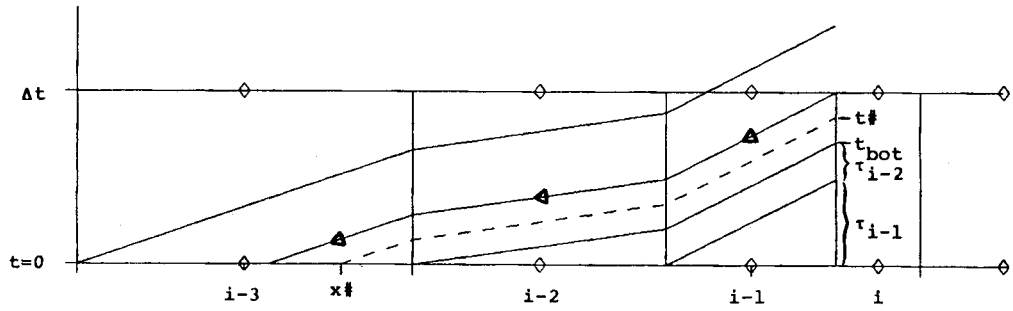

Figure 5. Flux-based MMOC methodology at interior point for $CFL>1$, illustrated for cell-wise constant characteristic (C^3) velocities. Unmarked solid characteristics are tracked forwards from the edges of the upstream computational cells. The characteristic marked ◁ is tracked backwards from the end of the time step Δt. The dashed characteristic is tracked backwards from the interpolated time level $t\# = \frac{1}{2}(\Delta t + t_{bot})$ to $x\#$, the location of the interpolated $f\#$

interpolation to $tc(i-ii)$ in time over $U(i-\frac{1}{2}, n)$ and $U(i-\frac{1}{2}, n+1)$. That is, once $tc(i-ii)$ has been determined from the geometry of Figure 5, we calculate

$$UC(i-ii) = U(i-\tfrac{1}{2}, tc(i-ii))$$
$$= U(i-\tfrac{1}{2}, n) + (tc(i-ii)/\Delta t)\,(U(i-\tfrac{1}{2}, n+1) - U(i-\tfrac{1}{2}, n)). \quad (12)$$

Higher-order interpolations over more time levels are also possible. For non-linear problems the time-step could be iterated for a predictor–corrector evaluation or the fluxing velocities could be simply lagged in time, i.e. all $Uc = U(i-\frac{1}{2}, n)$. This lagged value can also be used for linear problems, avoiding the computations for tcs and for equation (12). If the velocity field were slowly varying compared to the advected variable f, this would be recommended. It also improves the operation count for $CFL \gg 1$ (see below).

Note that by notation like '$i-\frac{1}{2}$' we mean the cell interface between cells i and $i-1$, which is not necessarily half-way in physical space between the cell centres. In the finite volume formulation used here, the discrete velocities are actually defined at interfaces between cells, not at the cell centres, so no spatial interpolation is involved in determining $U(i-\frac{1}{2}, n)$, etc. (In the actual Fortran implementation the velocity arrays are defined at the trailing faces of cells, so that the Fortran '$U(I, N)$' corresponds to '$U(i-\frac{1}{2}, n)$' here.)

Although the present methodology is also applicable to a node-centred finite difference formulation, the finite volume formulation, with heads (pressures) defined at cell centres and velocities at faces (the venerable marker-and-cell approach[44,45] or 'block-centred finite difference method'[9]), is a 'mixed' method which, like the 'mixed finite element' methods, has significant advantages.[9] When the Darcy flow continuity equation in terms of head is solved, a discrete continuity equation is satisfied over the smallest possible discretization ($\Delta x\ \Delta y$ rather than $2\Delta x\ 2\Delta y$) and convergence rates of both head and velocity components are second-order. Other (than 'mixed') finite element methods may be expected to give (say) second-order convergence for head but only first-order convergence for velocities.[9]

The characteristic-tracking velocities

The characteristics may be tracked by any trajectory method. (There is no need for consistency in evaluation of the characteristic- or trajectory-tracking velocities and the fluxing velocities.) Baptista[3] recommends high-accuracy methods, including fourth-order Runge–Kutta methods.[12] We have used fifth-order RKF (Runge–Kutta–Fehlberg) integration for passive scalar (radionuclide) transport,[41,46] but it is too expensive for the fluid dynamics calculation.

The particular method recommended for this flux-based MMOC methodology is the simple one of characteristic slopes evaluated from cell-wise constant (in space and time) velocities. Again, for an independently determined velocity field, the obvious choice consistent with second-order accuracy is bilinear interpolation in space and time:

$$UBAR(i-1) = \tfrac{1}{4}(U(i-\tfrac{1}{2}, n) + U(i-\tfrac{3}{2}, n) + U(i-\tfrac{1}{2}, n+1) + U(i-\tfrac{3}{2}, n+1)). \quad (13)$$

(Note that $UBAR$ is a cell-centred velocity, not face-centred.) For non-linear problems the time step could be iterated or the fluxing velocities could be lagged in time, i.e. $UBAR(i-1)$ interpolated between $U(i-\frac{1}{2}, n)$ and $U(i-\frac{3}{2}, n)$, or extrapolated in time.

The use of cell-wise constant velocities for characteristic tracking leads to very significant advantages in efficiently arranging the computations. The partial time increments $\tau(i)$ (which, it may be seen, are simply those local Δts which would give a local cell $CFL(i) = 1$) are calculated as

$$\tau(i) = \Delta x(i)/UBAR(i). \quad (14)$$

(See again Figure 5, which is drawn for this particular method of using cell-wise constant characteristic slopes.) These can be calculated prior to a time stepping and stored for each cell. From the evident geometric similarity of the parallelograms in Figure 5, it is seen that the terms $tc(ii)$ in equation (12) are just

$$tc(i-1)=\tfrac{1}{2}\tau(i-1), \tag{15a}$$

$$tc(i-ii)=tc(i-ii+1)+\tfrac{1}{2}\tau(i-ii), \tag{15b}$$

so that no real trajectory tracking or progressive construction of geometry is required.

The flux contribution from the core cell

The location of the foot of the characteristic, denoted $x\#$ in Figure 5, is found from the following process. The 'core' cell $i-iCFL$ has already been located (see above). Now $t\#$ is calculated as the centre of the last (partial) cell time interval:

$$t\#=\tfrac{1}{2}(\Delta t-t_{\text{bot}}), \tag{16a}$$

$$t_{\text{bot}}=\tau(i-1)+\tau(i-2)+\ldots+\tau(i-iCFL+1). \tag{16b}$$

Then $x\#$ is found by backward tracking of the characteristic through $(i-\frac{1}{2}, t\#)$ to time level n. The algebra is slightly complicated, but the geometry is clear.

For the constant u, constant Δx problem the contributions from the integer CFL cells are exact. The only discretization error comes with the evaluation of the flux contribution from the core cell. The larger CFL is, the less critical is this choice. (The foot of the characteristic is then relatively closer to some node.) Here we are free to choose a method from any of the usual interpolation methods used for explicit difference methods (or others such as high-order Lagrangian, Hermite, compact, etc., considered by Baptista[3]). As in the case (see above) of FB-MMOC derivations of difference methods for $CFL<1$, piecewise constant (upstream-biased) 'interpolation' yields the flux contribution $f\#$ of the explicit upstream differencing method, whereas linear interpolation yields the flux contribution $f\#$ of the Lax–Wendroff method.

Leonard's third-order upstream method[40] is a possibility promising higher accuracy at reasonable cost. One could also consider 'reach-back' (to earlier time levels) characteristic calculations.[13–15] However, the method recommended here is to evaluate both the upstream and Lax–Wendroff values and to combine them in an algebraic TVD flux limiter, discussed next.

Flux limiters

The techniques of flux limiting to achieve high accuracy and virtually non-oscillatory solutions are now highly developed, including[47] FCT, TVD, ENO and UL methods. Any of these developed for explicit difference methods restricted to $CFL<1$ can be applied within this FB-MMOC methodology to the core cell. Again, the larger CFL is, the less critical is this choice. The 'algebraic methods' are particularly easy to apply within the FB-MMOC methodology, since they only require the evaluation of the core cell flux contributions from upstream and Lax–Wendroff methods. We have experimented with eight TVD methods[47] in the FB-MMOC, and all work. (For $CFL<1$ the FB-MMOC just reverts to the chosen flux limiter method.) Of these, we agree with the evaluations of Leonard[40] that Van Leer's MUSCL algorithm[34] is the best. For limited applications (namely shock-tube-like problems where one expects slowly varying regions separated by discontinuities), Roe's 'Superbee'[29,30] gives slightly better results, but unfortunately it, like the geometric-based FCT methods,[25–28] unrealistically steepens smooth profiles, and more so in solution-adaptive grids.[48]

Leonard's 'ULTIMATE QUICKEST' method[40] is possibly the most accurate practical method presently available for passive scalar advection in 1D. It is in fact compatible with the present FB-MMOC methodology, but since it involves a geometric limiter (UL) and third-order differencing, the cost in code development time of incorporation for us would not be insignificant. In economic terms we have 'reached the point of diminishing returns', especially considering the base method to be the standard implicit upstream differencing. A further practical consideration is that the overall simulation accuracy will be limited by the accuracy of the advection velocity field, which at present is second-order. However, since the velocity field is often more slowly varying than the advected variable, it would definitely be of interest to incorporate Leonard's method into the FB-MMOC methodology. Especially if high-order trajectory calculations were used, the method would not be inexpensive, but for accuracy would likely justify the acronym 'ULTIMATE'.

RECOMMENDED METHOD

Within the FB-MMOC methodology, then, our particular method of choice, which we dub the C^3-MUSCL method, involves these features: (1) bilinear interpolation (in space and time) for the fluxing velocities, (2) cell-wise constant (in space and time) characteristic velocities and (3) core cell evaluation of non-integer CFL fluxes by both upstream and Lax–Wendroff interpolations, combined in (4) Van Leer's MUSCL TVD flux limiter.

Comparisons of methods for the constant u, constant Δx problem are shown in Figures 6–10. The problem is the advection of a semi-ellipse pulse over $210\Delta x$, calculated with $CFL = 0{\cdot}5$, $1{\cdot}5$ and $10{\cdot}5$. We also evaluated the performance on the step function profile and a smooth pulse based on a sine-squared function, but agree again (!) with Leonard[40] that the semi-ellipse pulse is most demanding, featuring both sharp corners and a rounded top, which features stress the ability of the method to avoid wiggles and not be overly compressive.

Figure 6 presents the results from Van Leer's MUSCL for $CFL = 0{\cdot}5$. (The FB-MMOC methodology is not operative for $CFL < 1$.) Figure 7 presents the results from C^3-MUSCL for $CFL = 1{\cdot}5$. The results only get better as CFL increases. For $CFL = 1{\cdot}5$ and greater a reasonable and simple method (Figure 8) is C^3-$(\frac{1}{2}(\mathrm{UP} + \mathrm{LW}))$, which is the C^3 FB-MMOC method with an ersatz flux limiter consisting of the core cell contribution calculated with a fixed 50% weighting of explicit upstream differencing and Lax–Wendroff. For $CFL = 10{\cdot}5$, even the C^3-UPSTREAM method, which is the C^3 FB-MMOC method with no TVD flux limiter applied but just explicit upstream differencing for the core cell, performs acceptably, as shown in Figure 9. However, the C^3-MUSCL results are very satisfying indeed, as shown in Figure 10, and this method is also robust for $CFL < 1$. For further comparison, also shown are the results for $CFL < 1$ from explicit upstream differencing and for $CFL > 1$ the pathetic results from the commonly used implicit upstream differencing. (It is not our intention here to justify the present method just by comparing it with implicit upstream differencing, but the results are of interest because this method is still in common use. A meaningful comparison with good methods, e.g. non-flux-based MMOC, must involve variable velocity multidimensional problems to assess the importance of the main features of the present method, namely full conservation and use of flux limiters, and must therefore await the development of a multidimensional FB-MMOC code.)

Although the C^3-MUSCL accuracy improves as CFL increases, the operation count per time step also increases, since some operations are required for every cell whose forward time characteristics influence the face at which the flux is being calculated. For similar treatments of the velocity field, the method is comparable in operation count to the conservative explicit upstream method for each incremental cell. Depending on many details of the implementations,

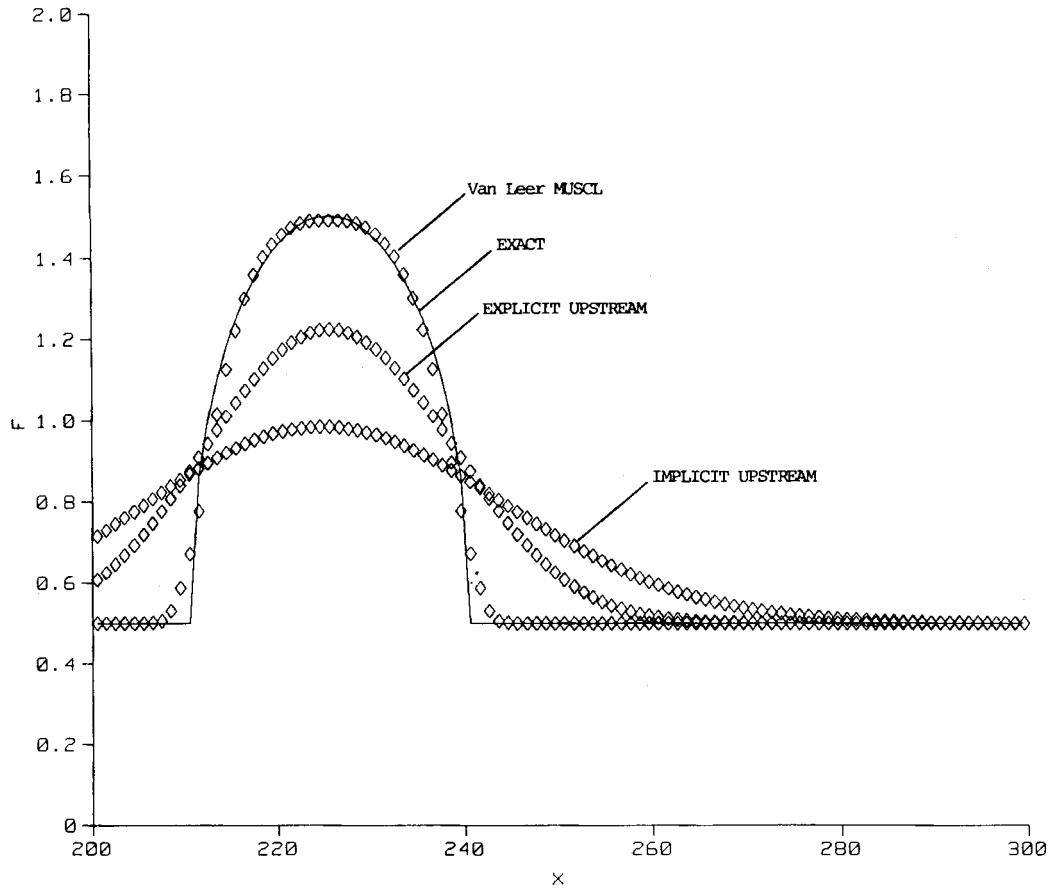

Figure 6. $CFL=0{\cdot}5$. Results for Van Leer MUSCL, explicit upstream and implicit upstream differencing. Pulse travel distance $210\Delta x$

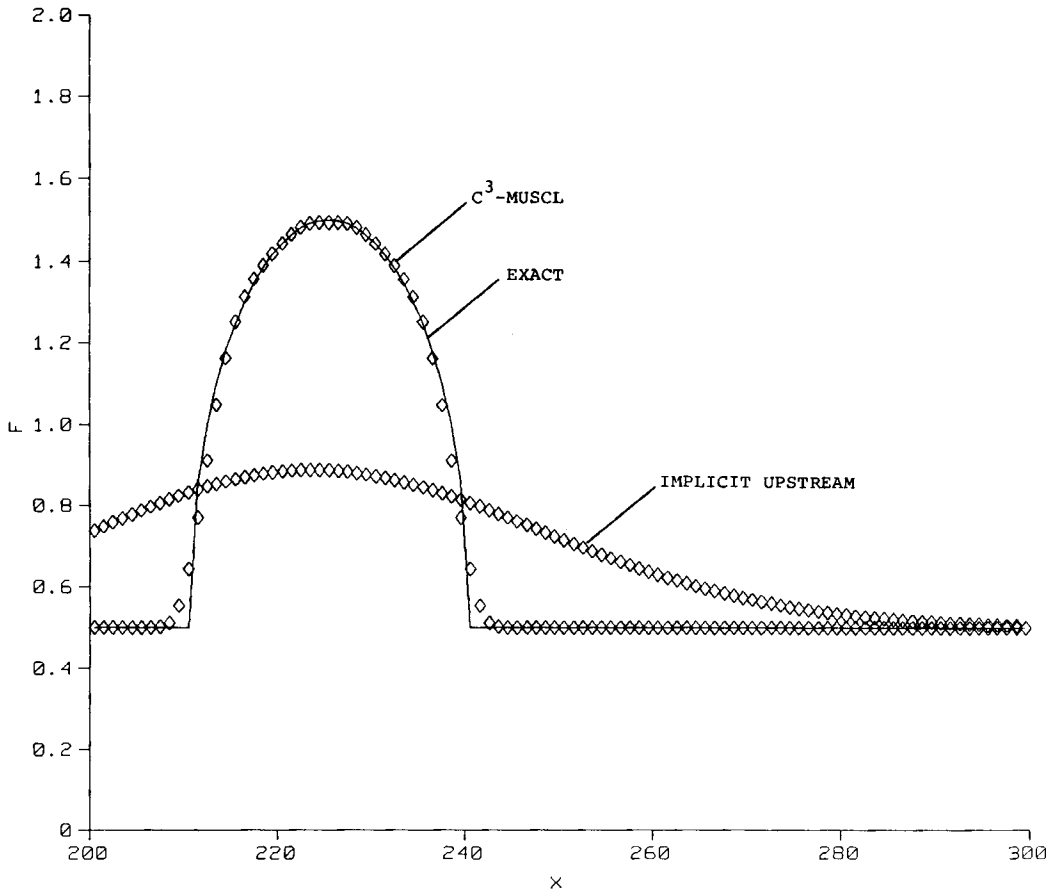

Figure 7. $CFL = 1{\cdot}5$. Results for C^3-MUSCL and implicit upstream differencing. Pulse travel distance $210\Delta x$

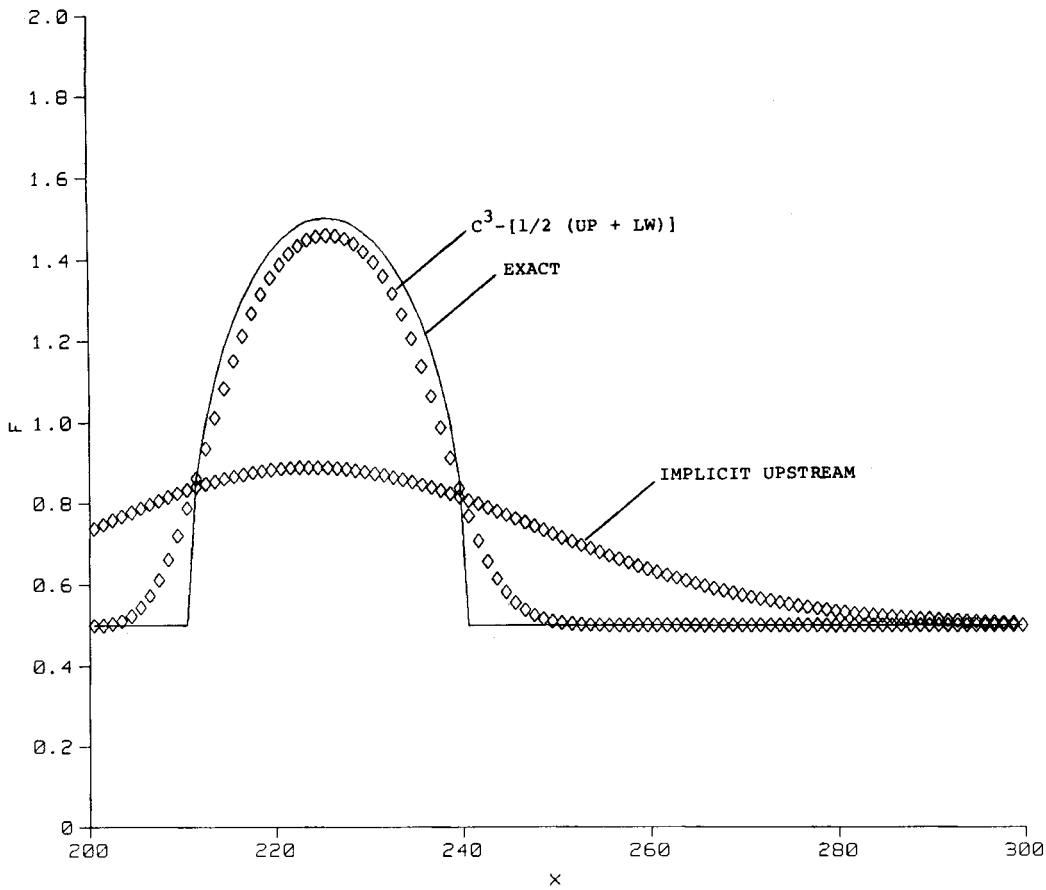

Figure 8. $CFL = 1{\cdot}5$. Results for C^3-($\frac{1}{2}$(UP + LW)) and implicit upstream differencing. Pulse travel distance $210\Delta x$

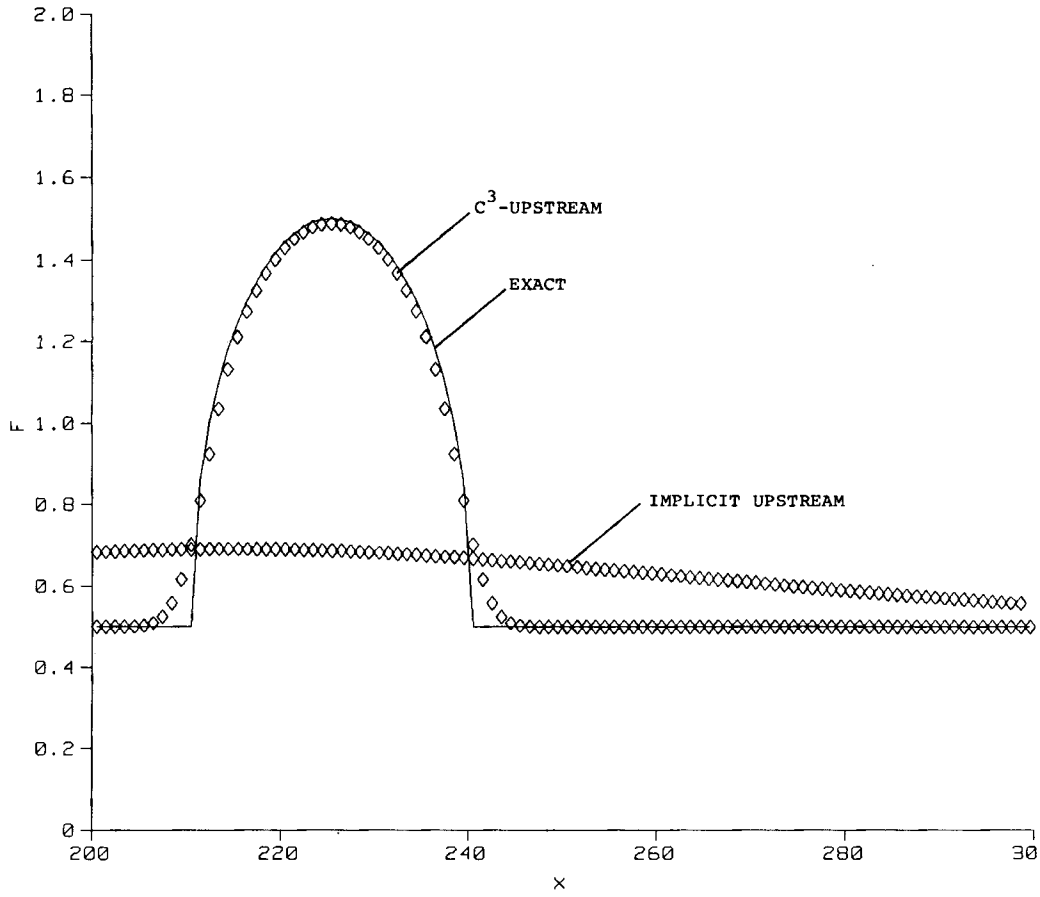

Figure 9. $CFL = 10{\cdot}5$. Results for C^3-UPSTREAM and implicit upstream differencing. Pulse travel distance $210\Delta x$

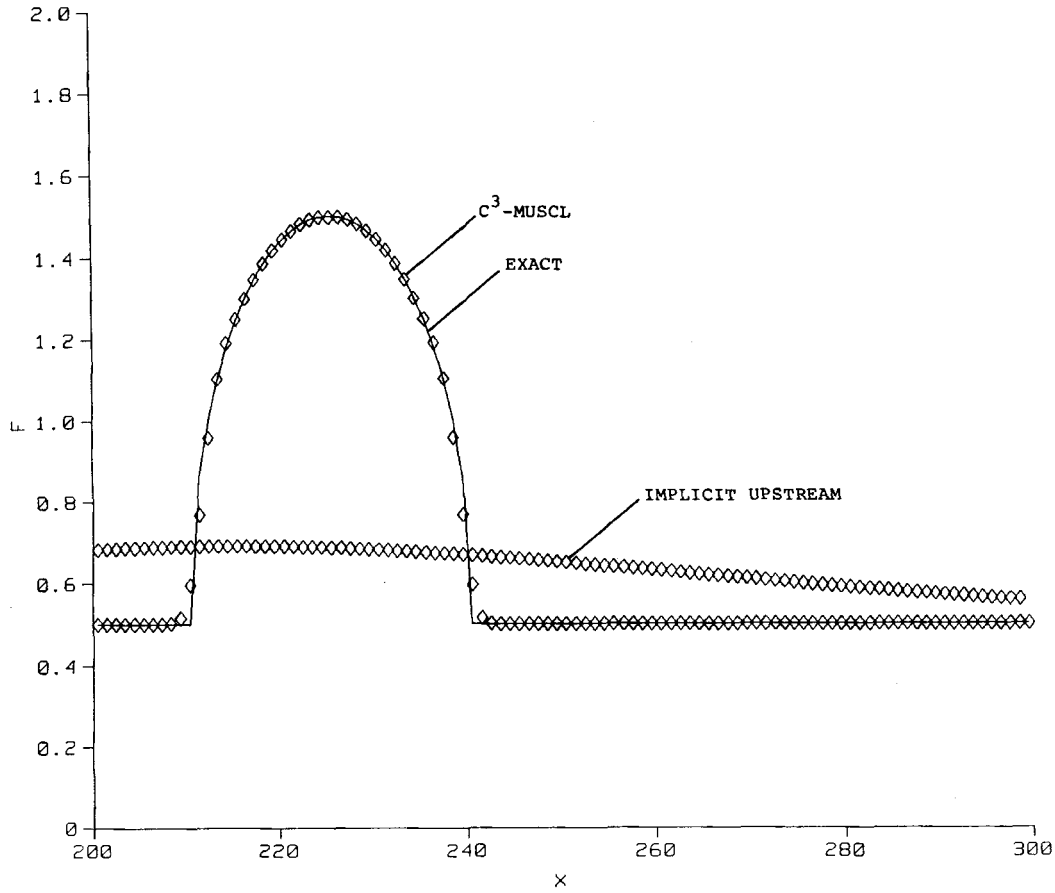

Figure 10. $CFL = 10{\cdot}5$. Results for C^3-MUSCL and implicit upstream differencing. Pulse travel distance $210\Delta x$

this method will be more expensive than implicit upstream differencing for $CFL > 3$–5 in 1D. The penalty is not so significant when $CFL \gg 1$ only locally owing to local grid clustering, which is the case with many of the groundwater flow simulations. Also, the operation count per simulation (i.e. out to a specified time) decreases as CFL increases.

Another approach to the pessimistic operation count is to modify the C^3 method by not interpolating the fluxing velocity Uc over Δt, but using a constant value over each face. While reducing the temporal accuracy, this approach allows each face flux summation to accumulate algebraically from face to face, so that the operation count does not increase proportionally to CFL. (Note that the non-flux-based semi-Lagrangian methods of trajectory tracking[20] use a single-chord-slope approximation over the entire time step to attain operation counts not proportional to CFL, but in the process sacrifice the spatial resolution of u.)

The real advantage of the method is its accuracy. As Russell and Wheeler[9] (see also References 5 and 16) point out, solutions will be smoother along characteristics than along x, so truncation errors (in a Taylor series sense) will be smaller. Note also that any MMOC, and more basically the theory of characteristics for hyperbolic PDEs, is incompatible with implicit upstream differencing and indeed with any implicit method. If one tries to interpret implicit upstream

differencing in terms of interpolation for $f\#$ at the foot of the characteristic, its incompatibility becomes evident. (The interpolation is done by calculating the *CFL*-proportional part of the increment between $f(i, n+1)$ and $f(i-1, n+1)$ at the advanced time level and subtracting it from $f(i, n)$ at the old time level, which makes no sense as geometric interpolation.)

For real problems, accuracy would be expected to deteriorate at much higher Courant numbers owing to variable velocity in the characteristic tracking and possibly round-off errors.

Extension to multidimensions and additional terms (diffusion, dispersion, radionuclide decay, dual porosity) is planned using operator splitting and LOD (locally one-dimensional) directional splitting for advection. The diffusion and reaction terms will be treated by non-directionally split implicit time differencing, which will not restrict the time step owing to stability considerations, but may of course impose additional constraints on Δt for accuracy. The diffusion/dispersion term requires care in the application of boundary conditions,[2] as does the LOD.[49] We prefer LOD splitting from the viewpoint of both simplicity and accuracy, as shown in the following example.

Consider the simple 2D problem of u, v, Δx and Δy constant. For the special case $u/\Delta x = v/\Delta y$ the spatial trajectories pass through diagonal node points. If the directional Courant numbers $CFL_x = u\Delta t/\Delta x = 1$ and $CFL_y = v\Delta t/\Delta y = 1$, it should be possible with an explicit method to obtain the exact solution $f(i, j, n+1) = f(i-1, j-1, n)$. As pointed out in Reference 1, the use of 2D operators for explicit upstream differencing does not give the exact answer, and in fact the stencil only involves $f(i, j, n)$, $f(i-1, j, n)$ and $f(i, j-1, n)$, so that the correct value $f(i-1, j-1, n)$ does not even enter into the calculation. (Consistency of the method depends on smoothness.) The same is true for 2D Lax–Wendroff, with the additional complication that the 2D interpolation must include cross-derivative terms to obtain stability; likewise in 3D. The use of LOD splitting with $CFL_x = CFL_y = 1$ does give the exact answer for explicit upstream and Lax–Wendroff, and requires only 1D interpolation operators to achieve stability in Lax–Wendroff.[1]

The operator splitting and LOD approach in this flux-based MMOC methodology will also preserve the symmetric positive definite property of the matrix resulting from implicit time differencing of the diffusion/dispersion term. For 1D the present method performs well for variable velocity, variable grid spacing and time-dependent boundary conditions.[50] However, the practical accuracy of LOD will degrade with variable velocity. A true multidimensional MMOC method (without LOD splitting) with some similarity to the present one is given by Arbogast *et al.*[51]

The more problematical aspect of multidimensional extension is the treatment of velocity reversals. Several approaches come to mind, including fifth-order RKF tracking only locally, but it is clear that accuracy will require adequate resolution of the velocity field near reversal, which implies local $|CFL| < 1$.

Extension to non-orthogonal co-ordinates appears to be quite difficult. Prospects for application to non-linear problems are optimistic, both because the MUSCL flux limiter is successful for the Burgers equation and shock equations[34,47] and because non-flux-based MMOC methods have been successfully applied to non-linear two-phase flow.[17,19] Finally, we note that the method is *fully* conservative, not 'conservative' only for continuous time discretizations, as the term is often used in meteorological and ocean modelling literature.

ACKNOWLEDGEMENTS

The development of the flux-based MMOC methodology owes much to my discussions with R. Ewing, K. Salari, S. Steinberg, R. Healy, J.-C. Yang and especially T. Russell. An early draft of this paper was reviewed by B. Van Leer and B. Leonard, who suggested several clarifications. My

colleagues K. Salari and S. Steinberg have coached me on the literature and actual practice of modern flux limiters; the initial test-bed code with the flux limiters was written by Dr. Salari. An anonymous reviewer suggested Reference 20. This work was supported by the U.S. Department of Energy through Sandia National Laboratories, Albuquerque, Dr. M. Marietta, Technical Monitor.

REFERENCES

1. P. J. Roache, *Computational Fluid Dynamics*, Hermosa, Albuquerque, NM, 1976.
2. M. A. Celia, T. F. Russell, I. Herrera and R. E. Ewing, 'An Eulerian–Lagrangian localized adjoint method for the advection–diffusion equation', *Adv. Water Resources*, **13**, 187–206 (1990).
3. A. M. Baptista, 'Solution of advection-dominated transport by Eulerian–Lagrangian methods using the backward methods of characteristics', *Ph.D. Thesis*, Department of Civil Engineering, MIT, 1987.
4. T. F. Russell, M. F. Wheeler and C. Y. Chiang, 'Large-scale simulation of miscible displacement by mixed and characteristic finite element methods', in W. E. Fitzgibbon (ed.), *Mathematical and Computational Methods in Seismic Exploration and Reservoir Modeling*, SIAM, Philadelphia, PA, 1986, pp. 85–107.
5. R. Healy and T. Russell, 'Efficient implementation of the modified method of characteristics in finite difference models of solute transport', *Proc. Conf. on Solving Ground Water Problems with Models*, Indianapolis, IN. February 1989, National Water Well Association, pp. 483–491.
6. S. P. Neuman, 'An Eulerian–Lagrangian scheme for the dispersion convection equation using conjugate space–time grids.' *J. Comput. Phys.*, **41**, 270–279 (1981).
7. S. P. Neuman, 'Adaptive Eulerian–Lagrangian finite element method for advection–dispersion', *Int. j. numer. methods eng.*, **20**, 321–337 (1984).
8. S. P. Neuman and S. Sorek, 'Eulerian–Lagrangian methods for advection–dispersion', in K. P. Holz, U. Meissner, W. Zeilke, C. A. Brebbia, G. F. Pinder and W. G. Gray (eds), *Finite Elements in Water Resources*, Vol. 4, Proc. Fourth Intern. Conf. in Hannover, Germany, Berlin, 1982, pp. 14.41–14.68.
9. T. F. Russell and M. F. Wheeler, 'Finite element and finite difference methods for continuous flows in porous media', in R. E. Ewing (ed.), *Mathematics of Reservoir Simulation*, SIAM, Philadelphia, PA, 1983, pp. 35–106.
10. R. E. Ewing and H. Wang, 'Eulerian–Lagrangian localized adjoint methods for linear advection or advection–reaction equations and their convergence analyses', *J. Computational Mechanics*, in review.
11. R. E. Ewing, H. Wang and T. F. Russell, 'Eulerian–Lagrangian localized adjoint methods for convection–diffusion equations and their convergence analysis', *IMA J. Numerical Analysis*, to appear.
12. A. M. Baptista, E. E. Adams and K. D. Stolzenbach, 'Eulerian–Lagrangian analysis of pollutant transport in shallow water', *MIT, R. M. Parsons Laboratory, Technical Report 296*, 1984.
13. C. Lai, 'Comprehensive method of characteristics models for flow simulation', *J. Hydraul. Eng., ASCE*, **114**, 1074–1097 (1988).
14. J.-C. Yang and E.-L. Hsu, 'On the use of the reach-back characteristics method for calculation of dispersion', *Int. j. numer. methods fluids*, **12**, 225–235 (1991).
15. F. M. Holly Jr. and A. Preissmann, 'Accurate calculation of transport in two dimensions', *J. Hydraul. Div. ASCE*, **103**, 1259–1278 (1977).
16. T. F. Russell, 'Galerkin time stepping along characteristics for Burgers' equation', in *IMACS Transactions on Scientific Computation*, Vol. 1, R. S. Stepleman, ed., North-Holland, Amsterdam, 1983, pp. 183–192.
17. R. E. Ewing, T. F. Russell and M. F. Wheeler, 'Simulation of miscible displacement using mixed methods and a modified method of characteristics', *Soc. Petrol. Eng. AIME, SPE 12241*, 1983, p. 71.
18. H. K. Dahle, M. S. Espedal, R. E. Ewing and O. Saevareid, 'Characteristic adaptive subdomain methods for reservoir flow problems', *Numer. Methods Partial Diff. Eqns.*, **6**, 279–309 (1990).
19. M. S. Espedal, R. E. Ewing, T. F. Russell and O. Saevareid, 'Reservoir simulation using mixed methods, a modified method of characteristics, and local grid refinement', *Proc. Joint IMA/SPE European Conference on Mathematics of Oil Recovery*, Cambridge Univ., 25–27 July, 1989, Oxford Univ. Press.
20. A. Staniforth and J. Côté, 'Semi-Lagrangian integration schemes for atmospheric models—a review', *Mon. Weather Rev.*, **119**, 2206–2223 (1991).
21. P. J. Roache, 'Recent developments and problem areas in computational fluid dynamics', in *Lecture Notes in Mathematics Series*, Vol. 461, Springer, Berlin, 1975, pp. 195–256.
22. R. Courant, K. Friedrichs and H. Lewy, 'On the partial difference equations of mathematical physics', *IBM J.*, **11** March, 215–234 (1967).
23. B. Van Leer, 'On numerical dispersion by upwind differencing', *Appl. Numer. Math.*, **2**, 379–384 (1986).
24. R. Ewing, personal communication, 1991.
25. J. P. Boris and D. L. Book, 'Flux corrected transport, I. SHASTA, a fluid transport algorithm that works', *J. Comput. Phys.*, **11**, 38–69 (1973).
26. D. L. Book, J. P. Boris and K. Hain, 'Flux-corrected transport II: Generalizations of the method', *J. Comput. Phys.*, **18**, 248–283 (1975).

27. S. T. Zalesak, 'Fully multidimensional flux-corrected transport algorithms for fluids', *J. Comput. Phys.*, **31,** 335–362 (1979).
28. S. T. Zalesak, 'High order 'zip' differencing of convective terms', *J. Comput. Phys.*, **40,** 497–508 (1981).
29. P. L. Roe, 'Characteristic-based schemes for the Euler equations', *Ann. Rev. Fluid Mech.*, **18,** 337–356 (1986).
30. P. L. Roe, 'Some contributions to the modeling of discontinuous flows', *Lectures in Applied Mathematics*, Vol. 22, American Math. Society, Providence, Rhode Island, 1985.
31. A. Harten, 'High resolution schemes for hyperbolic conservation laws', *J. Comput. Phys.*, **49,** 357–393 (1983).
32. H. C. Yee, 'Construction of explicit and implicit symmetric TVD schemes and their applications', *J. Comput. Phys.*, **68,** 151–179 (1987).
33. S. K. Godunov, 'A difference method for the numerical calculation of discontinuous solutions of hydrodynamic equations', *Mat.-sborn.*, **47,** 357–393 (1959).
34. B. Van Leer, 'Toward the ultimate conservation difference scheme. V. A second-order sequel to Godunov's method', *J. Comput. Phys.*, **32,** 101–135 (1979).
35. H. C. Yee, 'Upwind and symmetric shock-capturing schemes', *NASA TM 89464*, May 1987.
36. H. C. Yee, 'A class of high-resolution explicit and implicit shock-capturing methods', *NASA TM-101088*, February 1989.
37. A. Harten and S. Osher, 'Uniformly high-order accurate non-oscillatory schemes I', *SIAM J. Numer. Anal.*, **24,** 297–309 (1987).
38. A. Harten, B. Engquist, S. Osher and S. Chakravarthy, 'Uniformly high order accurate essentially non-oscillatory schemes, 3', *NASA CR-178101*, 1986.
39. P. Colella and P. R. Woodward, 'The piecewise parabolic method (PPM) for gas dynamical simulations', *J. Comput. Phys.*, **54,** 174–201 (1984).
40. B. P. Leonard, 'The ULTIMATE conservative difference scheme applied to unsteady one-dimensional advection', *Comput. Methods Appl. Mech. Eng.*, **88,** 17–74 (1991).
41. P. J. Roache, 'Computational fluid dynamics algorithms and codes developed for WIPP site simulations', in Y. K. Cheung, J. H. W. Lee and A. Y. T. Leung (eds), *Computational Mechdnics, Proc. Asian Pacific Conf. on Computational Mechanics*, Hong Kong, December 1991, Vol. 2, Balkema, Rotterdam, 1991, pp. 1325–1336.
42. T. F. Russell, 'Eulerian–Lagrangian localized adjoint methods for advection-dominated problems', *Proc. 13th Dundee Biennial Conf. on Numerical Analysis, Research Notes in Mathematical Series*, Pitman, Vol. 228, pp. 206–228, (1990).
43. S. F. McCormick and Z. Cai, 'On the accuracy for the finite volume element method for diffusion equations on composite grids', *SIAM J. Numer. Anal.*, **27,** 636–645 (1990).
44. F. H. Harlow and J. E. Welch, 'Numerical calculation of time-dependent viscous incompressible flow of fluid with free surface', *Phys. Fluids*, **8,** 2182–2189 (1965).
45. J. E. Welch, F. H. Harlow, J. P. Shannon and B. J. Daly, 'The MAC method', *LASL Report No. LA-3425*, Los Alamos Scientific Laboratory, Los Alamos, NM, 1966.
46. P. J. Roache, R. Blaine and B. Baker, 'SECO 2DH user's manual, version 2.1', *SAND90-7096*, Sandia National Laboratories, Albuquerque, NM, August 1991.
47. A. J. Przekwas and H. Q. Yang, 'Advanced CFD methodology for fast transients encountered in nonlinear combustion problems', *SBIR Phase I Final Report*, CFD Research Corporation, Huntsville, AL, 1989.
48. K. Salari and S. Steinberg, 'Flux-corrected transport in a moving grid', *J. Comput. Phys.*, accepted for publication.
49. R. J. LeVeque, 'Intermediate boundary conditions for LOD, ADI, and approximate factorization methods', *ICASE Report No. 85-21*, Institute for Computer Applications in Science and Engineering, NASA Langley Research Center, March 1985.
50. P. J. Roache, 'Validation exercises of a one-dimensional flux-based modified method of characteristics', in T. Russell (ed.), *Proc. IX Int. Conf. on Computational Methods in Water Resources*, Denver, CO, June 1992, Computational Mechanics Publications, Southhampton, 1992.
51. T. Arbogast, A. Chilakapati and M. F. Wheeler, 'A characteristic-mixed method for contaminant transport and miscible displacement', in T. Russell (ed.), *Proc. IX Int. Conf. on Computational Methods in Water Resources*, Denver, CO, June 1992, Computational Mechanics Publications, Southhampton, 1992.