

CHAPTER ONE HUNDRED SIXTY THREE

ACCURATE MODELLING OF TWO-DIMENSIONAL MASS TRANSPORT

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Any numerical solution of the convective transport equation in an Eulerian framework will exhibit inherent numerical dispersion and solution oscillations. The magnitude of such numerical errors is often so severe as to destroy the value of many computed solutions. A successful and economical algorithm for the convective transport equation in one spatial dimension has been published recently by one of the authors (RJS), in which an exact solution is achieved by means of a moving coordinate system. The present study describes the extension of this work to the more important and challenging two-dimensional case.

INTRODUCTION

Numerical methods for the solution of the two-dimensional convection-dispersion or advective-diffusion equation (ADE) abound in the literature of fluid dynamics. In Cartesian coordinates (x, y) the ADE has the form:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} = \nu \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right), \quad (1)$$

where $C(x, y, t)$ is the field of the substance that is re-distributed passively by the velocity field (u, v) , t is time and ν is the diffusion coefficient. The equation may also contain source and reaction terms.

The attention given to ADE is a measure both of its importance and ubiquity. Physically, an initial distribution $C_0(x, y) = C(x, y, 0)$ is given and the solution describes the field of C at any subsequent time over the solution domain, under the dual influences of advection and diffusion. In many instances, and certainly in estuarine and coastal environments, Eq. (1) is advection-dominated, and diffusive effects are minor. To a first approximation, ν can be ignored the problem reverts to passive scalar advection.

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More importantly however, it is the advective rather than the diffusive terms in Eq. (1) that present numerical problems. Indeed, considerable attention continues to be devoted to the one-dimensional ADE (6,7,12,14,15), a sure indicator of dissatisfaction with the current 'state-of-the-art'. The reasons for this are well known, but often ignored. Most solutions of Eq. (1) are Eulerian, in that they use a fixed computational grid. As pointed out by Fenton (6), solutions such as conventional finite difference or finite element schemes attempt to solve the equation, with no attempt to take account, let alone advantage, of the nature of the solution. In problems dominated by advection, the performance of Eulerian solutions is often most unsatisfactory. With many such schemes, numerical dispersion and solution oscillations completely degrade the value of the computed solution.

In view of the above, a satisfactory solution of the two-dimensional problem remains to be demonstrated. A successful and economical algorithm for the one-dimensional ADE has been presented recently by Sobey (15,16), in which an exact solution is achieved by means of a moving coordinate system. The present scheme is an extension of this Lagrangian scheme to two spatial dimensions. The primary aim in such an algorithm is to permit the accurate calculation of mass transport (biota, pollutants) in continental shelf waters. In such cases, the velocity field (u, v) that is applied to Eq. (1) would be provided by a conventional two-dimensional hydrodynamic model.

GOVERNING EQUATIONS

Setting $v = 0$ in Eq. (1) gives the advection equation:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} = 0. \quad (2)$$

As the prototype problem, Eq. (2) is to be solved on a square, $-1 \leq (x,y) \leq 1$, for $t > 0$ where the initial field of C is a cone of unit height, radius r and initial location (x_0, y_0) - by convention (10,18) these parameters are $r_0 = 1/4$, $x_0 = -1/2$ and $y_0 = 0$. The initial conditions are:

$$C(x, y, 0) = C_0(x, y) = \begin{cases} 1 - r/r_0, & r \leq r_0 \\ 0, & r > r_0 \end{cases} \quad (3)$$

where $r = [(x-x_0)^2 + (y-y_0)^2]^{1/2}$.

On the boundaries of the square, C is set equal to zero. The velocity field is solid body (anti-clockwise) rotation about the origin:

$$u = -\Omega y, \quad v = +\Omega x, \quad (4)$$

where Ω is the angular velocity. Perspective and plan views of the initial conditions are shown in Fig. 1.

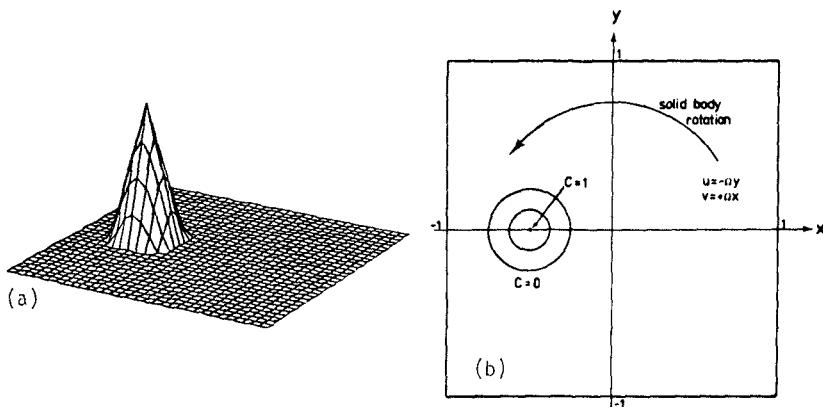


Fig. 1 (a) Perspective and (b) plan views of initial cone configuration.

In the absence of diffusion ($\nu = 0$), the cone should return, undistorted, to its original position after any integral number of periods, $nT = 2n\pi/\Omega$; elements of the cone describe concentric circles with constant angular velocity Ω , about the origin. The range of C should always remain $[0,1]$. The rotating cone problem has become the basic prototype problem for two-dimensional advection, and has been used widely as a test bed for numerical algorithms (3,4,10,18). It is undoubtedly demanding, since any dispersion (phase speed errors) immediately truncate the peak of the cone, as will be seen in the following section. However, if such schemes are to be capable of mapping the evolution of point-like sources such as a pollution outfall, then the requirement of high fidelity at short wavelengths is absolutely essential.

Jacobian Formulation

For incompressible flow a stream function ψ can be defined in the conventional manner by

$$u = - \frac{\partial \psi}{\partial y}, \quad v = + \frac{\partial \psi}{\partial x}. \quad (5)$$

This allows Eq. (2) to be expressed as

$$\frac{\partial C}{\partial t} + J(C, \psi) = 0, \quad (2')$$

where J is the usual two-dimensional Jacobian. In this form the equation can be expressed in a variety of ways so that certain quantities are conserved throughout the region of integration. Use of this has been made in particular for finite difference schemes beginning with the work of Arakawa (1), discussed in the following section.

EXISTING TECHNIQUES

Two finite difference (FD) schemes, representative of existing techniques for the solution of Eq. (2) are reviewed below. In order that an objective comparison of the performance and economy of the various schemes can be made with the proposed scheme, these two algorithms have been programmed and selected results are presented.

Arakawa/Jacobian scheme

The Jacobian formulation of Eq. (2') has been used widely to evaluate the advective terms in numerical weather prediction models as well as in a variety of other fluid dynamical applications. For homogeneous boundary conditions in the absence of dissipation, it can be shown that a number of quantities, averaged over the region of integration, must be conserved. For two-dimensional incompressible flow, if ζ is vorticity, then $\bar{\zeta}$, $\bar{\zeta}\psi$ (kinetic energy) and $\bar{\zeta}^2$ (enthalpy) must be conserved, where the overbar denotes the continuous spatial average. Arakawa (1) was able to show that certain aliasing interactions were minimised by particular second order FD formulations for the Jacobian, resulting in the global conservation of $\bar{\zeta}$, $\bar{\zeta}\psi$ and $\bar{\zeta}^2$.

The Jacobian, denoted here by J - see also Ref. (10) - conserves all three quantities. Numerical experiments showed that this formulation prevented instabilities that had caused numerical schemes to 'blow up' and the use of Arakawa Jacobians has become widespread. It is a relatively simple matter to extend this scheme to produce Jacobians that are fourth order accurate spatially. One such formulation (1,10) also conserves all three quantities, and will be referred to as J' . Although the conservative properties of J and J' apply over the entire region of integration, this does not necessarily hold locally, with the result that the undesirable numerical dispersion can still be severe, particularly at the important shorter wavelengths.

Two basic spatial grid spacings are used, $\Delta s = 1/8$ and $1/16$. These result in uniform 17×17 and 33×33 square grids applied to the given area of integration. These are denoted as cases A and B respectively. Both second order (J) and fourth order (J') Arakawa Jacobians are used, resulting in four cases altogether - A2, A4, B2 and B4. Time stepping is via the conventional 'leapfrog' scheme with periodic averaging to overcome time-splitting and appropriate re-initialisation. Thus, Eq. (2') is integrated by:

$$C_{i,j}^{n+1} = C_{i,j}^{n-1} + 2\Delta t J_{i,j}^n, \quad (6)$$

where $J_{i,j}^n$ is either $J_z(C_{i,j}^n)$ or $J_+(C_{i,j}^n)$. Temporal accuracy is of order $(\Delta t)^2$. The usual stability criterion applies to limit the size of Δt to $\Delta t < \Delta s/v_{\max} = \Delta s/(\Omega/2)$.

In Fig. 2 the progress of the cone as it rotates through one complete revolution is shown for case A2. In all cases, the perspective views are rotated back to the original position, with the centre at $(-1/2, 0)$,

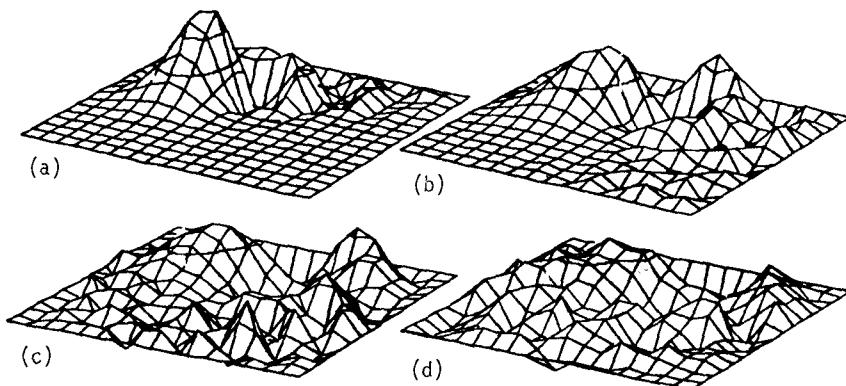


Fig. 2 Perspective views of cone at intervals of a quarter rotation for case A2 - see Table I.

for ease of comparison. The defects inherent in such a scheme are immediately apparent. In Fig. 2(a) after a quarter rotation, a wake is observed behind the cone proper for which only the 0.2 and 0.4 contours remain, even at this early stage - the range of C is $[-0.25, 0.54]$. This trailing wake continues to grow at the expense of the cone. By the end of one period - Fig. 2(d) - the structure of the cone is effectively unrecognisable, with the range of C now being $[-0.31, 0.30]$.

For some improvement, equivalent results for case B2 at twice the spatial revolution are presented in Fig. 3. Although a clear improvement, this second-order scheme is still totally inadequate. Numerical dispersion is so severe that short wavelength detail, particularly the cone's peak, trails behind in a wake of ever-increasing extent. After one revolution the original range for C of $[0, 1]$ has become $[-0.23, 0.52]$. In Fig. 4, the results for case B4 (fourth order Jacobian with $\Delta s = 1/16$) are presented after one and two revolutions. The range of C at these two times is $[-0.13, 0.83]$ and $[-0.16, 0.77]$ respectively. The well-recognised improvement with higher spatial order schemes (4, 8, 10) is apparent, but these results remain considerably short of theoretical expectations.

The overall results of these computations are listed in Table I. This gives the cone parameters (maximum and minimum values of C and the coordinates of the maximum C value) for the various cases at time $t = 2T$. These results can, to a limited extent, be compared with the results of a number of studies of the rotating cone problem that have been collated by Christensen and Prahl (3). Unfortunately, there is little uniformity amongst these, especially with regard to the times at which results are obtained. The present discussion will concentrate on the results at $t = 2T$ - c.f. Ref. (10).

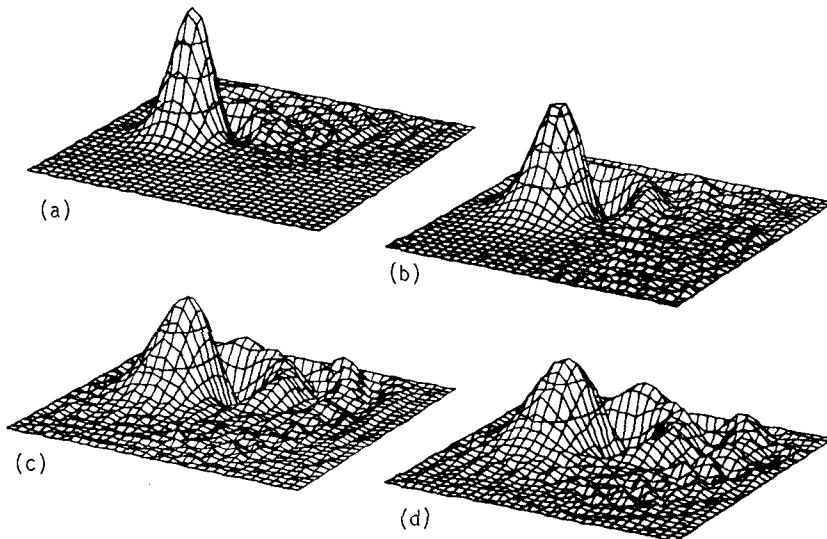


Fig. 3 As for Fig. 2, but case B2.

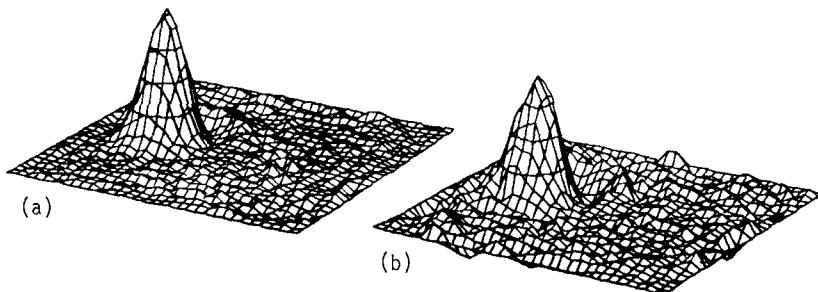


Fig. 4 Perspective views at (a) $t = T$ and (b) $t = 2T$ for case B4.

Lax-Wendroff Schemes

Consider the one-dimensional advection problem $\partial C / \partial t + u (\partial C / \partial x) = 0$, with u a constant. The standard Lax-Wendroff (LW) scheme (13) arises if, C is expanded as a Taylor series in time and the advection equation is then used to replace C_t and higher time derivatives by spatial derivatives. These are then approximated by centred FD approximations. Specifically, the one-dimensional scheme is:

$$c_i^{n+1} = c_i^n - \frac{\mu}{2}(c_{i+1}^n - c_{i-1}^n) + \frac{1}{2}\mu^2(c_{i+1}^n - 2c_i^n + c_{i-1}^n) \quad (7)$$

The LW scheme is both dissipative and quite strongly dispersive at short wavelengths (9). An equivalent two step scheme has also been derived (7). One advantage of the two-step formulation is the ease of extension to two or more spatial dimensions, as well as to higher spatial accuracy, as detailed in Gadd (7,8). In the second paper, Gadd noted that the scheme in two dimensions was not unconditionally stable and introduced a further modification. Like the fourth order Arakawa scheme above, calculations revert to second order at grid points adjacent to the boundaries. The final scheme (8) was shown to have a superior performance for the rotating cone problem over the earlier version.

Selected results for this scheme (8) and the standard second order LW method are presented. The cases that have been calculated are denoted by C and D for grid spacings of $\Delta s = 1/8$ and $1/16$ respectively, followed by the numbers 2 or 4 corresponding respectively to standard second order LW or the (fourth order) modified Gadd scheme (8). In Fig. 5 the progress of the cone over one rotation is shown for case D2. The overall impression is that these results are very similar to those exhibited by the corresponding second order Arakawa Jacobian experiments above. Quantitative details are listed in Table I. Again, doubling of spatial resolution does afford some improvement, but overall performance is poor. For example, after one revolution the C range in case D2 is [-0.20, 0.49] versus [-0.23, 0.52] for the corresponding case B2. In Fig. 6, case D4 is shown after one and two revolutions, the range for C at $t = 2T$ being [-0.07, 0.76], compared with [-0.16, 0.77] for the corresponding Arakawa case B4. The Gadd scheme is distinctly faster computationally, with two rotations for D4 taking 168 s on a DEC 10-21 mainframe versus 286 s for B4 - see also Table II. The performance of the Gadd scheme (8) does appear superior, since the negative values of C are not as extreme as those in case B4. However, it can be shown from Fourier analysis (9), that this can be attributed to increased dissipation and not necessarily to reduced dispersion at the shorter wavelengths.

It is apparent from Figs. 2-6 and Table I that the major problem is dispersion, although increased spatial accuracy in the representation of the advective terms can go a long way towards improving this situation. The effects of time differencing errors and spatial resolution are much less important. This defect (dispersion) is common to all Eulerian schemes; it is widely recognised and has been commented upon extensively, often in quite scathing terms (6,11,17). In spite of this, such schemes continue to enjoy widespread usage.

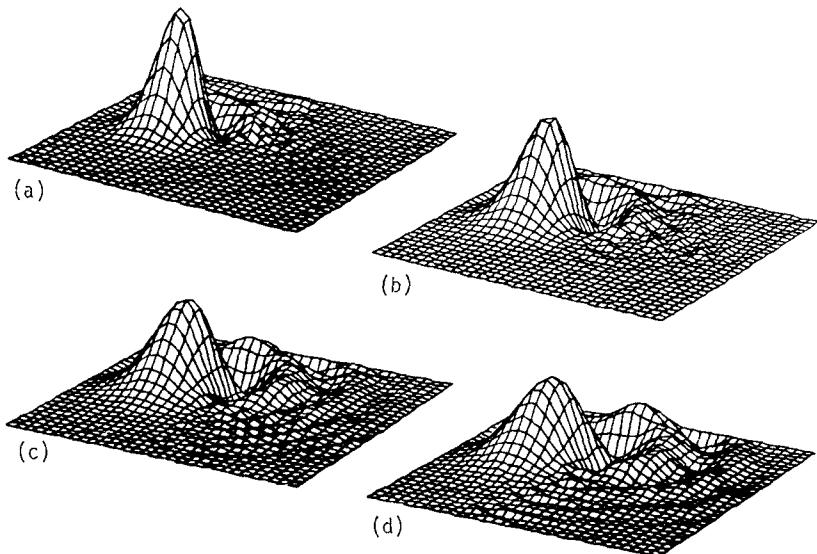


Fig. 5 As for Fig. 2, but case D2.

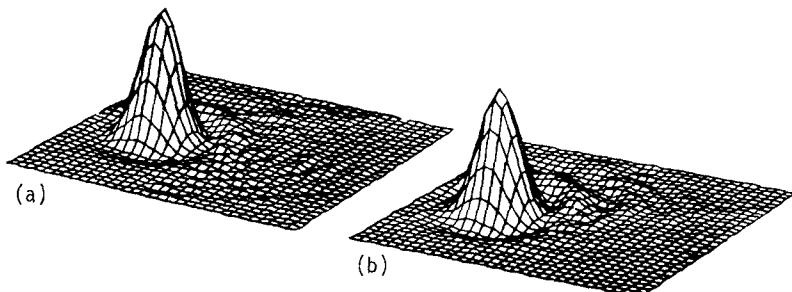


Fig. 6 As for Fig. 4, but case D4.

Spectral Methods

The major problem with the above FD methods, and indeed with all low order polynomial-based Eulerian methods is their failure to resolve spatial structure, particularly in the calculation of first derivatives. The spectral methods introduced by Orszag (10) have, by and large, been able to overcome this problem. They involve the expansion of the C field spatially in a set of suitable basis functions, chosen in general to satisfy the boundary conditions. Initial work used complex

two-dimensional Fourier series for the rotating cone problem which required the boundary conditions to be spatially periodic. Computations are sped up significantly by the use of the Fast Fourier Transform. Simple calculations reveal how with spectral methods, all available points enter the computation of derivatives, resulting in schemes that are markedly more accurate than second or fourth order FD methods. A substantial body of literature has arisen from this pioneering work of Orszag — see the review of Orszag and Israeli (11). The extension to less restrictive boundary conditions than the original periodic case follows with the use of alternative basis functions, such as Chebyshev polynomials.

There is, however, a major problem with spectral methods:- their lack of flexibility. The major motivation behind the present work was stated in the Introduction to be the need for an accurate algorithm for Eq. (1) where the velocity field (u, v) is provided by a two-dimensional hydrodynamic model. Often, the boundaries of such models are extremely irregular, since they follow the coastline. Neither Eulerian FD models nor the present Lagrangian scheme have any difficulty in coping with this problem. On the other hand spectral models are totally unable to handle this situation; indeed, they are crucially dependent upon a regular (usually rectangular) geometry. A further related constraint is the lack of flexibility with respect to imposed boundary conditions. Even with regular boundaries, there is no simple way by which spectral methods could cope with, say, time-dependent input of C at a given point on the boundary, meant to model, for example, a pollutant discharge. Accommodation of this situation by Eulerian FD methods is again straightforward and will be shown below to be the case for the present method. Overall, although it can be demonstrated that spectral methods provide superior performance over more commonly used Eulerian FD schemes, they can offer little in the way of general application to hydrodynamic modelling of two-dimensional mass transport.

TABLE IACCURACY OF THE VARIOUS NUMERICAL SCHEMES (at $t = 2T$)

Scheme	Description	Spatial Order	Grid Dimensions	C_{\max}	C_{\min}
A2	Arakawa	2nd	17 x 17	0.32	-0.29
B2	"	"	33 x 33	0.42	-0.24
A4	"	4th	17 x 17	0.39	-0.24
B4	"	"	33 x 33	0.77	-0.16
C2	Lax-Wendroff	2nd	17 x 17	0.20	-0.18
D2	"	"	33 x 33	0.36	-0.21
C4	Gadd (LW)	4th	17 x 17	0.41	-0.17
D4	"	"	33 x 33	0.76	-0.07
MC	Moving Coords	Exact	17 x 17	1.00	0.00

MOVING COORDINATE ALGORITHM

It is widely recognised (6,11) that Lagrangian or moving coordinate numerical schemes are the 'natural' method for the solution of the advection equation, Eq. (1). Nevertheless, it would seem that the advantages offered by the simplicity of Eulerian schemes have been allowed to overshadow their considerable disadvantages as highlighted in the previous section. Lagrangian schemes have been proposed only rarely (5), but such work does not appear to have been carried appreciably further.

Lagrangian Solutions of the Advection Equation

Eq. (1) is mathematically equivalent to:

$$\frac{dc}{dt} = 0 \quad (8)$$

along

$$\frac{dx}{dt} = u, \quad \frac{dy}{dt} = v. \quad (9)$$

This is the Lagrangian scheme that forms the basis of the present work. There are complicating factors involved in the use of a Lagrangian scheme and these will be described below, but they are often over-stated. The almost trivial simplicity of Eq. (8) demands further attention. It simply states the well known physical fact that values of C are conserved in time along trajectories or characteristics that are the paths of the fluid particles. The actual integration of Eq. (9) can be performed by any suitable algorithm for ordinary differential equations, once the velocity field is specified. Standard fourth order Runge-Kutta is chosen in the present study.

The basis of Lagrangian schemes is reviewed by Book and Boris (2). A number of disadvantages of such schemes are stated, chief among which is the distortion of an initially uniform grid by a non-uniform velocity field. In specific numerical computations, the flow and hence the grid might become so distorted that the 'bookkeeping' involved in keeping track of the positions of the individual nodes ultimately becomes intractable. However, this argument loses sight of the fact that the very distortion of the grid mirrors the gradients in the flow: it is in regions where either C or the flow varies rapidly that grid points must be concentrated in order to effect an accurate solution. Lagrangian schemes adapt to this situation naturally; Eulerian schemes are simply unable to do so and their consequent and often severe loss of fidelity as the Nyquist limit is approached, can hardly be unexpected.

Previous Lagrangian schemes appear to have concentrated on situations where flow variables altered rapidly. These include flows involving shocks and other large gradients in the flow, for which they are ideal theoretically, but apparently impractical because of mesh distortion. In the present case the proposal is to apply the scheme to mass

transport calculations in slowly varying velocity fields. In this case, the computational grid does not become unmanageably distorted. More importantly, however, the gradients of C can be preserved accurately and do not suffer from the artificial diffusion and solution oscillations associated with Eulerian schemes. It needs to be recognised that in order to solve Eq. (9) for each element of C, the velocity field needs to be specified at the actual location of each of these points. For the solid body rotation of the present problem, simple linear interpolation will accomplish this exactly. For slowly varying velocities a low order bivariate interpolation scheme should suffice. This contrasts with the situation for Eulerian schemes where, on a fixed grid, spatial derivatives of C cannot be calculated accurately by low order Taylor series, especially in regions of high gradients (6).

Another problem that has been associated with Lagrangian schemes, and which has been believed to be to their detriment is associated with inflow and outflow boundaries. At the latter, grid points must leave the computational region; at the former, they must be created. This is by no means an insurmountable obstacle and will be discussed below.

If the solution of the full ADE, Eq. (1) is required, then the question incorporating diffusion on a possibly distorted Lagrangian grid, that may be both gaining and losing mesh points, is obvious. A proposed treatment of this important extension of the present problem is also discussed below. All of the above questions (i.e. method of integration of Eq. (9); boundary conditions and the addition or removal of grid points; incorporation of the diffusion step) have been addressed by Sobey (15,16) in an algorithm for the solution of the one-dimensional ADE. The results of this work were most encouraging, in terms of the high accuracy attained, the relative computational efficiency and the inherent flexibility of the scheme, and suggest that the extension of this Lagrangian approach to the more important and challenging question of two-dimensional advection should be equally worthwhile.

Sample Computations

Eqs. (8,9) were solved for the rotating cone problem, with the same spatial resolutions employed for the tests of the two main Eulerian schemes above. The results of these computations for the 17×17 grid after two full rotations are presented in Table I and in Fig. 7. The timestep used for these results was $1/16$ of the period of rotation. This corresponds to a dimensionless timestep of 4.5, compared with 0.5 used for the above Eulerian schemes. The error, which can be measured by the maximum error in the position of the grid elements at $t = 2T$ was negligible (5×10^{-3}). It should be recalled that the range of C is always [0,1] with this scheme. It can be reduced by reducing the specified timestep in the solution of Eq. (9), but this increases the CPU time and the present parameters would appear to be satisfactory. The actual CPU times for the various schemes are shown in Table II and the moving coordinate scheme undoubtedly compares favourably with the much less accurate Eulerian methods. Should, on the other hand, the timestep be increased, inaccuracy results inevitably. For example, a dimensionless timestep of 18.0 results in errors of order unity in the position of grid elements at the boundary of the computational region.

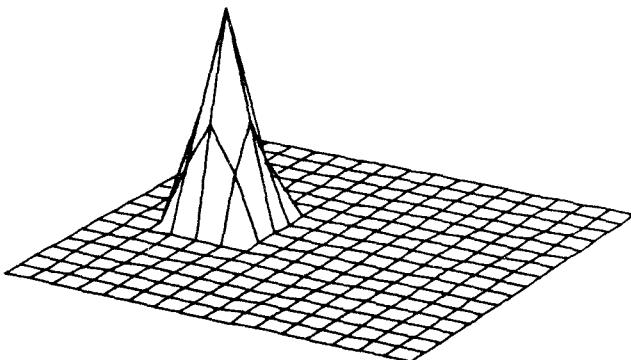


Fig. 7 Perspective view of cone at $t = 2T$ with the moving coordinate algorithm, with $\Delta s = 1/8$.

TABLE II

CPU TIMES FOR VARIOUS INTEGRATION SCHEMES ($t = 2T$)

Numerical Scheme	Dimensionless Timestep, λ	CPU(s)
Arakawa 2nd order	0.5	22.6
Lax-Wendroff 2nd order	0.5	10.9
Arakawa 4th order	0.5	32.3
Gadd (LW) 4th order	0.5	18.3
Moving Coordinates	4.5	6.7

$\lambda = v_{\max} \Delta t / \Delta s$, with all results for a spatial grid of $\Delta s = 1/8$.
All computations performed on a DEC 10-21 mainframe computer.

Boundary Conditions

The specification of boundary conditions is exactly analogous to the treatment used in the method of characteristics, and is detailed in Sobey (15). For the rotating cone problem, C is specified as zero along the boundary of the square computational region, but more general boundary conditions can just as easily be accommodated. Outflow boundaries present no problem. If over a given timestep an element of C is adjudged to have passed out of the computational region, that element is simply removed from further consideration. At inflow boundaries, additional grid points can be created by integration back along the characteristics, Eq. (9), to the particular inflow boundary (15).

Extension to the Advection-Diffusion Equation

The essence of this extension is the method of fractional steps employed by Sobey (15) for the one-dimensional ADE. Eq. (1) is equivalent to the following pair of equations:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} = 0 , \quad (10)$$

$$\frac{\partial C}{\partial t} = v' \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right) \quad (11)$$

Addition of Eqs. (10) and (11) gives Eq. (1), the two-dimensional ADE, provided $(u', v', v') = 2(u, v, v)$. Thus, the full ADE can be thought of as separate, but simultaneous advection and diffusion steps, but with twice the given velocity and diffusion. Numerically, it is simpler to take the two steps as sequential. The solution of C at $n\Delta t$ is advanced to $(n+1/2)\Delta t$ by the numerical solution of Eq. (10), the present Lagrangian scheme. The field of C at this intermediate step is then used to solve the diffusion (or heat) equation, Eq. (11).

Because of the Lagrangian solution of the advection equation, this second step necessitates the solution of the diffusion equation on a non-uniform grid. Sobey (16) has presented an optimised solution of this equation in one dimension. The results obtained were most satisfactory, but the extension of this method to two dimensions poses additional problems, and a more pragmatic but less sophisticated approach may be warranted. Although Eulerian schemes have been effectively rejected for the solution of the advective step, there is no reason to do so for the diffusive step. The solution of Eq. (11) by standard low order Taylor series approximations, either FD or FE methods, is satisfactory in this case. Further work is currently being pursued on this important aspect of the problem.

CONCLUSIONS

The moving coordinate method introduced in the present paper has been shown to have much higher accuracy than is available from conventional and widely-used Eulerian schemes. It is simple in both concept and implementation, and, in addition, it can be interfaced easily with hydrodynamic models used to provide the velocity field.

Extensions to include the diffusive component of Eq. (1) have to take account of the necessarily distorted computational grid. This has already been effected successfully for the one-dimensional equation - Refs. (15,16) - and an analogous procedure for the two-dimensional case has been proposed. With the slowly-varying velocity fields (e.g. continental shelf circulation) for which the method is intended, the mesh will distort, but not unmanageably so. Strategies have also been discussed for the removal or addition of mesh points, should they become too sparse or concentrated. It should be recalled however, that such

distortion mirrors the background gradients and gives a Lagrangian scheme natural advantages over any Eulerian approach. Overall, the present approach is meant to provide the first but also most important step towards the development of accurate and reliable methods for the solution of ADE problems in actual physical environments. Advection-dominated flows are the rule rather than the exception, yet too often the veracity of available solutions would appear to be compromised by an inadequate appreciation of the limitations of available numerical methods. A successful solution of the problem, based on the above principles, provides a resolution of this impasse.

ACKNOWLEDGEMENTS

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APPENDIX - REFERENCES

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