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Numerical Advection Algorithms and Their Role in Atmospheric Transport and Chemistry Models

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During the last 35 years, well over 100 algorithms for modeling advection processes have been described and tested. This review summarizes the development and improvements that have taken place. The nature of the errors caused by numerical approximation to the advection equation are highlighted. Then the particular devices that have been proposed to remedy these errors are discussed. The extensive literature comparing transport algorithms is reviewed. Although there is no clear cut "best" algorithm, several conclusions can be made. The judicious use of simple finite difference schemes (second-order time differences and even-order (>2) spatial differences) provides a minimum level of accuracy that is suitable for many atmospheric applications. More complex schemes can yield a significant improvement in accuracy, but sometimes at great computational expense. Spectral and pseudospectral techniques consistently provide the highest degree of accuracy, but expense and difficulties assuring positive mixing ratios are serious drawbacks. Schemes which consider fluid slabs bounded by grid points (volume schemes), rather than the simple specification of constituent values at the grid points, provide accurate positive definite results. The computer memory requirements of the volume schemes can be excessive. Recent attempts to maxmize accuracy while keeping cost low have lead to such useful schemes as the one proposed by P. K. Smolarkiewicz.

CONTENTS

1. INTRODUCTION

Advective processes are of central importance in all aspects of fluid dynamics. Because modern computing machines have made it possible to build realistic numerical models, there has been extensive work in the development of numerical algorithms to model advective processes. This effort has been multidisciplinary with well more than 100 numerical algorithms being reported from the fields of plasma physics, meteorology, oceanography, and computational physics.

The realization that man-made alterations of the atmosphere by trace gases might significantly affect the global biosphere has generated great interest in the development of constituent transport and chemistry models. In particular, the distribution of trace gases by the atmosphere is of importance in studies of stratospheric ozone depletion, acid deposition by rain, and climatic changes caused by radiatively active trace species. Large-scale, two- and three-dimensional transport and chemistry models are a fundamental tool in understanding these environmental problems and in projecting what the impact of additional contamination will be. It is necessary to model advection accurately within these models.

The numerical modeling of advection, however, is plagued with difficulties. All schemes have numerical errors, and it is commonplace for unrealistic negative constituent values to be generated. The most simple, straightforward schemes have such large errors associated with them that the inadequacies of the advection algorithm quickly dominate the model, and the model bears little resemblance to the physical situation that the model was built to represent. Furthermore, efforts to correct one error in an algorithm are frequently met with the magnification of another error; for instance, it is easy to devise a scheme that does not generate negative constituent densities, but it is likely that the numerical diffusion in the "corrected" scheme is intolerably high.

When faced with the prospect of choosing an advection algorithm, the scientist confronts a very large field of literature from which no clear best algorithm can be defined despite numerous intercomparison studies. This review is aimed at the practitioner who needs to incorporate advection into a constituent transport and chemistry model. It is not addressed at the numerical scientist, and it is not an original comparison and evaluation of all transport routines. A particular goal is to show how the errors in transport algorithms arise and what attempts have been made to reduce these errors.

The paper is divided into six sections. In section 2 the advection problem is defined, and the classical problems that are encountered when attempting to model advection are discussed. Also, the desirable physical and computational attributes of advection algorithms are considered.

In section 3 the numerical approximations used in modeling advection are presented. The section is divided into two subsections. The first subsection discusses four simple schemes

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that serve not only as a paradigm for the errors encountered in transport modeling but also serve as the fundamental schemes on which many of the more complex schemes are based. The second subsection then attempts to list and classify many of the more complex schemes. The classification is somewhat artificial, but it is an attempt to create order out of the literature in such a fashion as to elucidate what has been attempted in the effort to reduce errors in advection models.

Section 4 discusses comparisons of transport schemes. Much of the section is based on the work of *Chock* [1985] and *Chock and Dunker* [1983]. Aside from the papers explicitly devoted to comparison studies, the papers that introduce new schemes invariably contain comparisons to other accepted schemes. It will be seen that there are a few very good and a few very bad schemes and a host of schemes in the middle ground that are difficult to distinguish from one another in terms of general performance. It is difficult to determine which scheme is best. Part of the indetermination is due to the fact that some schemes do well when evaluated by restricted criteria, and part of the indetermination is due to the fact that there is no definitive, quantitative method of evaluation.

In section 5, sections 2–4 are discussed in light of the particular problems associated with atmospheric chemistry models. The detailed numerical problems of combining chemistry and transport are deferred to a second paper in preparation by this author. A summary is offered in section 6, and the most promising algorithms are highlighted.

It is necessary to limit the scope of the current review. Originally, an attempt was made to review the literature of plasma physics, meteorology, oceanography, computational physics, applied mathematics, and air pollution research. Well over 100 schemes were found, and during the research for this article, at least 10 new algorithms were introduced, and at least four new comparison studies were published. Many of the 100 or more schemes are just a reformulation of other schemes, sometimes obvious, sometimes subtle. Many of the schemes work well only for the special application for which they have been designed. An attempt is made here to limit the discussion to transport schemes which might be appropriate for two- and three-dimensional global models of the atmosphere.

The interested reader is referred to a survey by *Thompson* [1984] that was received after this review was finished in draft form. Thompson's work is an attempt at an exhaustive compilation of transport algorithms and studies of transport algorithms. The work is much more numerically oriented and touches on a wider range of material than contained in this review. In the final section of Thompson's survey, desirable features of transport algorithms are listed. The reader will find both the focus and the conclusions of these two reviews to be somewhat different.

Good introductory material to the advection problem can be found in the works of *Richtmyer and Morton* [1967], *Roache* [1976], *Haltiner and Williams* [1980], *Peyret and Taylor* [1983], and *O'Brien* [1986], among others.

2. Modeling Advection

2.1. *Advection Equation and Mixing Ratio*

In the absence of sources, sinks, and viscosity the rate of change of a constituent in a fixed volume in a fluid is equal to the amount of constituent transported across the boundaries into or out of the volume. This is expressed by the constituent continuity equation

$$\frac{\partial C}{\partial t} + \nabla \cdot \mathbf{u}C = 0 \tag{1}$$

where C is the constituent density and $\mathbf{u}$ is the fluid velocity (for instance, see *Gill* [1982, p. 67]). The quantity $\mathbf{u}C$ is defined as the constituent flux. Equation (1) is a particular form of the nonlinear conservation equation [*Courant and Hilbert*, 196 p. 147].

Equation (1) is the flux form (also called conservation form) of the constituent continuity equation. The equation can be rewritten in the advective form

$$\frac{dC}{dt} \equiv \frac{\partial C}{\partial t} + \mathbf{u} \cdot \nabla C = -C\nabla \cdot \mathbf{u}$$

where dC/dt is the substantive or material derivative. Advection is represented by $\mathbf{u}\cdot\nabla C$. For incompressible flows (or for pressure coordinates in the atmosphere) the velocity field is nondivergent, the right-hand side is zero, and the constituent is conserved following a fluid parcel.

A quantity frequently used in constituent transport modeling is the mixing ratio

$$\mu \equiv C/\rho$$

where ρ is the density of the fluid. By substituting $\rho\mu$ into (1) the continuity equation can be rewritten as

$$\frac{\partial \mu}{\partial t} + \mathbf{u} \cdot \nabla \mu = -\frac{\mu}{\rho}\left(\frac{\partial \rho}{\partial t} + \nabla \cdot \rho\mathbf{u}\right)$$

The quantity in the parentheses on the right-hand side is the mass continuity equation for the fluid and is formally equal to zero. Thus written in terms of the mixing ratio, the advective and flux forms are equivalent. Including all processes, the constituent continuity equation is written as

$$\frac{d\mu}{dt} = \frac{\partial \mu}{\partial t} + \mathbf{u} \cdot \nabla \mu = P - L + \nabla \cdot \kappa \nabla \mu$$

where P and L represent chemical production and loss, and κ is a "diffusion" coefficient which is meant to represent subgrid-scale irreversible processes.

Much of this review will concentrate on the analysis of the one-dimensional advection equation with constant positive velocity, namely,

$$\frac{\partial \mu}{\partial t} + u\frac{\partial \mu}{\partial x} = 0$$

With the assumption of constant positive velocity, (3) represents the shape-conserving movement of an initial distribution toward positive x. Since the analytic solution is known in this simple case, the numerical solution can be critically evaluated. Varying velocity fields, multidimensions, and nonrectangular coordinate systems all increase the difficulties in modeling (3), but if an algorithm cannot model (3) correctly, then it will be of little use in more complex situations.

The advection equation is often classified as a hyperbolic differential equation. The classification of differential equations as hyperbolic, parabolic, or elliptic is generally reserved for second-order differential equations. The classic second-order wave equation is hyperbolic and can be expressed as a coupled system of two first-order advection equations. The advection equation allows propagating solutions like the w

equation, but some care should be taken in assigning all of the properties of the advection equation to hyperbolic equations in general and vice versa [*Book*, 1981]. *Grotjahn and O'Brien* [1976] and *Sod* [1978], for instance, investigate the problems of calculating the numerical solutions of hyperbolic equations, and most of their results are pertinent to the advection equation. *Courant and Hilbert* [1962, chap. 5] offer a complete discussion of the conservation equation and hyperbolic equations in general.

The fundamental property of the advection equation that makes it more difficult to model than parabolic or elliptic equations is the formation and maintenance of fronts (shocks). Inaccuracies and instabilities in numerical methods are often hidden or corrected by numerical or artificial diffusion that smooths out the errors. In parabolic and elliptic systems this smoothing out has the same effect as the fundamental mathematics and therefore does not cause great difficulties. Diffusion counteracts the fundamental nature of advection to form shocks. Also, the fact that the numerical mechanisms that form shock fronts are similar to the mechanisms that cause numerical instability makes it difficult to write absolutely stable advection schemes for long-time integrations.

2.2. *Flux Form and Advective Form*

There has been some discussion in the literature about using the flux (or conservative) form rather than the advective form to model constituent transport (see section 2.1). The most rudimentary argument is that with the flux form it is simpler to assure that total mass is conserved. This is particularly obvious for a no-flux boundary condition. *Gordon* [1981] compares flux and advective formulations of spectral general circulation models and discusses many of the aspects of the two methods.

It has also been argued that by using the flux form it is easier to avoid the numerical nonlinear instabilities of the type reported by *Phillips* [1959]. Very specific numerical methods are used to calculate the flux $\mathbf{u}\mu$ [*Lilly*, 1965; *Arakawa*, 1966; *Hirt*, 1968; *Piacsek and Williams*, 1970; Zalesak, 1981*a*; *Orszag*, 1971*b*; *Arakawa and Lamb*, 1977; *Gary*, 1979] (see also section 3.2.3). The methodology proposed by *Hirt* [1968] and discussed by *Zalesak* [1981*a*] demonstrates that one type of nonlinear instability is proportional to the truncation error, and the differencing techniques proposed by these authors assure that the truncation errors will not grow exponentially. In a similar vein, *Smolarkiewicz* [1985] shows that extra accuracy can be acquired by reduction of the truncation error when the flux form is used.

In nonrectangular coordinate systems the flux form might actually prove more difficult to code than the advective form [*Thompson*, 1984, p. 232]. Differences between the flux form and the advective form will not be stressed here. In terms of the mixing ratio the two formulations are analytically equivalent. In the consideration of (3) with constant velocity, many advantages of the flux form are not realized. Also, because many of the schemes that will be discussed intrinsically avoid nonlinear instability, some of the motivation to use the flux form is lost. Actual implementation of a transport algorithm might benefit from consideration of the flux form.

Equation (3) states that μ is conserved following a fluid parcel, and most of the algorithms considered here conserve mass. Also, all of the moments of μ are conserved in the analytic case. In the development of numerical algorithms, particular interest has been given to the second moment, μ^2. In a highly diffusive scheme the second moment will be damped; hence the second moment is indicative of the diffusion in the scheme. Conservation of μ^2 is fundamental in A. Arakawa's differencing techniques to avoid nonlinear instability [*Arakawa*, 1966; *Arakawa and Lamb*, 1977]. *Mahlman and Sinclair* [1977] discuss how the conservation of various moments of μ benefit the numerical solution.

2.3. *Errors: Diffusion, Dispersion, and Monotonicity*

Two fundamental properties of a transport algorithm are stability and accuracy. In general, stability requires the estimated solution to remain bounded as the integration time extends to infinity. Accuracy requires that the calculated solution closely represents the actual solution of the differential equation. It will be assumed that all of the transport schemes to be considered in this paper are stable (or in some cases very weakly unstable) and that accuracy is the basic quest in the development of complex algorithms.

The classic problems of numerical dissipation and dispersion are illustrated in Figure 1 for the one-dimensional advection of rectangular and triangular distributions by a constant positive velocity. The analytic solution to this problem is the distribution simply moving to the right while preserving its shape. In Figures 1*a* and 1*b* the transport has been modeled using second-order centered spatial differences and centered (leapfrog) time differences (see section 3.1.4). Small-scale waves appear and rapidly dominate the solution. The production of the small waves is caused by dispersion, that is, different Fourier components of the original distribution propagating at different phase speeds.

In Figures 1*c* and 1*d* the same problem has been solved using the donor cell or upstream differencing scheme (see section 3.1.2). In this situation, no ripples, or dispersion errors, are generated, but the original rectangular distribution is rapidly dissipated until the field is constant throughout the entire domain. Because the dissipation error shows the qualitative features of diffusion, and because the dissipation error can frequently be shown to have the mathematical form of diffusion, the words dissipation and diffusion will be used synonymously.

Dissipation and dispersion are seemingly conflicting inaccuracies which arise in numerical estimates of (3). Much of the effort that has gone into the development of improved advection algorithms has simply been aimed at reducing dissipation and dispersion. The papers of *Leonard* [1979] and *Gresho and Lee* [1981] offer interesting discussions of the sources of errors in transport algorithms and the philosophy of how to deal with the errors.

Closely related to dispersion errors is the concept of monotonicity. For the special case that the velocity in (3) is constant, monotonicity implies that the finite difference scheme does not generate any new maxima or minima [*Godunov*, 1959; *van Leer*, 1973, 1974; *Boris and Book*, 1973]. In other words, for a constant positive velocity, if it is assumed that advection over more than one grid point in one time step is not allowed, then if μ_i^t is the value at time t of μ at grid point i and μ_{i-1}^t is the value at $i-1$, then the new value of μ at time $t+\Delta t$ at grid point i should be equal to, or lie between, μ_i^t and μ_{i-1}^t (this demonstrates the close relation between interpolation and advection modeling). Hence if the original distribution is positive definite, as will be the case for constituent fields, then the estimated solution will also be positive definite. Examination of Figure 1*a* shows that the dispersion errors

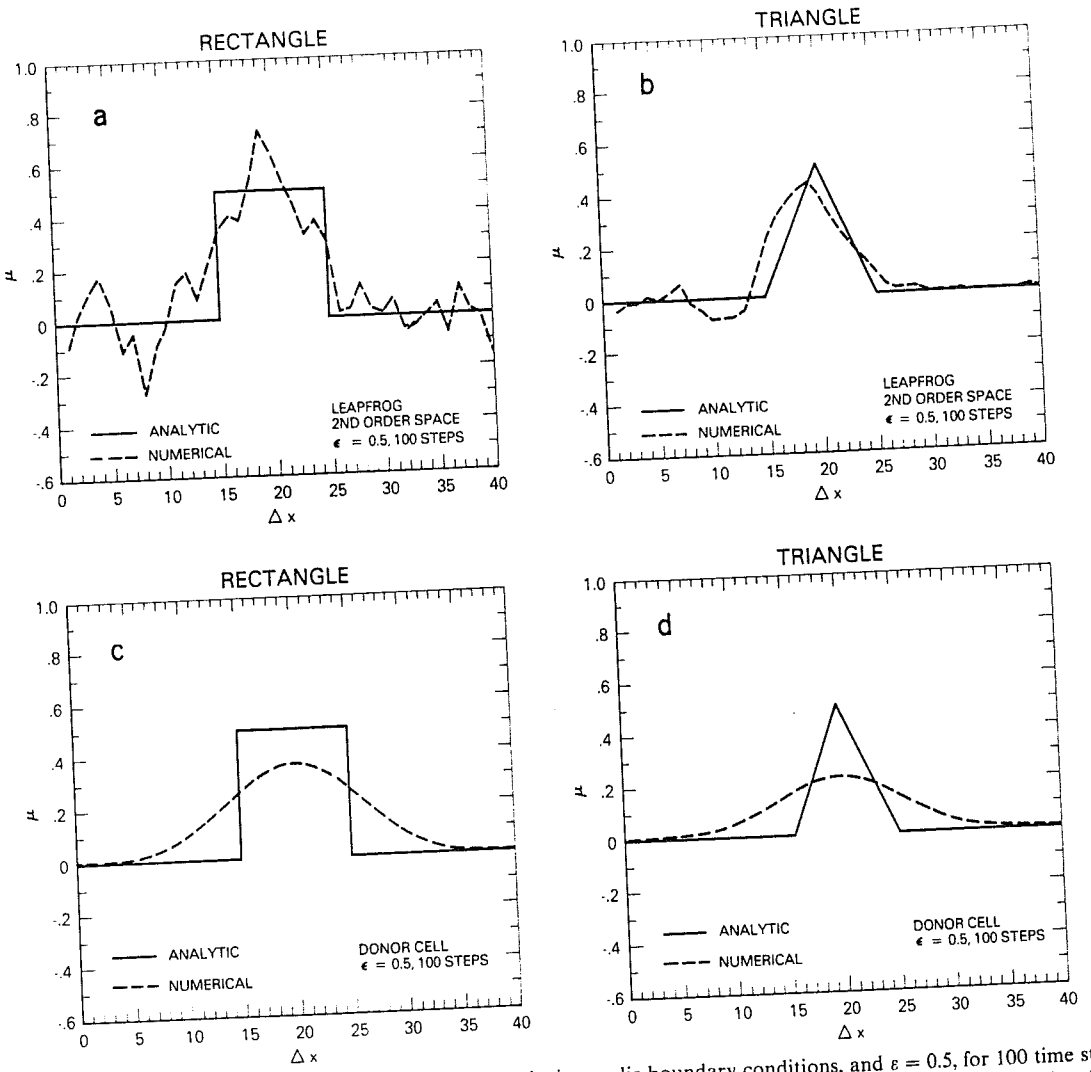

Fig. 1. Advection in one dimension, with constant velocity, cyclic boundary conditions, and $\varepsilon = 0.5$, for 100 time steps. (*a*) Rectangular distribution, using leapfrog time differences with second-order centered spatial differences (equation (15)). (*b*) Triangular distribution, using leapfrog time differences with second-order centered spatial differences (equation (15)). (*c*) Rectangular distribution, using donor cell (equation (11)). (*d*) Triangular distribution, using donor cell, (equation (11)).

lead to a lack of monotonicity and hence the production of nonphysical negative mixing ratios. (Monotonic and positive definite are not synonyms; positive definite means that positive mixing ratios are assured.)

A universally useful transport routine should transport all shape distributions with equal accuracy. Many of the schemes specifically designed to transport shocks quickly change other distributions into rectangular waves. Other schemes prefer to transport triangular-shaped distributions.

There are several practical reasons that influence the choice of a transport algorithms, for instance, applicability to more than one dimension, nonrectangular coordinate systems, and the ability to function under a wide variety of dynamical situations. Also, any transport scheme should be efficient in both its use of computer time and storage. These considerations are discussed in sections 5 and 6.

2.4. *Lagrangian and Eulerian Methods*

The use of Lagrangian (particle) methods rather than Eulerian (field) methods [*Lamb*, 1945; *Dryden et al.*, 1956; *Augenbaum*, 1984] eliminates the problem of advection per se, but because of the stretching and shearing of the original fluid parcels, it is necessary to either tag more parcels to resolve th scales of interest [*Mahlman and Sinclair*, 1977] or to reiniti lize the problem after a certain number of time steps. Th reinitialization process introduces many of the same trunc tion errors that would be present in Eulerian finite differen schemes [*Morton*, 1971]. Lagrangian transport algorithms ca be made very accurate, but generally at the expense of havi to transport an arbitrarily large number of particles. Still, L grangian schemes are useful for studying the evolution of pr cesses that are much smaller than finite grids can easily r solve (for example, turbulence) and for simple flows or sho time length integrations. For most global atmospheric pro lems, however, the time integration is so long that the init parcels become so intertwined and contorted that it c become difficult to interpret the results [*Hsu*, 1980]. Therefo the current emphasis is on Eulerian methods.

3. NUMERICAL MODELS

3.1. *Classic Schemes*

The formation of many transport schemes simply invol the method chosen to handle the derivatives in (3). In relat

to the spatial derivative, a small number of methods are used to estimate the time derivative. Therefore a great number of the recorded transport algorithms are merely different representations of the spatial derivatives. One of the basic philosophies invoked in deriving advection algorithms is to generate an algebraic representation of the spatial derivative and thereby reduce (3) to an ordinary differential equation in time so that well-known numerical techniques can be used. One common way of estimating the derivatives in (3) is to consider the Taylor series of μ about t (or x):

$$\mu(x, t \pm \Delta t) = \mu(x, t) \pm \Delta t \frac{\partial \mu(x, t)}{\partial t} + \tfrac{1}{2}\Delta t^2 \frac{\partial^2 \mu(x, t)}{\partial t^2} + \cdots \tag{4}$$

A time scheme (spatial derivative) is first-order accurate if the Taylor series is accurate to the term in Δt (Δx). It is second-order accurate if the Taylor series is accurate to Δt^2, and so on. In general, advection schemes that are accurate to an odd order are diffusive, and even-order accurate schemes tend to be dispersive [*Anderson and Fattahi*, 1974] (see particularly *Takacs* [1985]).

Another common (and often quite similar for the advection problem) method for generating estimates of the time derivative is the Runge-Kutta technique [*Carnahan et al.*, 1969; *Gerald*, 1978]. In this technique, rather than calculating higher derivatives as might be required in (4), more and more accurate approximations are developed by requiring that the solution be estimated at a number of intermediate steps during the time integration. Many of the methods in common usage are or can be interpreted as Runge-Kutta techniques.

The time integration of (3) can be carried out either explicitly, in which case the spatial derivative terms are only evaluated at known times, or implicitly, in which case the spatial derivative is evaluated at the same time at which the solution is being sought [see *Haltiner and Williams*, 1980]. The spatial derivatives can also be calculated at a combination of known and advanced times (for example, Crank-Nicolson and semi-implicit).

The characteristics of explicit and implicit time stepping are quite different. Explicit time stepping is conceptually simple, and the cost per time step is generally low. The source of the errors that arise in explicit time schemes are often readily identified and therefore can be alleviated or remedied. It is sometimes necessary to take prohibitively small time steps to assure that an explicit scheme is stable.

Implicit schemes are stable for any time step. However, implicit schemes are either iterative or require the inversion of matrices that reflect the size of the spatial grid. These techniques make the cost per time step high. Using computational expense as the criterion of decision can require comparing a large number of relatively cheap explicit steps to a smaller number of expensive implicit steps.

Implicit schemes tend to have dispersion errors caused by the retardation of shortwave features. These errors are particularly large when long time steps are taken. Therefore despite the unconditional stability of implicit schemes, careful consideration of the important time scales in the flow is required to assure an accurate algorithm.

Explicit time stepping will be considered in much more detail than implicit time stepping in this review. This is not meant, however, to underestimate the value of implicit and semi-implicit time schemes. Very accurate results can be obtained from implicit schemes [*Chock and Dunker*, 1983; *Long and Pepper*, 1981], and there are situations where their use is attractive.

From (4), rudimentary estimates for space and time derivatives can be derived, depending upon whether the series is expanded in Δx or Δt. By truncating after the first-order term, the following estimates are obtained:

$$\frac{\partial \mu}{\partial x} \approx \frac{\mu_{i+1}{}^t - \mu_i{}^t}{\Delta x} \tag{5a}$$

or

$$\frac{\partial \mu}{\partial x} \approx \frac{\mu_i{}^t - \mu_{i-1}{}^t}{\Delta x} \tag{5b}$$

$$\frac{\partial \mu}{\partial t} \approx \frac{\mu_i{}^{t+\Delta t} - \mu_i{}^t}{\Delta t} \quad \text{(forward)} \tag{6a}$$

or

$$\frac{\partial \mu}{\partial t} \approx \frac{\mu_i{}^t - \mu_i{}^{t-\Delta t}}{\Delta t} \quad \text{(backward)} \tag{6b}$$

The index i represents the spatial dependence. Equations (5) and (6) form what are often called one-sided or uncentered differences.

Second-order centered differences can be derived from (4) by subtracting the form of (4) written with the plus sign from the form written with the minus sign to yield

$$\frac{\partial \mu}{\partial x} \approx \frac{\mu_{i+1}{}^t - \mu_{i-1}{}^t}{2\Delta x} \tag{7}$$

$$\frac{\partial \mu}{\partial t} \approx \frac{\mu_i{}^{t+\Delta t} - \mu_i{}^{t-\Delta t}}{2\Delta t} \quad \text{(leapfrog)} \tag{8}$$

In order to discuss the nature of the numerical diffusion in the schemes detailed below, it is useful to derive the canonical form for the finite difference estimate to the second derivative. If the form of (4) using the plus sign is added to the form of (4) using the minus sign, then an estimate for the second derivative follows:

$$\frac{\partial^2 \mu}{\partial x^2} \approx \frac{\mu_{i+1}{}^t - 2\mu_i{}^t + \mu_{i-1}{}^t}{\Delta x^2} \tag{9}$$

This derivation of estimates of the derivatives in (3) serves as a basis for the discussion of the classic transport schemes below. Details on numerical analysis and the derivation of higher-order schemes can be found in many numerical analysis textbooks [e.g., *Ames*, 1977; *Lapidus and Pinder*, 1982; *Haltiner and Williams*, 1980; *O'Brien*, 1986].

Below, what may be considered classic techniques will be reviewed and discussed. When known, other names for a scheme will be given. As a note of caution, several of the schemes are equivalent when the velocity in (3) is constant; however, they are different in problems with nonconstant velocities. In this event the alternative name serves more as a reference to identify a similar scheme rather than to connote identity. There are many other schemes which could easily be interpreted as classic finite difference schemes for integrating nonlinear hyperbolic equations (see, for instance, *Kurihara* [1965], *Rubin and Burstein* [1967], *Emery* [1968], *Young* [1968], *Taylor et al.* [1972], *Richtmeyer and Morton* [1967], and *Haltiner and Williams* [1980]).

3.1.1. *Euler, forward in time.* The Euler scheme is simply a first-order Taylor approximation (also a first-order Runge-Kutta technique) and is represented by combining (6*a*) (forward) with (7):

$$\mu_i^{t+\Delta t} = \mu_i^t - \frac{\varepsilon}{2}(\mu_{i+1}^t - \mu_{i-1}^t)$$
$$\varepsilon \equiv \frac{u\Delta t}{\Delta x} \tag{10}$$

This scheme is unstable. Though unstable, the addition of diffusion to the Euler scheme stabilizes it, and the scheme is used in transport studies [*Leonard*, 1980; *Clancy*, 1981; *Garcia and Solomon*, 1983; *Gidel et al.*, 1983] (see also section 5.3). *Hirt* [1968] shows that the truncation error of (10) has the appearance of an exponential growth term (negative diffusion). The addition of too much diffusion to the scheme will also lead to instability [*Hirt*, 1968; *Clancy*, 1981]. The quantity ε is frequently called the Courant-Friedrichs-Lewy (CFL) parameter, or sometimes simply the Courant number.

3.1.2. *Upstream, one-sided, donor cell scheme.* This scheme can be viewed as (6*a*) (forward) combined with the particular specification that the spatial derivatives are evaluated as one-sided (equation (5)) from the direction of the flow. It is written as

$$\mu_i^{t+\Delta t} = \mu_i^t - \frac{\varepsilon}{2}[1 - \text{sign}\,(u_i^t)](\mu_{i+1}^t - \mu_i^t)$$
$$-\frac{\varepsilon}{2}[1 + \text{sign}\,(u_i^t)](\mu_i^t - \mu_{i-1}^t) \tag{11}$$

where

$$\text{sign}\,(\psi) \equiv 1 \qquad \psi \geq 0$$
$$\text{sign}\,(\psi) \equiv -1 \qquad \psi < 0$$

The donor cell scheme is very diffusive, and the diffusion can be shown clearly by rewriting (11):

$$\mu_i^{t+\Delta t} = \mu_i^t - \frac{\varepsilon}{2}(\mu_{i+1}^t - \mu_{i-1}^t) + \frac{|\varepsilon|}{2}(\mu_{i+1}^t - 2\mu_i^t + \mu_{i-1}^t) \tag{12}$$

The last term on the right-hand side has the canonical form of diffusion (equation (9)). The amount of diffusion in (12) is the least that can be added to the Euler scheme to assure monotonicity [*van Leer*, 1973]. For advection with a constant velocity this scheme is the same as *Courant et al.*'s [1952] scheme [see *van Leer*, 1977*a*], Lelevier's scheme [*Richtmeyer and Morton*, 1967], and *Godunov*'s [1959] scheme [see *van Leer*, 1973].

3.1.3. *Lax-Wendroff scheme.* The scheme of *Lax and Wendroff* [1960] is a second-order accurate Taylor series approximation in time and is derived most generally by substituting $-u\partial\mu/\partial x$ from (3) for the time derivatives in (4) to yield

$$\mu(x, t + \Delta t) = \mu(x, t) - u\Delta t\frac{\partial\mu(x, t)}{\partial x} + \tfrac{1}{2}u^2\Delta t^2\frac{\partial^2\mu(x, t)}{\partial x^2} \tag{13}$$

Now by substituting (7) and (9) into (13), the Lax-Wendroff scheme is obtained (for instance, *Gadd* [1978*b*]):

$$\mu_i^{t+\Delta t} = \mu_i^t - \frac{\varepsilon}{2}(\mu_{i+1} + \mu_{i-1}) + \frac{\varepsilon^2}{2}(\mu_{i+1} - 2\mu_i + \mu_{i-1}) \tag{14}$$

As with the donor cell, this scheme appears to be an Euler scheme stabilized by diffusion, but as discussed by *Haltiner and Williams* [1980], this interpretation is somewhat misleading, since (14) is in fact second-order accurate in time and (11) and (12) are only first-order accurate. The amount of diffusion in this scheme is the minimum amount to stabilize the Euler scheme, but this extensively utilized scheme is still quite diffusive [*Morton*, 1971]. The Lax-Wendroff scheme was also independently discovered by N. A. Phillips and C. E. Leith [*Gadd*, 1978*b*] and by *Godunov* [1959] (the tripod scheme).

3.1.4. *Leapfrog, centered time differences.* The above schemes can all be written as two-level schemes (one step); that is, only two time levels are involved, t and $t + \Delta t$. All Runge-Kutta schemes can be written as two-level schemes no matter what order accuracy is required. The leapfrog scheme is second-order accurate, like the Lax-Wendroff scheme, but requires three time levels (two step): $t - \Delta t$, t, and $t + \Delta t$. It is written as

$$\mu_i^{t+\Delta t} = \mu_i^{t-\Delta t} - \varepsilon(\mu_{i+1}^t - \mu_{i-1}^t) \tag{15}$$

This scheme is nondiffusive (see Table 1). The leapfrog technique has the disadvantage of producing not only a physical but a computational mode. In the linear case (constant u) the computational mode can be eliminated by the proper choice of the initial condition. In general, for long wavelengths the amplitude of the computational mode is small, and the physical mode dominates the solution [*Mesinger and Arakawa*, 1976; *Haltiner and Williams*, 1980, pp. 114, 118]. The computation mode may cause difficulties in problems rich in short-wave features, and some effort may be needed to suppress it [*Zalesak*, 1981*b*].

The leapfrog scheme exhibits the "weak instability" of producing two independent solutions at even and odd time steps. These split solutions can be brought together by occasionally averaging the even and odd time step solutions (for instance, *Orszag* [1971*b*, p. 80]) or by occasionally using a two-level scheme. The Asselin time filter is also frequently used to combine the split solutions and reduce the computational mode [*Haltiner and Williams*, 1980, p. 147; *Asselin*, 1972] (see also *Deque and Carriolle* [1986]).

The leapfrog scheme requires, as do all multistep schemes, a separate startup scheme, because μ is only known at one time. For advection it is not necessary to store three arrays in memory with the leapfrog scheme. However, when combining advection with chemistry and diffusion, it may prove necessary (or at least conceptually simpler) to store all three levels.

TABLE 1. Dissipation Error for a Fourier Component of Wave Number k

Algorithm	Order	Square of the Amplification Factor	Comment
Theory	∞	1	
Donor cell	1	$1 - 2\lvert\varepsilon\rvert(1 - \lvert\varepsilon\rvert)[1 - \cos(k\Delta x)]$	strong damping
Lax-Wendroff	2	$1 - (\varepsilon^2 - \varepsilon^4)[1 - \cos(k\Delta x)]^2$	weak damping
Leapfrog	2	1	no damping

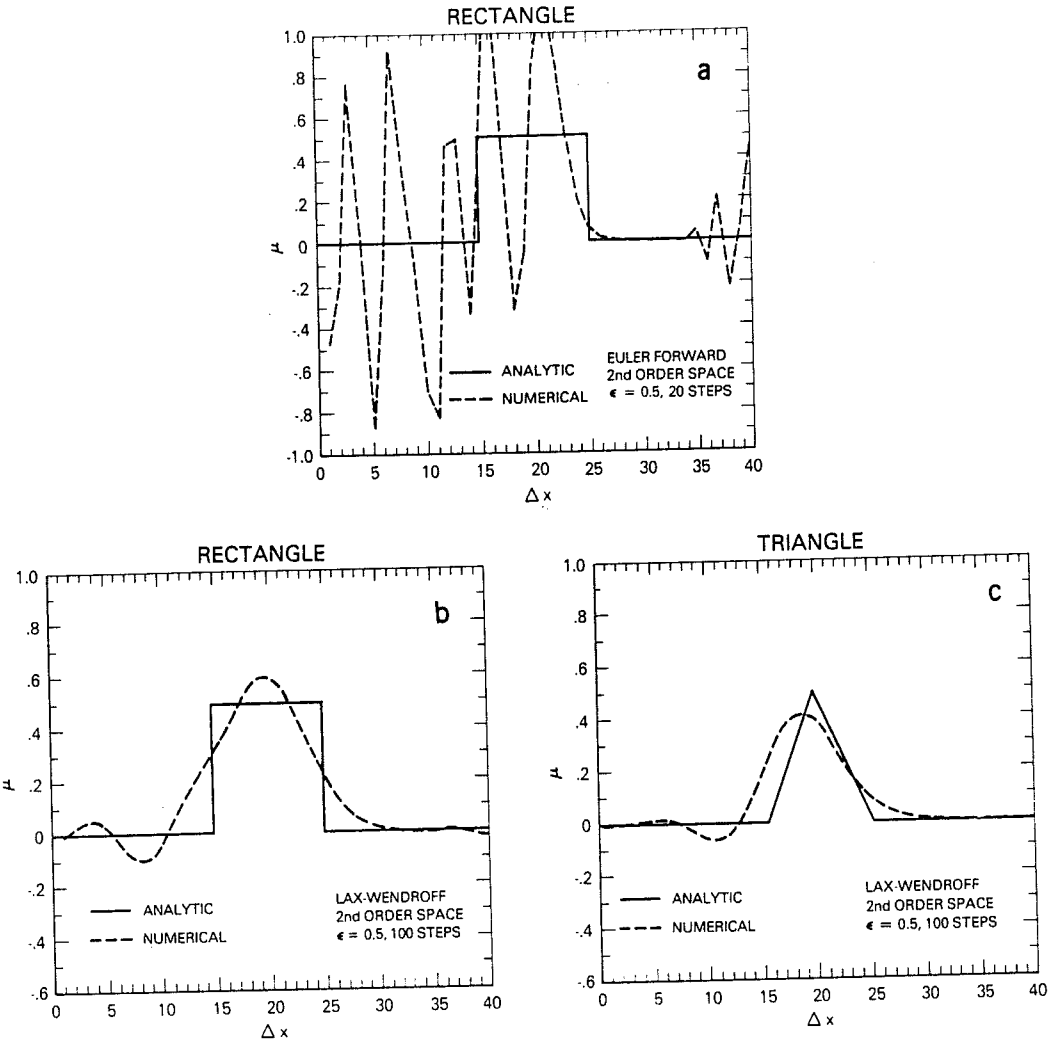

Fig. 2. Advection in one dimension, with constant velocity, cyclic boundary conditions, and $\varepsilon = 0.5$. (*a*) Rectangular distribution using Euler forward scheme (equation (10)) for 20 time steps; this scheme is unstable. (*b*) Rectangular distribution using Lax-Wendroff scheme (equation (14)) for 100 time steps. (*c*) Triangular distribution using Lax-Wendroff scheme (equation (14)) for 100 time steps.

thus increasing memory requirements in relation to those of two-level schemes.

Equations (10)–(15) will be considered the classic transport schemes. These schemes have been used by themselves, but more importantly, for this discussion they have been the conceptual basis for the development and interpretation of more sophisticated transport algorithms.

Comparison of the schemes (equations (10), (11), (14), and (15)) for one-dimensional advection by a constant velocity of a rectangular and triangular distribution is shown in Figures 1 and 2. The Euler scheme (equation (10)) is unstable, and the solution rapidly grows beyond the bounds of the graph (Figure 2*a*). The donor cell (equation (11)) does not generate negative densities, is highly diffusive, and rapidly diminishes the amplitude of the rectangle or triangle (Figures 1*c* and 1*d*). The Lax-Wendroff scheme (equation (14)) is not as diffusive as the donor cell but because of dispersion generates ripples that follow the distribution (Figures 2*b* and 2*c*). The leapfrog scheme (equation (15)) is not diffusive but like the Lax-Wendroff scheme is dispersive, and because of the lack of diffusion, the scheme is quickly dominated by the shortwaves (Figures 1*a* and 1*b*). None of these schemes adequately models the advection equation.

The dissipation errors and phase shift and phase errors (dispersion errors) for schemes (11), (14), and (15) are shown in Tables 1–3 [from *Boris and Book*, 1973]. In these tables the propagation of a single Fourier component is considered so that the amplification and phase errors can be analytically calculated. The donor cell has a first order in ε ($=u\Delta t/\Delta x$) dissipation error, and the Lax-Wendroff scheme has a second-

TABLE 2. Phase Shift for a Fourier Component of Wave Number k During One Time Step

Algorithm	Order	Phase Shift x_ϕ in One Cycle
Theory	∞	$kx_\phi = k\varepsilon\Delta x \qquad x_\phi = u\Delta t$ (correct answer)
Donor cell	1	$\tan(kx_\phi) = \dfrac{\varepsilon \sin(k\Delta x)}{\{1 - \lvert\varepsilon\rvert[1 - \cos(k\Delta x)]\}}$
Lax-Wendroff	2	$\tan(kx_\phi) = \dfrac{\varepsilon \sin(k\Delta x)}{\{1 - \varepsilon^2[1 - \cos(k\Delta x)]\}}$
Leapfrog	2	$\tan(kx_\phi) = \dfrac{\{1 - [1 - (\varepsilon^2/2)\sin^2(k\Delta x)]^2\}^{1/2}}{[1 - (\varepsilon^2/2)\sin^2(k\Delta x)]}$

TABLE 3. Relative Phase Error for a Fourier Component of Wave Number k During One Time Step

Algorithm	Order	Relative Phase Error
Theory	∞	$\frac{x_\phi - v\Delta t}{v\Delta t} = 0$ no error
Donor cell	1	$\frac{x_\phi - v\Delta t}{v\Delta t} = -\left(\frac{1}{6} - \frac{\lvert\varepsilon\rvert}{2} + \frac{\varepsilon^2}{3}\right)k^2\Delta x^2 + O(k^4\Delta x^4)$
Lax-Wendroff	2	$\frac{x_\phi - v\Delta t}{v\Delta t} = -\left(\frac{1}{6} - \frac{\varepsilon^2}{6}\right)k^2\Delta x^2 + O(k^4\Delta x^4)$
Leapfrog	2	$\frac{x_\phi - v\Delta t}{v\Delta t} = -\left(\frac{1}{6} - \frac{\varepsilon^2}{24}\right)k^2\Delta x^2 + O(k^4\Delta x^4)$

The x_ϕ is the phase shift given in Table 2.

order dissipation error (see (12) and (14)). There is no dissipation error in the leapfrog scheme.

The phase shift and the relative phase error are shown in Tables 2 and 3. None of the schemes propagate the shortest resolvable wavelength (the $2\Delta x$ wave, $k\Delta x = \pi$) for all ε. For long-waves, all of the schemes do an adequate job, but the phase error increases as the wavelength decreases. The donor cell and Lax-Wendroff schemes have no phase errors for $\varepsilon = 1$. Also, the donor cell scheme has no dispersion error for $\varepsilon = 0.5$, and for values close to 0.5 the linear term in the dispersion error tends to cancel the constant term. These features lead *Boris and Book* [1973] to conclude that the phase characteristics of the donor cell are acceptable.

Hirt [1968] proposed expanding each term of the finite difference equation in a Taylor series in order to reveal information about the stability and error characteristics of a particular scheme. Application of Hirt's method frequently reveals the cancellation of truncation errors so that a scheme may be more accurate than it would appear to be by the methods considered in the production of Tables 1–3. Hirt's method is not considered in detail here. *Cloutman and Fullerton* [1978] discuss automated analyses based on Hirt's method.

The phase errors associated with space and time finite difference approximations are shown in Figure 3 [from *Zalesak*, 1981*b*]. In the upper part of the figure the phase error derived from leapfrog time differencing and an exact spatial representation is shown. The time differencing errors have a tendency to advance the phase (as opposed to implicit methods which retard the phase). The phase advance associated with shortwaves is larger than the phase advance associated with long-waves.

In the lower part of Figure 3 the phase error caused by the spatial truncation error is shown. It is seen that all schemes propagate the long wavelengths accurately. As the order of the spatial truncation increases, shorter and shorter wavelengths are more accurately propagated, but none of the finite differences schemes or the pseudospectral scheme (see section 3.2.3) propagates the shortest wavelength ($2\Delta x$ wave). Because the phase errors that arise from finite difference approximations are worse for shorter wavelengths, it can be argued that the short wavelengths should be selectively diffused to eliminate those modes which are not accurately modeled [*Zalesak*, 1984].

The schemes that have been labeled as the classic time schemes have several valuable attributes on which to base the development of more sophisticated schemes. The Lax-Wendroff scheme represents the minimum amount of diffusion that must be added to the simple Euler scheme to yield stability. The donor cell scheme represents the minimum amount of diffusion that must be added to the Euler scheme to make it monotonic. The leapfrog scheme has no diffusive errors but has large dispersion errors. The donor cell has large diffusive errors but has relatively good dispersion characteristics. It is easily seen how a wealth of transport schemes could be devised by weighing the various advantages and disadvantages of these basic schemes.

Godunov [1959] [see *van Leer*, 1973] proved that no linear scheme of second-order or higher accuracy can be made free of dispersion errors. Therefore the development of a perfect transport algorithm implies some sort of nonlinearity which usually involves a "filtering" algorithm that goes through the grid and searches for areas where dispersion errors are a danger and then prevents these errors from occurring. It is such nonlinear schemes that are the subject of sections 3.2.5 and 3.2.6.

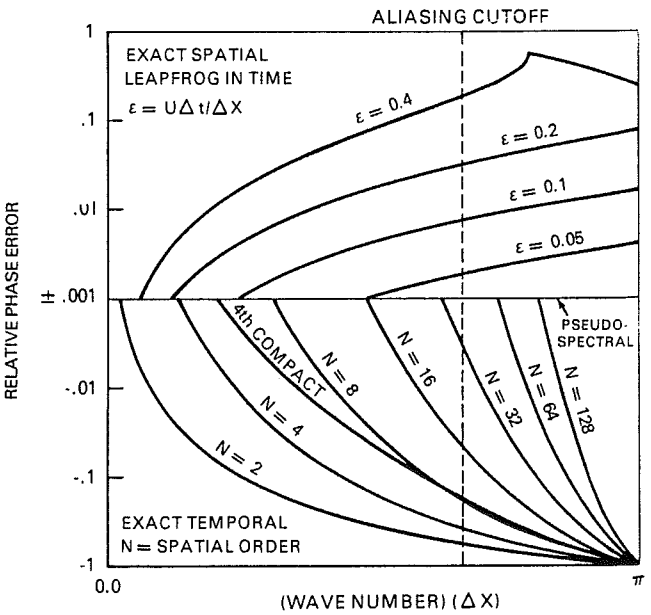

Fig. 3. "Plot of the relative phase error as a function of the Fourier wave number $k\Delta x$ for various schemes applied to the linear advection equation. The upper and lower halves of the plot refer to two distinct families of idealized schemes: the upper half to a scheme discretized in time but continuous in space, and the lower half to a scheme discretized in space but continuous in time" [from *Zalesak*, 1981*b*].

TABLE 4. Transport Algorithms

Classification	Reference	Comments
Finite difference	*Burstein and Mirin* [1970]	Third-order in space and time; Runge-Kutta.
Centered	*Clark and Hall* [1979]	Hybrid scheme with nonlinear switch.
	Crowley [1967]	Improved Lax-Wendroff.
	Fromm [1968]	Zero average phase error.
	Gadd [1978*a*, *b*]	Improved Lax-Wendroff, fourth-order accurate.
	Harten [1978]	Hybrid of low- and high-order schemes with switching.
	Kutler et al. [1972]	Combined *Rusanov* [1970] and *MacCormack* [1969].
	MacCormack [1969]	Noncentered Lax-Wendroff
	Rusanov [1970]	Third-order Runge-Kutta, like *Burstein and Mirin* [1970].
	Schneider [1984]	Square root scheme; avoids negative constituent values.
	Smolarkiewicz [1982]	Improved *Crowley* [1968] scheme.
Quasi-Lagrangian, upstream, and upstream biased	*Bates and McDonald* [1982]	Similar to *Krishnamurti* [1962].
	Crowley [1968]	Quasi-Lagrangian, three- and five-point interpolation.
	Godunov [1959]	Monotonic schemes; a classic paper.
	Krishnamurti [1962]	Quasi-Lagrangian.
	Pudykiewicz and Staniforth [1984]	Robert's method with an emphasis on iterative methods.
	Robert [1981, 1982]	"Semi-Lagrangian."
	Schlesinger [1985]	Upstream-biased Crowley scheme.
	Takacs [1985]	Empirical error reduction; upstream bias.
	van Leer [1973, 1974, 1977*a*]	Monotonic versions of Fromm's scheme.
Expansion function	*Christensen and Prahm* [1976]	Pseudospectral.
	Fleischer and Worley [1978]	Orthogonal collocation.
	Orszag [1971*a*, *b*]	Spectral and pseudospectral.
	Orszag [1972]	Comparison of spectral and pseudospectral.
	Wengle and Seinfeld [1978]	Orthogonal collocation.
	Wengle et al. [1978]	Orthogonal collocation.
Finite element	*Chock* [1985]	A comparison paper with a variety of formulations.
	Gelinas et al. [1981]	Moving element, very accurate, one-dimension only.
	Hasbani et al. [1983]	Combined characteristics and finite elements.
	Hughes [1979]	A book on advection and finite elements.
	Pepper et al. [1979]	Chapeau functions.
	Piva et al. [1980]	Reduction of dispersion by considering element details.
	Taylor and Hood [1973]	A fairly early application to advection.
FCT (antidiffusive)	*Boris and Book* [1973]	SHASTA.
	Book et al. [1975]	Generalization of FCT beyond SHASTA.
	Boris and Book [1976]	New flux limiters to reduce diffusion.
	Smolarkiewicz [1983, 1984]	Antidiffusion.
		Multidimensional *Smolarkiewicz* [1983].
	Zalesak [1979, 1981*b*, 1984]	Fully multidimensional FCT.
		High-order and pseudospectral spatial differences.
		High-order Lax-Wendroff with and without FCT.
Volume	*Egan and Mahoney* [1972]	Second moments.
	Pedersen and Prahm [1974]	Second moments with width correction.
	Pepper and Baker [1980]	Three-dimensional second moments.
	Pepper and Long [1978]	Second moments with and without width correction.
	Hain [1978]	Partial donor method.
	Russell and Lerner [1981]	Slopes scheme.
	Prather [1986]	Extension of slopes scheme; uses second-order moments.
	van Leer [1977*b*, 1979]	Linear representations within slabs, coupled with monotonicity algorithm.
	Colella [1982]	MUSCL; generalization of *van Leer* [1977*b*, 1979].
	Colella and Woodward [1984]	Piecewise parabolic method.
	Woodward and Colella [1981]	Piecewise parabolic method.

3.2. *Transport Schemes*

Transport schemes that have been specifically developed for modeling advective processes are listed in Table 4. These are all Eulerian schemes which have been classified according to whether they are straightforward finite difference algorithms, expansion function algorithms, flux-corrected transport (FCT) algorithms, volume algorithms, or finite element methods. The classification is somewhat arbitrary and is meant to convey the feature intrinsic to the scheme that is supposed to yield a significant improvement over the classic schemes discussed above. As is mentioned in section 1, it is impossible and impractical to expect that all advective algorithms have been included. Table 4 represents what sort of algorithms are available, and by discussion of the entrants in Table 4 demonstrates what methods have been tried in the improvement of advective schemes.

3.2.1. *Finite difference schemes.* In the algorithms that are classified as finite difference schemes in Table 4, much of the effort has gone into reducing the errors caused by dispersion. A straightforward way to improve the simple schemes (section 3.1) is to go to higher-order accuracy. *Rusanov* [1970] and *Burstein and Mirin* [1970] have considered a third-order Runge-Kutta method that is consistently accurate to third

order in both Δx and Δt. One feature of the Runge-Kutta technique is that for "n"th-order accuracy there are $n + 1$ parameters. Therefore there is one arbitrary parameter that can be chosen by the user. This parameter can be chosen to minimize some measure of error such as dispersion (see *Anderson and Fattahi*'s [1974] evaluation of the Rusanov scheme, for instance).

The idea of using a tunable parameter to reduce errors is carried further by *Wesseling* [1973]. Wesseling assumes that the solution of (3) can be written in the following finite difference form:

$$\mu_i^{t+\Delta t} = \sum_{k_1}^{k_2} a_k \mu_{i+k}^{t} \tag{16}$$

Wesseling calculates the error in (16) associated with the propagation of a single Fourier component and then in conjunction with Parseval's theorem generates an algorithm for producing finite difference schemes that minimize the error with regard to some weighting function. Wesseling shows how the schemes of *Lax and Wendroff* [1960], *Courant et al.* [1952] (see section 3.1.2), and *Fromm* [1968] can be derived as methods to reduce a particular form of error in the finite difference estimate. Fromm's scheme, called the "zero average phase error," is the second-order scheme that minimizes dispersion. The most accurate scheme derived by Wesseling was a modified version of the Rusanov-Burstein-Mirin third-order Runge-Kutta technique.

Takacs [1985] uses the same expansion as (16), truncated to be second-order accurate. Takacs then includes one more point than needed to ensure second-order accuracy, yielding a free parameter that is used to empirically minimize errors by comparing estimated solutions to known analytic solutions. Takacs' scheme is upstream biased (see section 3.2.2) and is third-order accurate in the case of constant velocity.

Several schemes have been introduced that explicitly address inadequacies in the Lax-Wendroff scheme [*Gadd*, 1978*b*; *van Leer*, 1974; *MacCormack*, 1969; *Kutler et al.*, 1972]. *Crowley* [1967, 1968] developed a popular second-order scheme that avoids some of the problems of the Lax-Wendroff scheme. *Smolarkiewicz* [1982] has considerably improved *Crowley*'s [1968] scheme and applied it to nonconstant velocities in two and three dimensions. *Schlesinger* [1985] investigates improvements to the Crowley scheme by adding third-order upstream-biased terms (see section 3.2.2).

Increasing the order of accuracy of the spatial derivatives in (3) reduces the dispersion error and can lead to dramatic improvement in an advection algorithm. This has been clearly demonstrated by *Roberts and Weiss* [1966] and *Mahlman and Sinclair* [1977] with fourth-order spatial derivatives combined with the leapfrog time scheme (see also *Kreiss and Oliger* [1972]). A caveat pointed out by *Zalesak* [1981*b*] is that for distributions which are rich in high wave number components, use of high-order accurate differences may actually reduce the accuracy of the solution.

3.2.2. *Quasi-Lagrangian, semi-Lagrangian, upstream, upstream-centered, and upstream-biased methods.* Another approach for using finite difference schemes to model advection is the quasi-Lagrangian method as discussed by *Krishnamurti* [1962]. In this technique the question is asked (assuming positive velocity), what is the value of the advected function upstream at the point $x_i - u\Delta t$? This should be the value at the grid point on the next time step. In practice, an interpolation technique is used to estimate the required value residing between grid points. Because of the interpolation requirements, quasi-Lagrangian schemes are expected to have the same characteristics as normal finite difference algorithms. In the techniques discussed by *Krishnamurti* [1962], *Crowley* [1968], and *Mahlman and Sinclair* [1977], the numerics are centered around the grid point of interest, and both upstream and downstream points are used in this interpolation.

Recent quasi-Lagrangian schemes have developed around the work of *Robert* [1981]. These schemes are biased to include points upstream from the grid point of interest. Such schemes are classified as "upstream biased." *Pudykiewicz and Staniforth* [1984] investigate many quasi-Lagrangian schemes and show that their technique of using multiple iterations to determine the departure point significantly improves the accuracy of the calculation (see also *Bates and McDonald* [1982, 1985] and *Staniforth and Pudykiewicz* [1985]). These methods have received much recent attention in general circulation modeling because they can be run with a much larger time step than conventional finite difference techniques [*Robert et al.*, 1985; *Ritchie*, 1986; *McDonald*, 1986]. *Staniforth and Temperton* [1986] have applied upstream-biased techniques to the method of finite elements (section 3.2.4).

The difference between the two types of quasi-Lagrangian methods discussed above is detailed by *van Leer* [1977*a*], who discusses upstream-centered (i.e., upstream biased) and central difference schemes. In upstream-centered methods, attention is focused away from the grid points onto the point $x_i - u\Delta t$, that is, the point from which the particle has been advected. In central difference schemes the new values of the advected quantity are centered on the old values at the grid points. In upstream-centered schemes the choice of grid points to calculate the advection is dependent on the direction of the flow. Upstream-centered schemes are known for their intrinsically small phase errors. The donor cell technique (section 3.1.2) is the upstream-centered scheme derived using linear interpolation.

3.2.3. *Spectral and pseudospectral global expansion function techniques.* The most accurate way to estimate the spatial derivatives is to use expansion functions to estimate the distribution of μ and then calculate the derivatives in (3) analytically. Expansion function techniques can be applied in either a global fashion or in the finite element method (section 3.2.4). Much of the theory and discussion of expansion function techniques was introduced by *Orszag* [1971*a*, *b*]. Excellent reviews are given by *Gottlieb and Orszag* [1977], *Machenhauer* [1979], and *Merilees and Orszag* [1979].

In the expansion function techniques it is assumed that μ can be expressed as a summation of basis functions:

$$\mu(x, t) = \sum_{0}^{N} A_n(t) \Upsilon_n(x) \tag{17}$$

where the Υ represent a complete set of orthonormal basis functions and are presumed to be chosen suitable for a particular domain and boundary conditions.

Expansion function techniques are traditionally classified in three ways, depending on how the errors are handled. The spectral or Galerkin method requires that the error in (3), arising from representing μ by (17), is orthogonal to the basis functions Υ_n. The orthogonality requirement is equivalent to requiring that the mean square integral of the error be a minimum [see *Machenhauer*, 1979].

The pseudospectral or collocation technique requires the expansion functions to equal μ at a finite number of points (collocation points or grid points). For constant velocity the spectral and pseudospectral representations of (3) are identical. In essence, the pseudospectral technique uses the basis functions Υ_n as a high-order accurate interpolation function to represent the constituent field. The spatial derivatives are calculated analytically from the basis function fit. The pseudospectral technique does not propagate the shortest wave ($2\Delta x$), because there is no phase information at this wavelength for an even number of collocation points (an odd number of points does not allow determination of a $2\Delta x$ component at all).

A major difference between the spectral and pseudospectral technique involves the treatment of the aliasing errors [*Orszag*, 1971*b*, 1972]. Aliasing errors are those errors that arise when it is attempted to resolve high wave number features on a grid that is too coarse to resolve the features. High wave number features arise naturally in (3) because of the product of the velocity and the constituent field. In Galerkin or spectral methods the aliasing errors are identically zero because of the requirement that the error be orthogonal to the basis functions. In the pseudospectral method the aliasing is included in the estimated numerical solution.

In some problems the aliasing terms can cause inaccuracies or even instabilities [*Phillips*, 1959]. Spectral techniques avoid this instability by eliminating the aliasing errors. In spectral methods the second moment is exactly conserved. In pseudospectral models the presence of aliasing errors can cause long-term stability problems. Pseudospectral techniques are easier to apply to nonlinear problems. *Peyret and Taylor* [1983, p. 103] list among the advantages of the pseudospectral approach (compared to the spectral approach) ease in prescribing boundary conditions and ease in application to compressible flow.

Both the spectral and the pseudospectral techniques can be viewed as particular cases of the method of weighted residuals [*Zienkiewicz and Morgan*, 1983]. If the error is defined as e_n, then an attempt can be made to reduce the error according to

$$\int_x e_N W_N \, dx = 0 \tag{18}$$

where W_N is some weighting function. The choice of W_N as the basis functions themselves leads to the Galerkin technique. The choice of W_N as the Dirac delta function, $\delta(x - x_N)$ where x_N are N points in the domain where the series approximation exactly equals the data, leads to the pseudospectral or collocation technique.

A third classification of expansion function techniques is the "tau" approximation [*Gottlieb and Orszag*, 1977]. This method differs from the spectral technique in that the expansion functions are not required to satisfy the boundary conditions explicitly. Instead, a series representation is used to meet the boundary conditions.

Of the schemes listed in Table 4 as expansion function techniques, most of them would fall under the classification of pseudospectral. Most are time advanced using leapfrog time stepping.

3.2.4. *Finite element method.* In the expansion function techniques discussed in section 3.2.3, the expansion functions were used to represent μ over the entire domain. In the finite element technique the domain is divided into many subdomains called elements, and then an expansion function representation is used within each element. With this technique, very accurate results can be obtained with series expansions that use very few basis functions. Excellent descriptions of the finite element method are offered by *Zienkiewicz and Morgan* [1983] and *Lapidus and Pinder* [1982].

One of the most commonly used basis functions is the chapeau function (hat function) which is defined by

$$\Upsilon_i(x) = 0 \qquad x > (i+1)\Delta x \tag{19a}$$

$$\Upsilon_i(x) = 0 \qquad x < (i-1)\Delta x \tag{19b}$$

$$\Upsilon_i(x) = [x - (i-1)\Delta x]/\Delta x \qquad (i-1)\Delta x \le x \le i\Delta x \tag{19c}$$

$$\Upsilon_i(x) = [(i+1)\Delta x - x]/\Delta x \qquad i\Delta x \le x \le (i+1)\Delta x \tag{19d}$$

A sample chapeau function is shown in Figure 4. The chapeau functions are not orthogonal, so that the neighboring cells are not independent of each other.

The general application of the finite element method involves using a small number of basis functions (for instance, a single chapeau function) to represent the constituent within each element. Therefore accuracy is not achieved by using a large number of basis functions as would be required in the expansion function techniques discussed in the previous subsection, but accuracy is achieved by increasing the numbers of elements used to resolve the domain. Traditionally, the greatest advantage of the finite element method is flexibility. There is no restriction upon the choice of the element shape or size. Therefore elements can easily be made smaller in regions where high resolution is required, and complex boundary conditions, such as an accurate topography, can be formulated in the same fashion as the interior points. The disadvantages frequently cited include complexities in coding and a relatively high cost of computer time and memory in comparison to the increased accuracy. As will be shown in section 4, however, finite element methods can be accurate and efficient.

Like the global expansion function techniques, finite element methods are applied by the method of weighted residuals (equation (18)). Another technique that appears in the finite element literature is the Petrov-Galerkin technique [*Hughes and Brooks*, 1982]. In this technique the weighting functions are not the same as the basis functions, and in particular, weighting functions are chosen such that the short wavelength features of the distribution are selectively damped, thereby reducing dispersion errors.

Finite element methods have a long and successful history in modeling of parabolic and elliptic equations, and only rela-

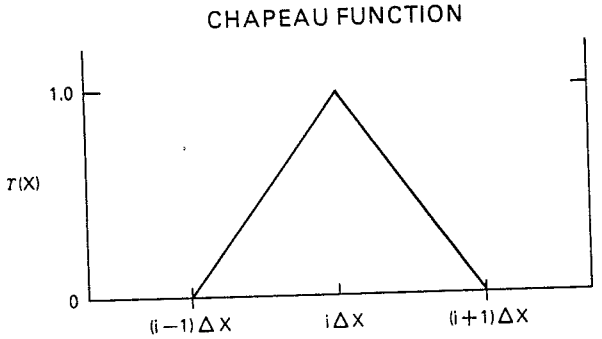

Fig. 4. Sample chapeau function (equation (19)). A single chapeau function is frequently used in the finite element method to represent the constituent field within each element.

tively recently has the method been extended to hyperbolic equations. The development of accurate finite element schemes is proceeding in a similar fashion to that followed by finite difference algorithms, with the advantage that the long history of finite difference methods can be used as a guide.

There are many similarities between finite difference and finite element schemes, particularly in applications that have regular grid spacing. *Runca et al.* [1985] compare finite difference and finite element formulations of the advective diffusion equation (equation (2)) and obtain similar results with the two methods. The entries in Table 4 under finite elements do not reflect the amount of literature available on finite elements. Finite element techniques are relatively rare in atmospheric tracer applications (particularly nontropospheric applications).

3.2.5. *Monotonicity, flux-corrected transport, filling, and filters.* As was mentioned in section 2.3, one approach to dealing with numerical dispersion is to develop special algorithms that force a numerical scheme to be monotonic. The fact that dispersion errors are present even with very high order approximations for the spatial derivatives means that monotonicity cannot be obtained just by increasing the accuracy of the numerical techniques [*Godunov*, 1959].

The upstream-centered schemes of *van Leer* [1977*a*] (see section 3.2.2) are based on an extension of the method of *Godunov* [1959] (see also *Richtmyer and Morton* [1967]) which requires that a scheme be expressed not only in conservative form but also be monotonic. Because of the favorable phase characteristics of upstream-centered schemes, the choice of such a scheme in the development of advanced transport algorithms is logical, but special effort has to be made to assure monotonicity.

Monotonicity algorithms are not as straightforward as pure advection algorithms. The monotonicity algorithm has to identify danger zones where monotonicity might be violated and then keep the rippling from occurring. The suppression of high wave number structure in certain regions by monotonicity algorithms has the same effect as nonlinear diffusion. *Van Leer* [1974] uses *Fromm*'s [1968] scheme to develop a new conservative, monotonic method with very small phase errors. This scheme requires the calculation of a smoothness function to determine the danger zones. In these danger zones, additional terms are added to Fromm's scheme in order to insure monotonicity. In a method similar to *van Leer*'s [1974], *Harten and Zwas* [1972] introduce the self-adjusting hybrid technique. In this method a high-order, accurate scheme is used in the smooth regions of the constituent profile (where dispersion is small because of a lack of high wave numbers), and a low-order routine (such as the monotonic donor cell scheme) is used in regions of sharp gradients. A switch, similar to van Leer's smoothness parameter, automatically switches from one scheme to another. To deal with the excessive diffusion of the low-order scheme in regions of large constituent gradients, *Harten* [1977, 1978] has introduced the artificial compression method which is similar in concept to flux-corrected transport discussed below.

Flux-corrected transport is more of a philosophy of how to develop a transport scheme than a particular numerical algorithm [*Boris and Book*, 1973, 1976; *Book et al.*, 1975]. FCT has been applied to ordinary finite difference transport methods and to pseudospectral techniques with varying degrees of success. The basic concept is to use an accurate, but dispersive, high-order scheme in conjunction with a monotonic, but diffusive, low-order scheme. The two schemes are combined with an "antidiffusion" operator to produce a high-order monotonic scheme. The formal algorithm, taken from *Zalesak* [1979], is in the following steps (where i represents the spatial grid):

1. Compute ${F_{i+1/2}}^L$, the transportive flux given by a low-order scheme guaranteed to give monotonic results (such as the donor cell).
2. Compute ${F_{i+1/2}}^H$, the transportive flux given by some high-order scheme (such as the leapfrog scheme with high-order spatial derivatives).
3. Define the "antidiffusive flux":

$$B_{i+1/2} = {F_{i+1/2}}^H - {F_{i+1/2}}^L$$

4. Compute the transported and diffused solution:

$${\mu_i}^{TD} = \mu_i - ({F_{i+1/2}}^L - {F_{i-1/2}}^L)/\Delta x$$

5. Limit B from step 3 such that $\mu^{t+\Delta t}$ to be computed in step 6 is free of extrema not found in μ^{TD} or μ^t:

$${B_{i+1/2}}^C = C_{i+1/2} B_{i+1/2} \qquad 0 \le C_{i+1/2} \le 1$$

where $C_{i+1/2}$ is called the flux limiter.

6. Apply the "limited antidiffusive flux" calculated in step 5 to yield

$${\mu_i}^{t+\Delta t} = {\mu_i}^{TD} - ({B_{i+1/2}}^C - {B_{i-1/2}}^C)/\Delta x$$

The scheme of *Harten and Zwas* [1972] mentioned above when combined with artificial compression (read antidiffusion) incorporates both the idea of *van Leer* [1974] to identify regions where monotonicity might be violated and the idea of antidiffusion to correct this violation.

The FCT algorithm can be interpreted as the nonlinear average of a high- and low-order accurate finite difference scheme. The algorithm described above suggests that this is not a simple averaging technique and that the averaging operator is a function of grid location. *Clark* [1979] and *Clark and Hall* [1979] describe a simple hybrid scheme which is the weighted average of the donor cell and *Crowley*'s [1968] scheme.

The choice of the flux limiter in step 5 above requires intervention by the developer of the transport algorithm and is a highly nonlinear procedure. The original FCT codes developed by *Boris and Book* [1973] used a flux limiter that preserved square wave distributions almost perfectly. Unfortunately, this limiter quickly turned other distributions into square waves. *Zalesak* [1979, 1981*b*] has developed a line of flux limiters that do not distort the profile as much as the original flux limiters and thus lead to very accurate transport routines. In an attempt to develop flux limiters that preserve peaked distributions, care must be taken not to violate the monotonicity constraints.

Smolarkiewicz [1983, 1984] has developed a fast positive definite advection algorithm that calculates an antidiffusion velocity to correct implicit numerical diffusion. This antidiffusion counteracts most of the numerical diffusion, and accurate results are obtained. *Book et al.* [1975] offer a detailed discussion of antidiffusion.

The preceding schemes are general in that they can be applied to any fluid advection problem. Two other approaches, specific for constituent transport, prohibit the generation of negative mixing ratios but not in a monotonic manner. The square root scheme [*Schneider*, 1984] is a positive definite

scheme but has dispersion errors. In the scheme the square root of the concentration is advected using a quadratic conserving modification of the Lax-Wendroff scheme. Then the square is taken, which removes the negative densities generated in the first step, but also generates high-frequency noise.

The second approach for dealing with negative densities is the filling process discussed by *Mahlman and Sinclair* [1977] and *Mahlman and Moxim* [1978]. Filling algorithms require that when negative densities are generated, mass is borrowed from the surrounding grid points, in a user-determined way, to remove the negative constituent value. This method is not monotonic and can be very time consuming. Filling is a nonlinear diffusive process.

One filling algorithm, called "downstream borrowing," was described by *Mahlman and Sinclair* [1977]. In this filling scheme a time step is completed, and then negative constituent values are identified. If a negative value is found, then mass is borrowed from a downstream point to fill the negative region. If there is not enough mass at the downstream point, then mass is borrowed from an upstream point. If the hole has still not been filled, then mass is borrowed from more distant points. Downstream borrowing attempts to fill locally, that is, from the vicinity of where the negative value was created. A characteristic of local filling is that many decisions have to be made by the transport routine; therefore local filling is frequently expensive.

Two global (as opposed to local) filling algorithms that are less time consuming are what might be called the subtractive and multiplicative methods. In the subtractive method, negative constituent values are searched for, and then these values are corrected in some fashion (for example, they are set to zero, or the absolute value is taken). The extra mass added to this system is then uniformly subtracted from all of the grid points from which the mass can be subtracted without producing negative constituent values. Once again, this method requires quite a bit of comparison to assure that the new distribution is positive definite.

The multiplicative method is positive definite by its very nature. The negative values in the transported distribution are found and corrected. The total mass of the corrected distribution is calculated, and then the corrected distribution is multiplied grid point by grid point by the ratio of the mass of the original distribution to the mass of the corrected distribution.

Once again, both the subtractive and the multiplicative methods are diffusive. Their intrinsic value lies with the use of very accurate transport schemes, so that negative constituent values are small, and therefore the redistribution of mass over the entire domain is small and rapidly computed.

A potentially attractive method for filling can be derived by observing the general nature of the inaccuracies generated in either the triangular or rectangular distribution advection problem (Figure 1). The amplitude of the ripples following the main part of the distribution decreases with distance from the rectangle or triangle. The negative value nearest the distribution is either the largest or second largest of the ripples. The first step in the filling algorithm is to identify and set all of the negative values equal to zero (this adds mass to the system). Then all of the remaining constituent values are checked, and the values with magnitudes less than the absolute value of the most negative grid point are set to zero (this removes mass from the system). This procedure provides a nonlinear diffusion on the shortest wavelengths. The discrepancy in mass that remains after the above procedure is then corrected by the multiplicative method described above.

This filling algorithm is tested for leapfrog time differences with both second- and fourth-order centered spatial differences (Figure 5). As compared to Figure 1, the second-order scheme has been improved tremendously. The superiority of the fourth-order scheme over the second-order scheme is particularly evident in the square wave simulation. This filling algorithm prefers to transport triangular distributions.

Monotonicity and filling algorithms can be viewed as a subset of numerical filters that attempt to deal specifically with numerical dispersion errors. *Forester* [1977] introduced a filtering technique that like filling and the FCT algorithm can be applied to transport routines in general. Forester's filter is a diffusionlike, iterative filter with two parameters for the "highly discriminate smoothing" necessary in advection modeling. The filter can be tuned to smooth out ripples with wavelengths less than some specified wavelength. The applications of the filter presented by *Forester* [1977] show very promising results which remove negative constituent values while preserving peaks much better than the original *Boris and Book* [1973] FCT (see also *Chock* [1985]).

3.2.6. *Lagrangian schemes and volume schemes.* In the schemes that are classified as volume schemes in Table 4 the modeling concept has been shifted away from the grid points themselves to the boxes or elements defined by the grid points. The constituent is assumed to be continuously distributed within each grid box with discontinuities between the boxes.

Mathematically, the volume schemes have their basis in Lagrangian mass coordinates [*van Leer*, 1979; *Russell and Lerner*, 1981; *Dryden et al.*, 1956]; that is, the evolution of the flow is written in terms of a coordinate system that is based on the location of a particular fluid slab at some point in time. In practice, the coordinate system is usually reinitialized at the beginning of every time step. The attention is placed on fluid slabs (ensembles of particles) rather than on individual fluid "particles." The algorithms classified as volume schemes in this review are sometimes classified as Lagrangian. However, no attempt is really made to follow the evolution of particular slabs for long periods of time (there is frequent reinitialization to model the interaction of slabs); therefore it is felt that a classification distinct from the more particle-oriented schemes is in order; hence the term "volume." The volume schemes are by their very nature upstream centered (section 3.2.2).

Consider the case demonstrated in Figure 6*a*. An ideal transport scheme would simply move the square distribution to the right (for positive velocities) the distance ($\varepsilon\Delta x$). The donor cell scheme (equation (11)) can be rewritten for constant positive velocities as

$$\mu_i^{t+\Delta t} = (1 - \varepsilon)\mu_i^t + \varepsilon\mu_{i-1}^t \tag{20}$$

For $\varepsilon = 1$ the donor cell scheme shifts the constituent distribution one grid point to the right and is therefore an exact transport routine. Referring to Figure 6*b*, for $\varepsilon = 0.4$ it is easy to see from (20) that after the first time step a positive value of μ is predicted at point $i + 1$. After the second time step a nonzero value of μ is predicted at point $i + 2$. In the analytic solution, even after two time steps, the constituent should not have reached the $i + 1$ point. This example graphically demonstrates the numerical diffusion associated with the donor cell scheme.

The basic premise of the volume scheme approach to modeling advection is to produce a scheme that transports slabs of

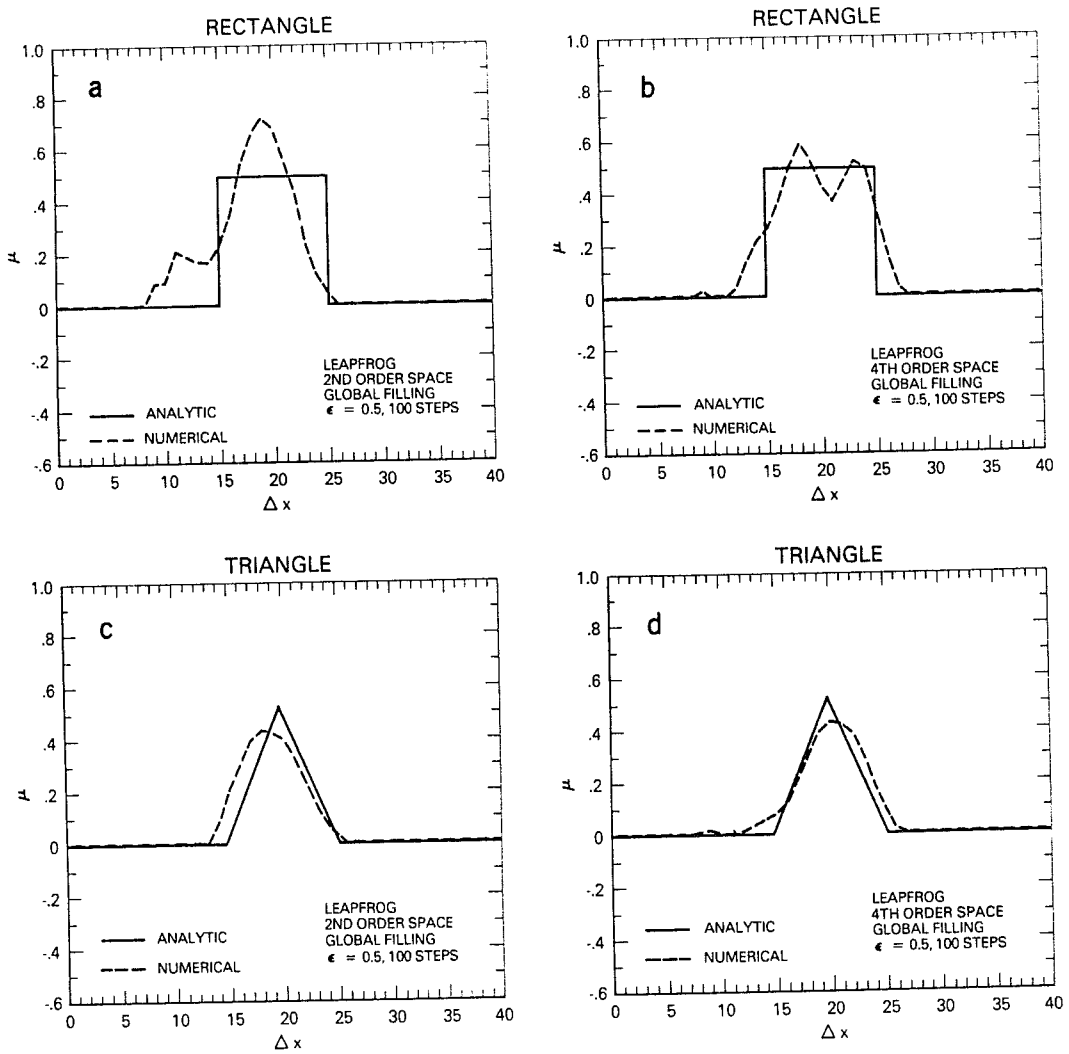

Fig. 5. Advection in one dimension, with constant velocity, cyclic boundary conditions, $\varepsilon = 0.5$, 100 time steps, and global filling algorithm described in section 3.2.5. (*a*) Rectangular distribution using leapfrog time differences with second-order centered spatial differences (equation (15)); compare to Figure 1*a*. (*b*) Rectangular distribution using leapfrog time differences with fourth-order centered spatial differences. (*c*) Triangular distribution using leapfrog time differences with second-order centered spatial differences (equation (15)); compare to Figure 1*b*. (*d*) Triangular distribution using leapfrog time differences with fourth-order centered spatial differences.

material in such a manner that the slabs maintain their original shape. If it could be generally assumed that ε could be maintained at 1, then the donor cell scheme would be ideal. However, this restriction is not realizable, and schemes always have to deal with the movement of slabs some fractional distance of a spatial grid length. The variation of velocity in space and time means that slabs will interact; that is, they will overlap and spread out. It is the accurate interaction of slabs on which is focused much of the effort in the development of volume schemes.

The donor cell scheme can be interpreted as the simplest of the volume schemes, with the assumption that the constituent is distributed uniformly within a numerical box. In the partial donor method [*Hain*, 1978] an attempt is made to produce a simple, high-speed algorithm to yield that portion of the mass that was moved from cell to cell at each time step. This technique reduces the diffusion of the donor cell method. As is defined by Hain, essentially three simple estimates of $\mu^{t+\Delta t}$ are computed, and then one is chosen such that the transport is monotonic. Operationally, the results of the partial donor method are very similar to the early version of flux-corrected transport (SHASTA [*Boris and Book*, 1973]).

The partial donor method, like the donor cell, is based on the interpretation of the constituent being uniformly distributed within each numerical box. In the method of moments [*Egan and Mahoney*, 1972; *Pedersen and Prahm*, 1974; *Pepper and Long*, 1978], not only the mean concentration in a box but the center of mass (the first moment) and the second moment, which is used as a measure of width, are considered.

Assuming a box of width unity, the zeroth, first, and second moments are defined as

$$\mu_i = \int_{-0.5}^{0.5} \mu(\xi_i)\, d\xi$$

$$F_i = \left[\int_{-0.5}^{0.5} \mu(\xi_i)\xi_i\, d\xi\right] \Big/ \mu_i \tag{21}$$

$$R_i^2 = \left[\int_{-0.5}^{0.5} \mu(\xi_i)(\xi_i - F_i)^2\, d\xi\right] \Big/ \mu_i$$

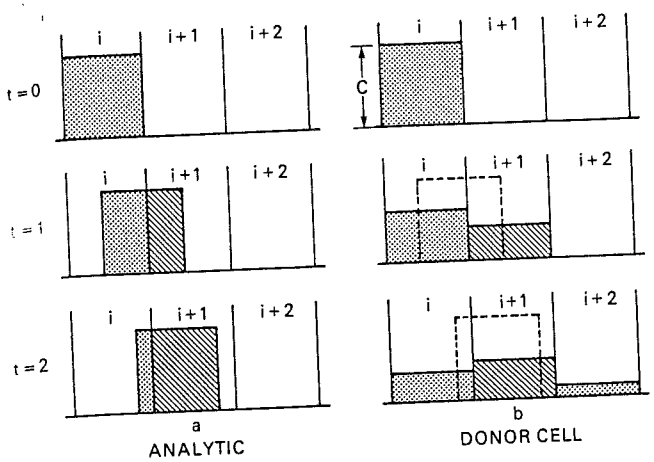

Fig. 6. (*a*) Idealized advection of a rectangle, with $\varepsilon = 0.4$. (*b*) Donor cell advection for a rectangle, with $\varepsilon = 0.4$. Note the diffusion associated with the donor cell (adapted from *Egan and Mahoney* [1972]).

where the mass coordinate ξ is measured from the center of the box. Figure 7 gives a graphical representation of the meaning of each of the moments within a rectangular distribution. Simple advection (u = const) should move the constituent a distance of $u\Delta t$, and all of the moments (equation (21)) should be conserved. In Figure 7 at the start of the advection the right-hand boundary of the cell is located at $F_i + R_i/2$. Assuming advection to the right ($u > 0$), then after the advection the right boundary of the cell is at $F_i + R_i/2 + \varepsilon$. The part of the distribution that has moved into the $i + 1$ cell is $F_i + R_i/2 + \varepsilon - 0.5$. This quantity can be normalized by R_i to yield a portioning parameter $(F_i + R_i/2 + \varepsilon - 0.5)/R_i$ which represents the portioning of the constituent between the i and $i + 1$ boxes. *Egan and Mahoney* [1972] derive a scheme based on the proportioning parameter that conserves the moments of the initial distribution. As is originally derived by Egan and Mahoney, the scheme is biased toward a rectangular distribution; therefore the scheme has a tendency to turn all distributions into rectangular waves. *Pedersen and Prahm* [1974] developed a width correction algorithm in an attempt to remedy the bias toward rectangular distributions. *Pepper and Long* [1978] show that width correction degrades the method of moments for generalized velocity fields. *Pepper and Baker* [1980] discuss an accurate three-dimensional moments algorithm. The computation of all the moments significantly increases the storage requirements of the algorithms.

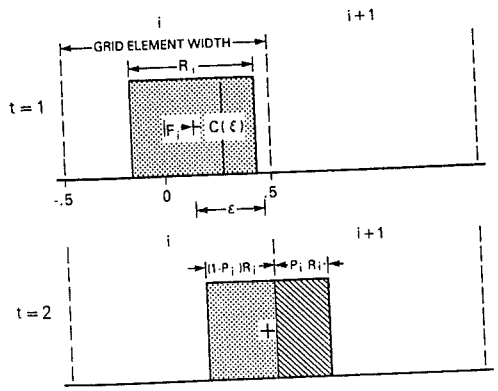

Fig. 7. Graphical representation of the method of moments [from *Egan and Mahoney*, 1972]. The constituent is assumed to be distributed within a grid element "i" in a slab of width R_i centered at F_i with a uniform value of C_i (equation (21)). The portion of the slab that moves to the next element is given by the portioning parameter P_i, and the portion that remains is given by $(1 - P_i)$.

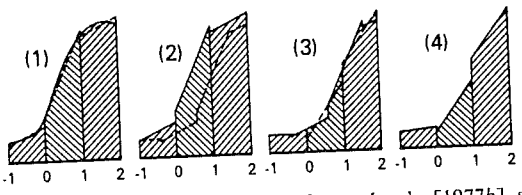

Fig. 8. Graphical representation of *van Leer*'s [1977*b*] scheme that represents the constituent within each grid element as a linear function. This scheme is similar to the slopes scheme of *Russell and Lerner* [1981]. Compare to Figure 7, where the constituent is considered to be of constant value within each grid element. The following explanation is from *van Leer* [1977*b*]: "(1) approximating the initial-value distribution (solid line) in each slab by a linear distribution (broken line) with the same mesh integral. In this case the slopes are determined by least-squares fitting. (2) The approximate initial value distribution before (solid) and after (broken) convection over a distance $\varepsilon\Delta x$. (3) Determining the new linear distributions (broken) in each mesh by least-squares fitting to the convected distribution (solid). (4) The initial values for the next step."

Van Leer [1973, 1974, 1977*a*] deduced that upstream-centered schemes are the most natural schemes for modeling (1). In the works by *van Leer* [1977*b*, 1979] and *Colella* [1982], the emphasis is shifted away from the grid points to the grid elements. In the volume schemes described previously, the constituent was assumed to be distributed in rectangular blocks within each cell. Rather than represent the grid boxes as rectangular slabs, *van Leer* [1977*b*] uses a polynomial expression to represent the constituent within each box (Legendre polynomials, for instance). Then a monotonic upstream-centered conservative scheme is used to advect the piecewise continuous function. A graphic example of this scheme is shown in Figure 8. Higher-order polynomial schemes are discussed by *van Leer* [1977*b*, 1979], and the piecewise parabolic method has been developed and tested by *Woodward and Colella* [1981, 1984] and *Colella and Woodward* [1984]. The interaction of the slabs is treated as individual Riemann problems (shock fitting) (see also *Roe* [1981], *Colella and Glaz* [1985], and *Richtmyer* [1978, p. 386]).

The slopes scheme [*Russell and Lerner*, 1981] is similar in concept to the piecewise linear approximation version used by *van Leer* [1977*b*] and *Colella* [1982]. In this scheme a linear approximation is made to the constituent distribution. The interaction between the squares is handled by a separate equation to transport the slope which reduces the diffusion that would otherwise be in the system. The slopes scheme is not monotonic.

Prather [1986] reports an extension of the slopes scheme that models the tracer slabs with second-order polynomials. Prather's scheme conserves first and second moments and is stable for ε close to 1. Prather also presents a method to assure positive tracer distribution.

4. COMPARISON OF TRANSPORT SCHEMES

There have been many papers devoted specifically to comparing advection algorithms. Also, with the development of a new transport algorithm the inventor generally evaluates the new algorithm against one or more standard methods. Considering all of the various desirable attributes of any advection routine (section 2), it is not surprising that there is no consensus on which routine is best. The ever increasing power of

computing machines also has its effects on advection algorithm evaluation, because routines that were too costly 20 years ago are today considered to be rather primitive. An interesting insight into the development of computing power lies in the statement of *Emery* [1968] that the difficulties involved with the Lax-Wendroff scheme "render it useful only to those interested in numerical methods for methods for their own sake."

Two standard ways of evaluating routines have developed. In the first, a complicated problem, such as a 24-hour weather forecast, is verified against observations. If the forecast with a new and improved numerical technique is better than the old one, then the new transport routine is considered to be more accurate than the old one. It then comes down to evaluating the various cost benefits ratios to decide whether or not the new algorithm is in fact "better."

Another, more precise and more common, method of evaluating routines is by comparing numerical solutions to known analytic solutions. In this approach, therefore, transport algorithms are evaluated by how well they represent one-, two-, and three-dimensional advection of various geometric shapes by a constant velocity or angular velocity. Three problems have more or less become standard. The first is one-dimensional advection of a triangular distribution (see Figure 1). The second is the one-dimensional advection of a rectangular wave or a step function (shocks; see Figure 1). The final, more or less standard test, is two-dimensional rotation of a peaked distribution such as a cone or a cosine hill [*Pepper and Long*, 1978; *Orszag*, 1971*b*]. There are other tests that have been used, but these three appear most frequently. *Smolarkiewicz* [1982, 1984] considers the three-dimensional solid body rotation of a spherical distribution.

Frequently, when a new routine is introduced, it uses only one of the one-dimensional tests. If the routine is meant for general use, both one-dimensional tests and at least one multidimensional test should be performed. Many schemes translate a triangular distribution well and have a strong tendency to generate peaked distributions out of rectangular waves (see Figure 5*a*). Similarly, many of the schemes that transport rectangular waves well rapidly turn other distributions into rectangles (see Figure 10*a*). Finally, most schemes transport long-waves accurately, but this should be explicitly tested, particularly those schemes that have been derived by forcing exact agreement with a specific problem (see Figure 10*a*).

The one-dimensional problems provide stringent tests for dispersion, diffusion, and accuracy. The two-dimensional and three-dimensional tests give some indication of how difficult it is to extend a particular algorithm to multidimensional situations. These tests also allow for easy evaluation of computer time and memory requirements.

Tables 5 and 6 represent a large cross section of the comparison studies of numerical advection algorithms. Table 5 summarizes those studies that are an evaluation or survey of schemes that are different finite difference estimates of (3). Table 6 summarizes the studies in which algorithms that are fundamentally and philosophically different in their formulation are compared.

The comments in Table 5 point out some of the more important schemes that carry different names depending on the authors. Several of the schemes are derived as Runge-Kutta techniques, and given the free parameter of the Runge-Kutta technique, many of the two-level schemes can be shown to be Runge-Kutta schemes.

The results summarized in Table 5 are not too surprising. Basically, the more accurate the approximation of the time derivative, then the more accurate the computed transport. However, a third-order accurate Runge-Kutta scheme requires more time to compute the solution than does a second-order scheme. By looking at a paper such as *Kurihara*'s [1965], it is interesting to see how rather subtle changes in the time derivative formulation can change the numerical results.

The basic conclusion that might be drawn from these studies is that second-order accurate time derivatives are sufficient for most atmospheric applications. If the leapfrog scheme is used, then extra memory may be required over two-level schemes, some technique must be used to prevent splitting of the solutions, and care must be taken to reduce the computational mode. Second-order schemes such as *Takacs*' [1985] and *Fromm*'s [1968], which are two-level schemes which minimize errors, and *Gadd*'s [1978*b*] extension of the Lax-Wendroff scheme are perhaps more appropriate if it is impossible to carry three time levels.

Of the schemes presented in Table 5, leapfrog in time with fourth-order centered spatial derivatives (LF4) is about the most cost effective [see *Mahlman and Sinclair*, 1977]. It is conceptually simple and easy to program in three dimensions. *Gadd*'s [1978*b*] fourth-order extension of the Lax-Wendroff method performs similarly to LF4. Neither method is monotonic, so if the production of negative constituent values is a danger, then some method of filling or a monotonicity algorithm will have to be used with the transport routine.

The schemes presented in Table 6 are more sophisticated in their approach to the advection problem than those given in Table 5. Much effort has been made to insure monotonicity and/or produce accurate spatial derivatives. The concepts of FCT and artificial compression (see section 3.2.5) can be applied to any of the routines presented in Table 5 (for instance, *Smolarkiewicz* [1982]).

The results of *Chock and Dunker* [1983] supply the best starting point for evaluating the transport routines. The original FCT algorithm (SHASTA) proved to be unacceptably diffusive, as can be seen from Figure 9. The flux-limiting algorithms defined in the original codes have a strong tendency to produce square waves; therefore the peaks in the Chock and Dunker tests are quickly removed. On the other hand, the fully multidimensional FCT (MFCT) algorithms which use the flux limiters derived by *Zalesak* [1979] are much less diffusive and maintain the peak better than SHASTA. SHASTA is strictly monotonic. The Zalesak flux limiters are not strictly monotonic, but with the flux limiters used by Chock and Dunker, negative constituent values are small. Flux limiters can be derived that eliminate virtually all diffusion, but the production of negative constituent values can become a problem.

The second-moment method (SM) is also positive definite and consistently performed better than either SHASTA or MFCT. However, in the version that Chock and Dunker tested, SM required large amounts of storage and large amounts of computer time. SM is still diffusive, and like the FCT algorithms prefers to advect square distributions.

Several authors describe orthogonal collocation methods distinct from pseudospectral methods (Table 4). In general, the distinction seems to be based on the selection of interpolation polynomials. *Chock and Dunker* [1983] compare three orthogonal collocation (OC) methods which differ by virtue of their time schemes (see Table 6). Chock and Dunker eliminate the

TABLE 5. Comparison Studies for Schemes Based on Finite Difference Techniques

Reference	Methods Compared	Comments
Anderson and Fattahi [1974]	MacCormack's method, Rusanov's method, and Kutler-Lomax-Warming method.	The Kutler-Lomax-Warming seems to be the best. All of the schemes are diffusive and not positive definite.
Emery [1968]	Lax, Rusanov, Landshoff, Lax-Wendroff, and Richtmyer's.	Concludes Lax-Wendroff is best but too complex. Therefore recommends Rusanov.
Haltiner and Williams [1980]	Euler scheme, upstream/downstream, trapezoidal implicit scheme (trapezoid in the work by *Young* [1968]), Euler backward/Matsuno, leapfrog/second order, leapfrog/fourth order, forward/backward scheme, pressure averaging, time averaging, semi-implicit, and Lax-Wendroff.	Textbook that outlines a lot of routines but does not explicitly compare and evaluate the methods.
Kurihara [1965]	Backward implicit, trapezoidal implicit, partly implicit 1, leapfrog, partly implicit 2, Euler backward iteration (Euler method and backward correction), modified Euler backward iteration (modified Euler method and backward correction), leapfrog trapezoidal iteration (leapfrog method and trapezoidal correction), and leapfrog backward iteration (leapfrog method and backward correction).	Modified Euler backward same as *Schneider* [1984] modified Lax-Wendroff. Kurihara offers a comparison and evaluation of all the listed schemes in tabular form. This is an interesting paper because it tests the propagation of a sine wave instead of a sharp shock.
Rubin and Burstein [1967] *Taylor et al.* [1972]	Several variations of Richtmyer's two-step methods Godunov, Rusanov (first order and third order), MacCormack, and Richtmyer.	Taylor et al. like the first-order Godunov scheme better than the first- order Rusanov scheme. The third-order Rusanov is the best tested but has twice the computation time of Godunov.
Young [1968]	Euler's modified (trapezoidal), Heun (double forward), method A (double forward, centered), method A′ (method A, variable time step), method B (forward, centered), method C, Kutta, method D (two forwards, latest values, reversed variable order), method D′, Euler (forward), Adams-Bashforth, centered (uncorrected), and centered (correction A).	Euler's modified is not the same as modified Euler [see *Kurihara*, 1965]. Heun is a second-order Runge-Kutta; it is the same as modified Euler for constant velocity advection. For method D, see angled derivative scheme by *Roberts and Weiss* [1966]. Young likes method A and the Kutta method. However, these schemes require more time than the single-step schemes. Of the three-level schemes, the Adams-Bashforth is preferred. Young recommends "multipart, one-step schemes probably from the Runge-Kutta family."

TABLE 6. Comparison Studies for Schemes Based on Technique Differences

Reference	Methods Compared	Comments
Chock [1985]	Chapeau function (forward Euler with balancing diffusion (CF/FED)), chapeau function with mass lumping (forward Euler with balancing diffusion (CFML/FED)), Forester applied to CF/FED (forward Euler with balancing diffusion (FCF/FED)), Forester applied to CF/I (implicit Crank-Nicolson (FCF/I)), FRAM diffusion applied to CF/FED (forward Euler with balancing diffusion (FRAM1/FED), FRAM diffusion applied to CF/I (implicit Crank-Nicolson (FRAM1/I)), FRAM donor cell applied to CF/FED (forward Euler with balancing diffusion (FRAM2/FED)), FRAM donor cell applied to CF/I (implicit Crank-Nicolson (FRAM2/I)), Hermite cubic orthogonal collocation (forward Euler with balancing diffusion (HCOC/FED)), Hermite cubic orthogonal collocation (implicit Crank-Nicolson (HCOC/I)), and quadratic function (forward Euler with balancing diffusion (QF/FED)).	*Chock* [1985] compares finite element techniques and finds FCF/FED to be the best all-around method, considering accuracy and computer resources. For problems with small gradients CF/FED. CF/I is the chapeau function method with implicit Crank-Nicolson time integration from *Chock and Dunker* [1983].
Chock and Dunker [1983]	Flux-corrected transport (explicit Euler (SHASTA)), fully multidimensional flux-corrected transport (explicit leapfrog trapezoidal (MFCT/LT) and modified Euler predictor-corrector (MFCT/PC)), orthogonal collocation (modified Euler predictor-corrector (OC/PC), implicit Crank-Nicolson (OC/I), and implicit backward Euler (OC/BE)), second-moment method (explicit (SM)), pseudo-spectral method (explicit leapfrog (PS/L)), and chapeau function method (implicit Crank-Nicolson (CF/I), implicit Crank-Nicolson (CFD/I), and modified Euler predictor-corrector (CFD/PC)).	CFD/PC has been eliminated only with respect to CFD/I. All the orthogonal collocation routines are eliminated. SHASTA is eliminated. Chock and Dunker say it is difficult to evaluate the rest of the schemes. PS/L is the most accurate, and SM is accurate, but requires a lot of computer time and storage (but see entry for *Pepper and Cooper* [1983]). There is a mild recommendation for CF/I, particularly in problems with small constituent gradients.
Crowley [1968]	Interpolation on three points (second order), interpolation on five points (fourth order), upstream, and Crowley.	Crowley notes dramatic improvement when using fourth-order instead of second-order estimates of the spatial derivatives.
Long and Pepper [1981]	Donor cell, fully implicit, Crank-Nicolson, cubic spline, Akima quasi-Lagrangian, chapeau function (Galerkin), and second moment.	Cubic spline, Akima, second moment, and chapeau are reasonable. Second-moment conserved mass is positive definite but diffused. Chapeau a bit dispersive but small. Cubic spline selectively damps dispersive waves. Spline phase speed exceeds chapeau phase speed. Akima maintains peak well but is inferior to cubic spline.
Mahlman and Sinclair [1977]	Polynomial algorithms (second order and fourth order (LF4)), quasi-Lagrangian algorithms, cubic spline algorithm, pseudospectral algorithms, and Lagrangian trajectory algorithms.	Second-order polynomial seriously inferior. Fourth order is better. Fourth-order quasi-Lagrangian and cubic spline do not show significant improvement over fourth-order polynomial. Pseudospectral shows the best results, but at high cost because of high number of waves and small time step.
Molenkamp [1968]	Upstream (upstream N and upstream $N + 1$), leapfrog, Lax-Wendroff, Roberts-Weiss, and Arakawa (Euler and Adams-Bashforth).	Molenkamp finds the Roberts and Weiss scheme, which is second-order accurate in time and fourth-order accurate in space, to be the most accurate of these schemes.
Pepper and Cooper [1983]	Chapeau function, method of moments, particle in cell, and pseudospectral.	In analytic tests, all of these schemes are good. In field tests it is hard to evaluate them. A slight preference for the method of moments because of computational efficiency (see entry for *Chock and Dunker* [1983]).

Pepper et al. [1979] *Scheri* [1983]	Cubic splines and chapeau functions. SHASTA, fully multidimensional FCT, and BIQUINTIC.	Both are good. FCT best here, but none of the schemes are outstanding. BIQUINTIC has inferior conservation qualities.
Sod [1978]	Godunov, Lax-Wendroff, MacCormack, Rusanov, upwind, Harten and Zwas (hybrid method), and Glimm.	Glimm's method is a random choice method. Sod also considers the artificial compression method of *Harten* [1978] applied to several algorithms. Sod notes the improvement of the schemes when Harten's method is applied. Glimm's method is accurate but difficult to evaluate.
Woodward and Colella [1984]	Piecewise parabolic method, MUSCL, flux-corrected transport, BBC (artificial viscosity), MacCormack, and Godunov.	This is a comparison focused specifically at shock propagation, and the six schemes listed are representative of classes of schemes. The piecewise parabolic method is the most accurate tested.

implicit schemes as being generally inferior to the explicit Euler predictor-corrector scheme. While the diffusion in this scheme is quite small, the dispersion errors are large, and large negative concentrations are generated. The overall accuracy of OC is poor in comparison to the other schemes, and OC methods as distinguished in Table 4 will be eliminated from further consideration.

Chock and Dunker eliminate the chapeau function finite element method (section 3.2.4) which uses explicit time stepping with respect to similar schemes that use implicit time stepping because the implicit methods allow for a much longer time step without significantly reducing the accuracy of the model. The most serious disadvantage of the chapeau function method is the rippling and the formation of negative constituent values. The chapeau function methods require relatively small amounts of both computer time and memory. Considering all aspects of the code, Chock and Dunker conclude that the chapeau function methods are perhaps the best methods to use in the absence of large concentration gradients or when there is a significant amount of physically derived diffusion in the problem.

The most accurate transport algorithm tested by Chock and Dunker is the pseudospectral method with leapfrog time differences (section 3.2.3.). The pseudospectral method is not intrinsically monotonic, but even in problems with large gradients the ripples associated with the method are small if enough expansion functions are used to sufficiently resolve the constituent field. The most serious problem with the method seems to be that very small time steps are required to make the system accurate.

Chock [1985] focuses on finite element methods. Chock emphasizes two time integration techniques, the semi-implicit Crank-Nicolson scheme and the explicit Euler forward scheme stabilized with diffusion (FED) (see sections 3.1.1–3.1.3; also see section 5.3). Chock considers the chapeau function (CF) finite element method, the CF combined with *Forester*'s [1977] filter (section 3.2.5), the CF combined with the filtering remedy and methodology described by *Chapman* [1981] (similar to that of *Harten and Zwas* [1972]) and the finite element techniques which use basis functions other than chapeau functions.

Chock and Dunker [1983] concluded that CF with implicit time stepping, while not the most accurate technique, might be the best overall choice for advection modeling. *Chock* [1985] finds CF using the explicit FED time scheme an attractive alternative. The results of the two methods are very similar, with the FED method damping the peak more but also producing smaller negative values. The addition of Forester's filter to the CF/FED method removes the negative constituent values and does only minimal damage to the peak concentrations.

While some of the finite element schemes considered by Chock were more accurate than the CF method, on consideration of complexity in coding and time constraints, most of the other methods are eliminated. The combination of *Forester*'s [1977] filter with CF, according to Chock, is a method with "high accuracy with good peak retention and minimal requirements on execution time and storage." These attributes led Chock to strongly recommend this technique. These results also indicate the quality and power of Forester's filtering technique, particularly when combined with an intrinsically accurate advection algorithm.

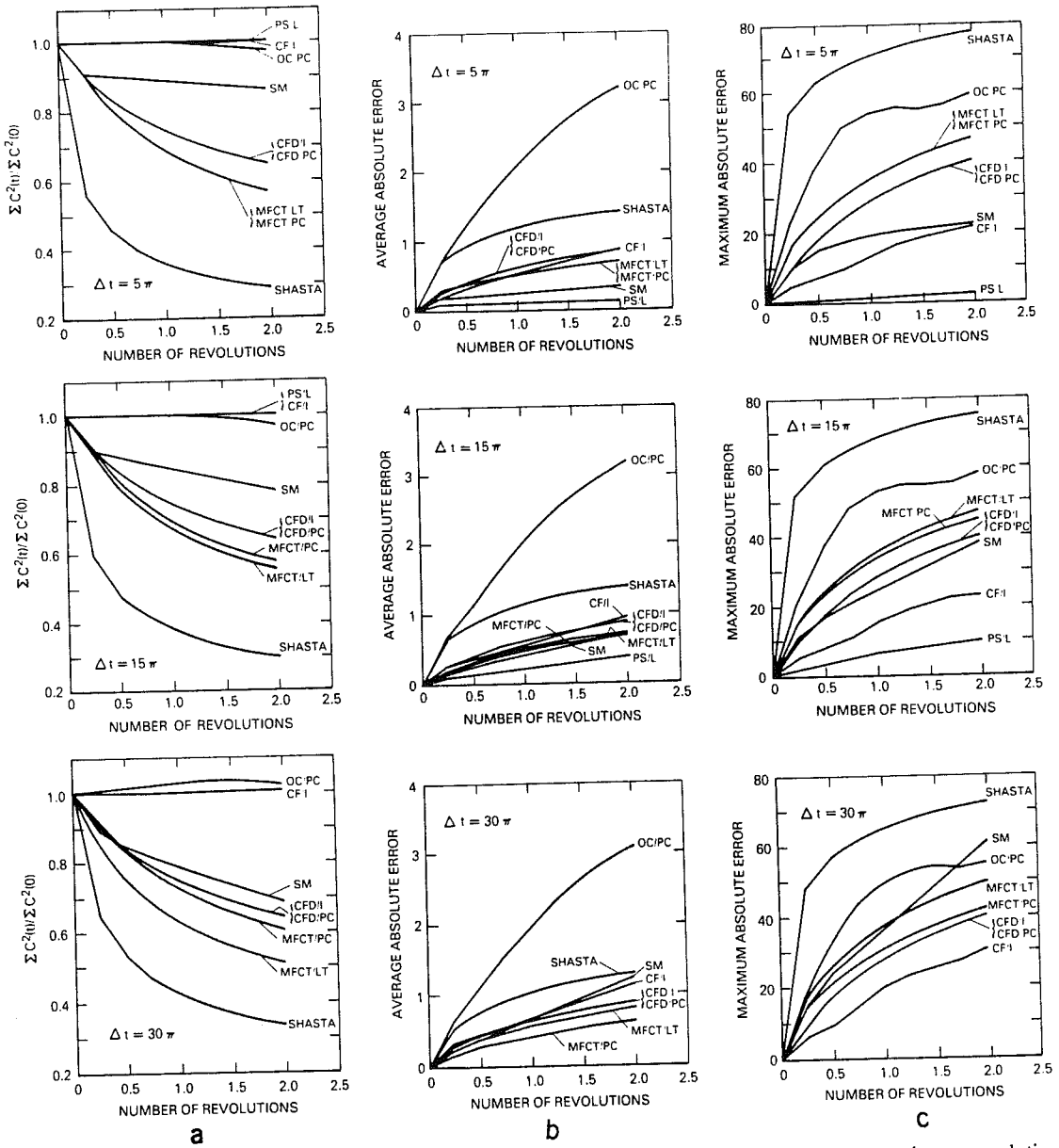

Fig. 9. Comparison of transport algorithms; abbreviations are given in Table 6. There are 7200π units per revolution. Therefore 5π corresponds to $\varepsilon = 0.07$; $15\pi \rightarrow \varepsilon = 0.21$; and $30\pi \rightarrow \varepsilon = 0.42$. (*a*) The ratio of the calculated to the initial squared concentrations (mass distribution ratio) for time steps of 5π, 15π, and 30π. This is a measure of dissipation errors. (*b*) The absolute error averaged over all grid points for time steps of 5π, 15π, and 30π. (*c*) The maximum absolute error at any grid point for time steps of 5π, 15π, and 30π [from *Chock and Dunker*, 1983]. Figures 9*d* and 9*e* are the same as Figures 9*a* through 9*c*, but for the schemes from *Chock* [1985]. (*d*) The ratio of the calculated to the initial squared concentrations (mass distribution ratio) for time steps of 5π, 15π, and 30π. This is a measure of dissipation errors. (*e*) The absolute error averaged over all grid points for time steps of 5π, 15π, and 30π. (*f*) The maximum absolute error at any grid point for time steps of 5π, 15π, and 30π [from *Chock*, 1985].

Mahlman and Sinclair [1977] concluded that the programming difficulties and time requirements of the cubic spline methods and the quasi-Lagrangian methods more than offset the small increases in accuracy gained over leapfrog time differences with fourth-order centered spatial differences (LF4). Mahlman and Sinclair also find that the pseudospectral technique is most accurate but requires many members in the basis function expansion and requires the use of a much smaller time step. For $\varepsilon = 0.3125$, Mahlman and Sinclair conclude that the pseudospectral technique is not significantly better than LF4. For $\varepsilon = 0.03125$ the results with LF4 actually deteriorate, and the results from the pseudospectral technique are nearly indistinguishable from the analytic result.

The explanation that Mahlman and Sinclair offer for the deterioration of the LF4 method with the reduction of ε (i.e., reduction of Δt) lies in the cancellation of space and time truncation errors (see Figure 3). When $\varepsilon = 0.3125$, the phase lag associated with the space truncation error nearly cancels the phase advance associated with the time truncation error. When Δt is reduced, the spatial truncation error remains the same while the time truncation error is reduced; therefore the balance ceases to exist. The same phenomenon explains why the results of the pseudospectral technique for $\varepsilon = 0.3125$ are so disappointing. In the pseudospectral case the space truncation error has been significantly reduced in comparison to lower-order finite difference representations, but the time error

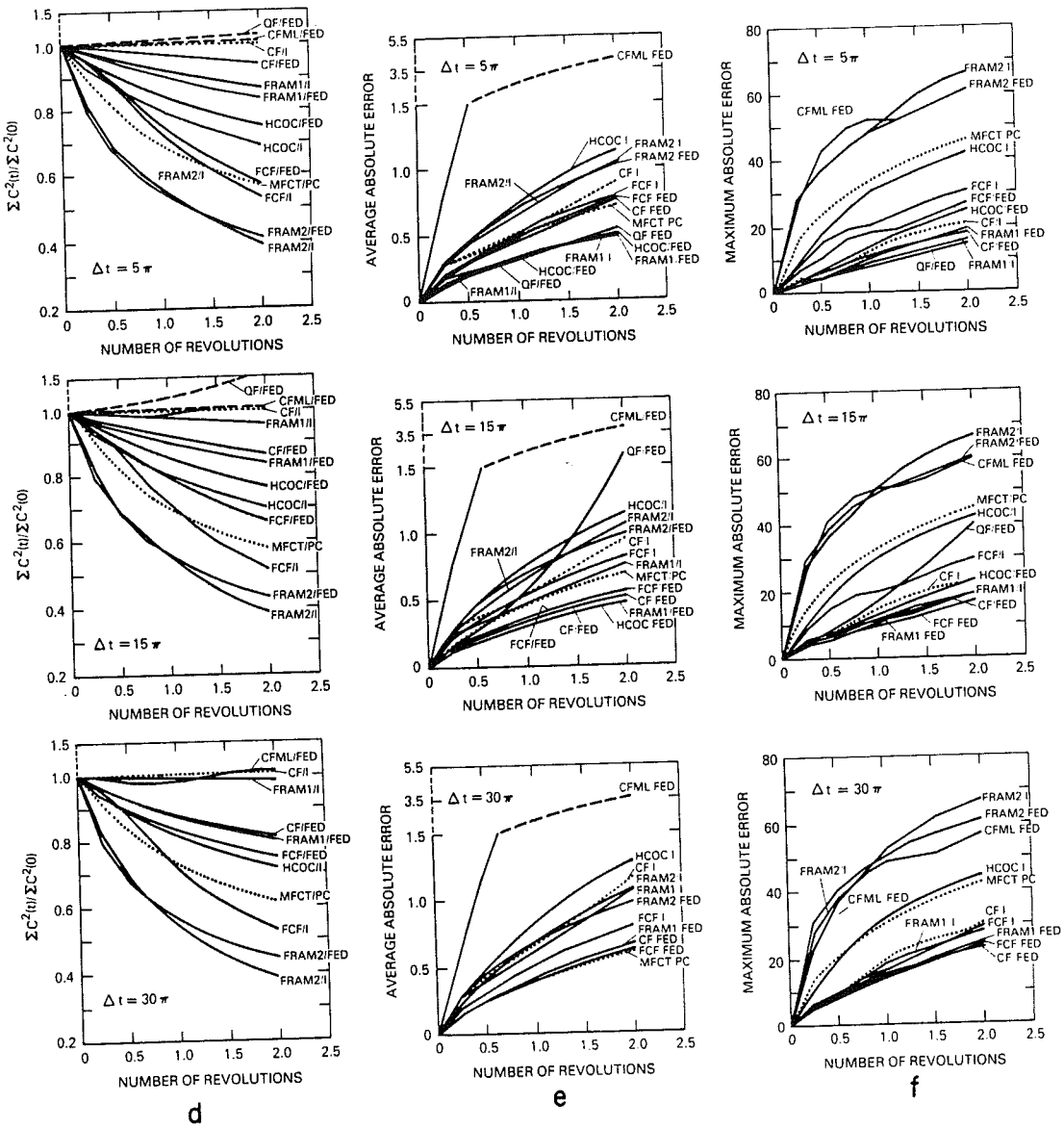

Fig. 9. (continued)

has not been similarly reduced. The lack of cancellation between space and time truncation errors also explains the notable difficulties with dispersion errors found with implicit time schemes.

Pepper and Cooper [1983] have tested the method of moments, the chapeau function method, the pseudospectral method, and the particle-in-cell technique on both analytical and field problems. All of these methods are accurate transport schemes. The particle-in-cell method is a particle method which follows the transport of particles between numerical boxes [*Sklarew et al.*, 1971]. The accuracy of the method ultimately depends on the tagging of many particles, and the method becomes prohibitively expensive. It is difficult to distinguish as to which of the remaining schemes are best. The method of moments algorithm used by Pepper and Cooper fairs much better than the algorithm used by *Chock and Dunker* [1983]. It is computationally the fastest, maintains peak values well, and does not produce negative mixing ratios. Once again, however, the pseudospectral method comes out as the most accurate of the tested methods, though at the cost of more computation time.

There are several recently developed schemes that have not been presented in the comparison studies above. The square root scheme, the slopes scheme, *Prather*'s [1986] second-order moments scheme, and *Smolarkiewicz*'s [1983, 1984] scheme. Also, the schemes of B. van Leer and the new schemes based on van Leer's methods are noticeably absent.

The square root scheme [*Schneider*, 1984] compares very favorably to the LF4 with filling as tested by *Mahlman and Sinclair* [1977] but does not require the computer time needed in local filling algorithms. The major disadvantage of the square root scheme is that conservation of mass is violated of the order of ε^4. In the implementation of the scheme this generally small violation is calculated with no extra effort, and when the violation reaches some small number (1 part in a million, for instance), the entire mass distribution is adjusted to conserve mass. There is the generation of small-scale noise caused by the squaring operation, which may have an influence on the long-term stability of the scheme.

Prather's [1986] scheme is an extension and improvement of the slopes scheme [*Russell and Lerner*, 1981]. Both schemes are relatively difficult to code. Prather offers a comparison of

both schemes to some of the schemes tested by *Chock and Dunker* [1983]. The second-order moments scheme produces very accurate results.

The tests described by *Smolarkiewicz* [1984] show good results in two and three dimensions. Smolarkiewicz's scheme is cost effective and positive definite.

The tests with the simple rectangular and linear versions of van Leer's scheme show that the scheme changes distributions into a square wave distribution in much the same manner as FCT. The higher-order versions (i.e., the piecewise parabolic method) are difficult to code because of the treatment of nonlinear Reimann problems at zonal interfaces but are very accurate [*Woodward and Colella*, 1984; *Colella and Woodward*, 1984]. These schemes were originally derived for shock propagation problems, and the coding necessary, balanced against the gain in accuracy for the higher-order schemes, seems to be beyond the level of effort necessary for natural atmospheric phenomena.

5. Discussion and Special Problems

The material in the previous sections primarily focused on the development of transport routines and their application in idealized circumstances. The problems that have been solved in the comparison studies provide very stringent tests, and it is assumed that if a particular transport algorithm does not do well in these tests, then it will not do well when applied to realistic problems. Unfortunately, if a scheme does do well in these tests, it does not assure that it is a generally useful scheme. This section will address the basic numerical difficulties of modeling advection when the constraints of a realistic atmosphere are considered.

A subtle point to remember in building a chemistry and transport model, which has a special algorithm for trace constituents, is numerical consistency between the constituent continuity equation and the equations used in the dynamical model. This point is easily overlooked in an offline transport model. Offline modes use wind fields from an independent dynamical model for transport velocity fields [see *Mahlman and Moxim*, 1978].

5.1. *Conservation of Mass and Boundary Conditions*

Conservation of mass is the most basic requirement of an advection algorithm. Given the situation of cyclic boundary conditions, then the vast majority of the algorithms discussed in the previous sections conserve mass without any special effort. Some schemes such as BIQUINTIC [*Schere*, 1983] and the square root scheme [*Schneider*, 1984] do not conserve mass. If the errors in mass conservation are very small, then the special attributes of a transport scheme might justify its use. In such a scheme the lack of mass conservation should be calculated as a diagnostic of how well the transport algorithm is performing. When chemical source and sink terms are added, it becomes more difficult to evaluate the role of nonconservation of mass.

As a general rule, it is best to avoid algorithms that do not conserve mass. In long integrations an appreciable part of the total mass might be lost, gained, or redistributed arbitrarily over the domain by a mass correction algorithm. This damages the credibility of the result. When a filling or monotonicity algorithm is needed, it must be carefully constructed to conserve mass.

Instrumental to the conservation of constituent mass is the conservation of total fluid mass,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0 \tag{22}$$

This equation relates the velocity field to the fluid density ρ, and it has been tacitly assumed in all previous discussions that (22) is satisfied. If (22) is not satisfied, then mass conservation, both total fluid mass and trace constituent mass, will be violated. Some finite difference algorithms that have been designed specifically for constituent transport require that specific numerical approximations be used in (22). The choice of such an algorithm may result in a tracer model that has, for instance, a different vertical velocity field than in the original dynamical model.

The choice of flux or advective form (section 2.2) can affect the ease with which mass conservation is coded. When no flux boundary conditions are given ($u\mu = 0$, at the boundary), the specification of the boundary condition is trivial in flux form. *Gordon* [1981] discusses the mass conservation properties of a flux form general circulation model. *Smolarkiewicz* [1985] discusses the high level of accuracy that can be obtained by using the flux form.

The implementation of boundary conditions frequently creates mass conservation problems. Most finite difference schemes must be altered at the boundaries in order to close the system. Therefore the symmetry amongst all of the grid points is lost. Two frequent mechanisms used at boundaries are one-sided differences [*Lapidus and Pinder*, 1982] and difference schemes that are of a lower-order accuracy than those used in the rest of the domain. Both of these mechanisms tend to generate errors, and since hyperbolic systems allow the errors to propagate undamped, the errors can propagate throughout the entire domain. An otherwise stable scheme can be made unstable by the improper specification of the boundary points.

By choosing a scheme that does not require a large cluster of points to calculate the spatial derivatives, the application of boundary conditions is simplified. Therefore the upstream volume (see Table 4 and section 3.2.6) schemes which generally look only one point upstream may be simply applied at the boundaries. Finite element methods (section 3.2.4) are known for their ease of application at boundaries. If the basis functions exactly meet the boundary conditions, then spectral or pseudospectral techniques have good characteristics.

5.2. *Dispersion, Atmospheric "Shocks," and Locality*

In section 2.3, dissipation and dispersion errors were portrayed as the two most fundamental errors encountered in trying to numerically model advection. Attempts to correct one of these errors frequently enhanced the appearance of the other error (Figure 1, for example). Dispersion errors are most important in regions of sharp gradients. Sharp gradients require short waves to resolve them, and it is a fundamental fact of finite difference schemes that shortwaves are not modeled as accurately as long-waves.

In natural atmospheric applications there are certain regions where sharp gradients are maintained, frequently due to the presence of a localized source or sink. Plumes from volcanos or power plants provide sharp constituent discontinuities which are very difficult to model. Ripples and

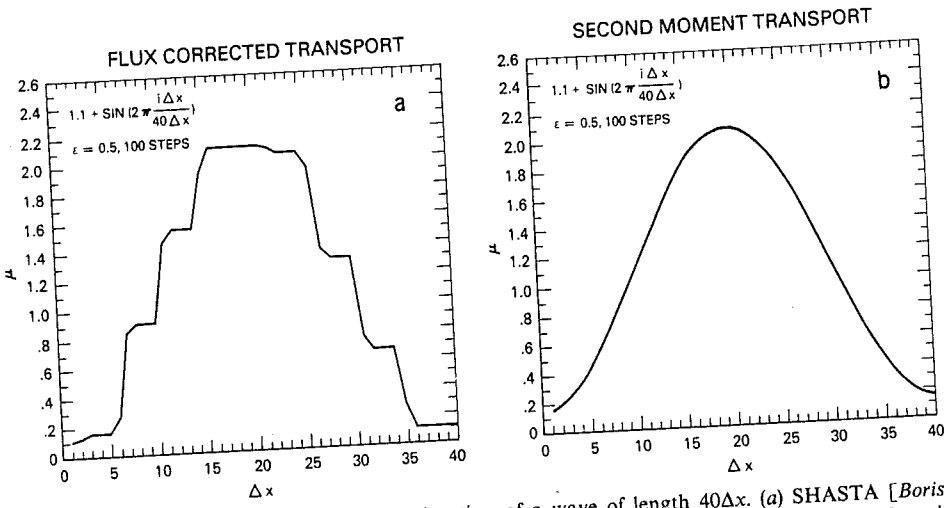

Fig. 10. Two positive definite schemes and the advection of a wave of length $40\Delta x$. (*a*) SHASTA [*Boris and Book*, 1973], the original flux-corrected transport which was derived to transport rectangular shocks exactly. Note the tendency for the scheme to fracture the distribution into a series of shock fronts. (*b*) The method of moments [*Egan and Mahoney*, 1972]. This scheme also transports rectangular waves exactly and has a tendency to square off rectangular distributions; however, it transports long-waves faithfully.

negative mixing ratios can appear around the plume. Attempts to reduce the ripples by adding diffusion might cause unrealistic spreading of the source.

For photochemically active constituents a region of particular difficulty is the terminator between day and night. For a constituent that exists only in light or dark, the terminator represents a shock. Numerical errors in the area of such a shock lead to the unrealistic presence of the constituent in an area where it should not be.

For tropospheric/stratospheric models the region of the tropopause represents a stationary shock for some constituents. Ozone, for instance, generally exists in much larger quantities in the stratosphere than in the troposphere. A numerical model has to be able to maintain this stationary shock without unrealistically propagating the shock to other parts of the domain. Also, the presence of the tropopause cannot be allowed to continuously generate negative mixing ratios.

The shocks discussed above are maintained by various processes that can be viewed as external to the advection problem. The single fact of advection that makes it difficult to model is that hyperbolic equations can form and maintain regions of sharp gradients. An important mechanism of transport of ozone between low and high latitudes is the advection of ozone in tongues around the high- and low-pressure cells of planetary waves. This transport manifests itself as the formation of tracer tongues that exhibit very large gradients [*Leovy et al.*, 1985]. Observations therefore suggest that in order for a transport scheme to accurately simulate the atmosphere, it must be able to form and maintain shocks without destroying the model with excessive dispersion errors.

If the maintenance of shock fronts is of critical importance, then schemes like FCT, the method of moments, and the piecewise parabolic method are perhaps appropriate (sections 3.2.5 and 3.2.6). Care, however, must be considered when applying these schemes. The most simple ones like SHASTA [*Boris and Book*, 1973] quickly fracture the entire distribution into a series of steps (Figure 10*a*). The more complex schemes may require significant effort to code and significant computer time. The method of moments also has a tendency to transport rectangular distributions, but Figure 10*b* indicates that the tendency to distort long-waves is much less than with SHASTA. The preference for many of the shock-conserving schemes to transport rectangular waves is the reason that many of these schemes preserve peaks so poorly (see Figure 9).

Another concern that frequently arises is the locality of a scheme; that is, from how many grid points away is information needed to calculate the spatial derivatives? If very many grid points are needed, and a shock is present, then constituent values that are unrealistic of the local situation are used in the calculation of the derivatives. The upstream geometric schemes only use local information and therefore avoid the problems of such contamination. *Pepper et al.* [1979] specifically discuss the disadvantages of the spline techniques, because each derivative involves other node points to some extent.

The view taken here is that based on the presence of sharp gradients, locality is not a required attribute. *Zalesak* [1984] explicitly shows that by going to higher-order accuracy, which requires more grid points, the resolution and the modeling of shock propagation is improved (see also *Orszag and Jayne* [1974]). The most accurate advection simulations are realized with spectral and pseudospectral techniques. Pseudospectral techniques draw information at each grid point from the entire domain. The advantage of having a local scheme are felt much more strongly when it comes to specifying boundary conditions.

5.3. *Diffusion*

Advection has the capability of stringing out and shearing off small-scale features that may ultimately be mixed [see *Welander*, 1955; *Tennekes*, 1978; *Mied and Lindemann*, 1984]. The formation of tracer shocks (fronts) by advection in a deformational velocity field is the instrumental mechanism for generating small-scale mixable structure. Diffusive or viscous processes are ultimately responsible for mixing the small-scale features generated by sheared velocity field. The atmosphere is not observed to generate and maintain shocks in constituent fields away from sources and sinks. Furthermore, high-resolution observations show the mixing of tracers to small scales (for instance, *Nastrom et al.* [1986]). Therefore diffusive processes must be included to properly model atmospheric transport.

In a numerical approximation, once the flow reaches the spatial scale of the numerical grid, some sort of parameterization has to be invoked to represent subscale processes. This is generally assumed to be diffusion. The transport studies of *Mahlman* [1985] clearly show that once advection has formed small-scale features, the subgrid parameterization quickly mixes the constituent. Since the blobs and strings caused by hyperbolic processes are not necessarily mixed [see *Clough et al.*, 1985], the specification of subgrid parameterizations remains largely an art.

While diffusion is a necessary physical process, it has been shown in sections 2 and 3 that numerical diffusion is often a great intrinsic source of error in an advection algorithm. Some schemes such as the donor cell scheme are so diffusive that numerical diffusion quickly dominates the solution. The donor cell and the Lax-Wendroff scheme have both been shown to appear as the unstable Euler scheme stabilized by diffusion. While the Lax-Wendroff scheme has the minimum amount of diffusion to stabilize the Euler forward scheme, the amplitude of a perturbation with wavelength equal to $6\Delta x$ is reduced by one half over 15 time steps for $\varepsilon = 0.5$ [*Morton*, 1971].

Not only is diffusion a necessary physical process and a source of error in advection algorithms, it is frequently touted as a necessary part of a transport algorithm to reduce dispersion errors. Finite difference schemes transport shortwaves with less accuracy than long-waves. Therefore it has been argued that since these waves are not accurately modeled, and that since this frequently leads to the unpleasant formation of negative mixing ratios, a highly scale dependent diffusion (or some other type of filter that can be interpreted as nonlinear diffusion) should be added to damp the shortwaves [*Thompson*, 1984; *Zalesak*, 1984]. Others argue that such corrections should not be made [*Gresho and Lee*, 1981; *Mesinger and Arakawa*, 1976].

The role of diffusion is confounded even more by the parameterization of transport processes in one- and two-dimensional chemistry models. In these models, part or all of the wave transport is modeled as diffusion. This is often a poor assumption. Recent work has shed some light on how it might be appropriate to use two-dimensional models to represent the zonal mean structure of the atmosphere [*Plumb and Mahlman*, 1987; *Strobel*, 1981; *Holton*, 1981; *Garcia and Solomon*, 1983; *Stordal et al.*, 1985].

Figure 11 illustrates how numerical and physical diffusion complicate each other. In Figure 11 the analytic problem solved by *Clancy* [1981] is considered. In this problem a wave of length $10\Delta x$ is being advected and diffused. In Figure 11*a*, forward Euler stabilized by diffusion is used with second-order spatial differences (sections 3.1.1–3.1.3). A very small ε is required in this case. The phase errors and the overestimation of the amplitude by the second-order scheme are obvious. Part of the diffusion must be used to stabilize the instability of the scheme; therefore the real diffusion is underestimated. In the event where there is little or no physical diffusion, Euler forward stabilized by diffusion overestimates the diffusion. Figure 11*b* shows that by using fourth-order differences (section 3.2.1) the results are improved. The phase error almost disappears, and even though this scheme is still unstable, the instability grows at a much slower rate, and the amplitude of the wave is more faithfully represented. Figure 11*c* shows the numerical results to be indistinguishable from the analytic result. For this example, leapfrog time differences (no numerical diffusion) have been used with fourth-order spatial differences, and the time step has been increased by a factor of 10. The diffusion is calculated using forward time differences.

Given that diffusion is a necessary physical process, and that its quantification in the atmosphere is unknown and very controversial, it must be concluded that numerical diffusion has to be minimized when writing an advection algorithm. The numerical scheme should be stable without a mechanism that maintains the characteristics of diffusion. If the scheme is held together by diffusion, then the task of assuring that the diffusion only very precisely operates on the mechanisms of instability must be undertaken. *Smolarkiewicz* [1983, 1984] uses carefully prescribed antidiffusion to counter intrinsic numerical diffusion. The addition of highly scale selective diffusion to damp out improperly modeled waves is recommended, but this diffusion must be carefully monitored and kept to a minimum. If these steps are taken, then physical diffusion can be added to the system in such a way that the magnitude of the diffusion is known, and the constituent variance is properly modeled.

There have been algorithms with small amounts of diffusion discussed in all of the generic classifications in section 3.2. The

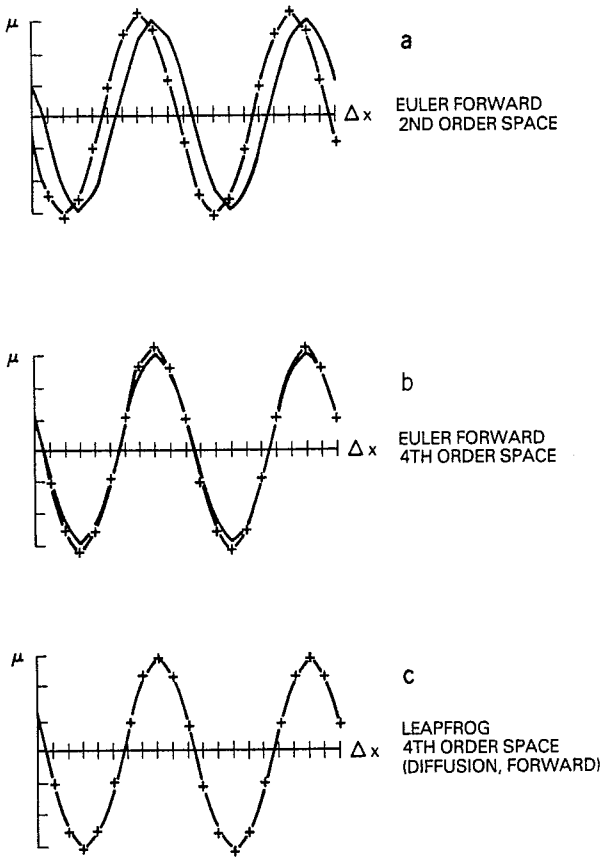

Fig. 11. Comparison of the analytic and numerical solutions of the "oceanic" advection-diffusion problem described by *Clancy* [1981] using three numerical techniques. The wavelength is equal to $10\Delta x$. The numerical solution is denoted by the plus signs. (*a*) Euler forward stabilized by diffusion (same as *Clancy* [1981, Figure 2]). (*b*) Euler forward time differencing with fourth-order estimates of the spatial derivatives. Note the significant improvement in the phase estimate. (*c*) Leapfrog time differences (with respect to the advective derivative, forward with respect to diffusion) with fourth-order centered spatial derivatives and an increase in Δt by a factor of 10 over that used in Figures 11*a* and 11*b*; note the nearly exact agreement between the analytic and numerical solution.

leapfrog scheme (section 3.1.4) has no intrinsic diffusion. Some of the shock-preserving, monotonic (sections 3.2.5 and 3.2.6) schemes have an unusual diffusion, because once peaked distributions are converted into rectangular distributions, the transport is exact.

5.4. *Multidimensions, Deformational Velocities, and Spherical Coordinates*

Many advection algorithms are derived for the idealized constant velocity, one-dimensional cases depicted in Figures 1 and 2. When the schemes are applied to realistic multidimensional situations, the quality realized in the simple situation is lost. Similar problems are found when nonrectangular coordinate systems are used.

One method of generating codes for multidimensions is illustrated by *Arakawa*'s [1966] formulation of the two-dimensional advection equation. Basically, a two-dimensional configuration of grid points is set up, and a numerical scheme to simultaneously calculate the spatial derivatives in both directions is specified. *Smolarkiewicz* [1982] generates a combined form of the *Crowley* [1968] advection scheme (that is, the x and y advective are combined in one step).

A second method for performing multidimensional calculations is the method of time splitting (or the method of fractional steps [*Yanenko*, 1971; *Marchuk*, 1974; *Strang*, 1968]). Time splitting involves calculating each process in a procedure separately and in a specific order. The modified results from the first step are used as the input parameters for the second step. In the comparison studies of *Chock* [1985] the two-dimensional transport is calculated with a time-splitting algorithm that calculates the x advection and then the y advection during one step; then on the next step the y advection is calculated first. *Thompson* [1984] discusses the various time-splitting algorithms that have been proposed and tested. *Smolarkiewicz* [1982, 1984] offers an interesting discussion of time split and combined formulations of multidimensional advection. Not all schemes take well to time splitting, and many schemes lose either their accuracy or stability when simple time-splitting algorithms are used [*Peyret and Taylor*, 1983]. *Prather* [1986] states that the cross terms, which consistently describe the interaction between the advection operators in each dimension, are necessary to the stability of his scheme. *Smolarkiewicz* [1982] discusses the importance of cross terms to the accuracy of the multidimensional *Crowley* [1968] scheme. Overall, however, time splitting is a proven efficient method for extending one-dimensional transport codes to two and three dimensions.

The shape-conserving tests in one, two, and three dimensions do not test the ability of an algorithm to function in deformational (sheared) velocity fields. Accurate performance in deformational fields is essential because deformational velocities are responsible for building up constituent fronts which may be mixed by irreversible diffusive processes. The most frequent failure in the presence of deformational velocities is instability. Instabilities in deformational flow might be expected because the numerical processes that build shocks are very similar to the processes that cause instability. *Smolarkiewicz* [1982] offers a discussion of deformational velocity fields that is applicable to finite difference techniques.

The final generalization of a scheme is the jump from rectangular to spherical coordinates. Conservation of mass and possible advantages supplied by the flux form may be lost when the metrics of the curvilinear coordinate system are incorporated into the numerical scheme. Also, the convergence of the meridians of longitude at the poles effectively reduces the spatial increment to zero, placing severe restraints on the time step. Polar filters, which attempt to remove the unstable modes while leaving the physical modes undisturbed, are frequently used in general circulation models, but care must be taken to assure that the filters do not unrealistically alter the flow [see *Takacs and Balgovind*, 1983]. A major advantage of spectral methods is that no special consideration has to be made at the poles (section 3.2.3). Some of the upstream volume schemes (section 3.2.4) do not require $\varepsilon \leq 1$ and therefore may exhibit favorable properties at singular boundaries. Implicit schemes remain stable near the pole.

5.5. *Numerics of Combined Chemistry and Transport*

Some effort has been put into the numerics of transport and chemistry, though the literature is not nearly as rich as either the transport algorithm literature or the literature concerning the integration of chemical equations. Much of the material that is available exists in laboratory reports and seems to be concentrated in the field of combustion [*Oran and Boris*, 1981]. As with the extension of advection algorithms from one to three-dimensions, the entire numerical procedure can be written as a single entity, or the process can be time split.

In time split techniques the chemistry and transport calculations are performed separately [*McRae et al.*, 1982]. This is sometimes referred to as process splitting and is a method that is commonly used to add diffusion to an advection calculation and to add radiation to atmospheric dynamics models. Process splitting has also been used to calculate wave-wave interaction terms in atmospheric dynamic models and to separate fast-moving wave modes from the slower-moving meteorological waves [*Chao*, 1982; *Gadd*, 1978*a*, 1980; *Bates and McDonald*, 1982].

Figure 12 shows the results of an idealized integration of chemistry and transport. In the idealized problem, rectangular distributions of odd oxygen ($O_x = O_3 + O$) and N_2O_5 with concentrations characteristic of middle latitudes are being advected in an environment representative of high latitudes. Total odd nitrogen is held constant. The background field in which the rectangular distribution is advecting is found by integrating the initial values for 10^6 s with a chemistry integrator. For an integration of 10^6 s the constituent in the rectangle is expected to approach the value of the initial background. The original background value is expected to reach the value obtained by integrating the initial values for 2×10^6 s. Only the results for O_x are shown (see Figure 12*a*).

Three experiments are presented. In the first the integration is represented schematically by

$$\mu^{t-\Delta t} = \mu^t + \Delta t(\text{advection})^t + \Delta t(\text{production} - \text{loss})^t \tag{23}$$

In the second experiment,

$$\begin{aligned} \mu^* &= \mu^t + \Delta t(\text{advection})^t \\ \mu^{t+\Delta t} &= \mu^* + \Delta t(\text{production} - \text{loss})^* \end{aligned} \tag{24}$$

where the chemistry is calculated with the asterisked values. In both of these experiments the Lax-Wendroff scheme is used with $\varepsilon = 1$ (the transport is exact). The third experiment is the same as the first with $\varepsilon = 0.5$.

Figure 12*b* shows that the straightforward method depicted in (23) generates errors. Since the transport is exact, it is the

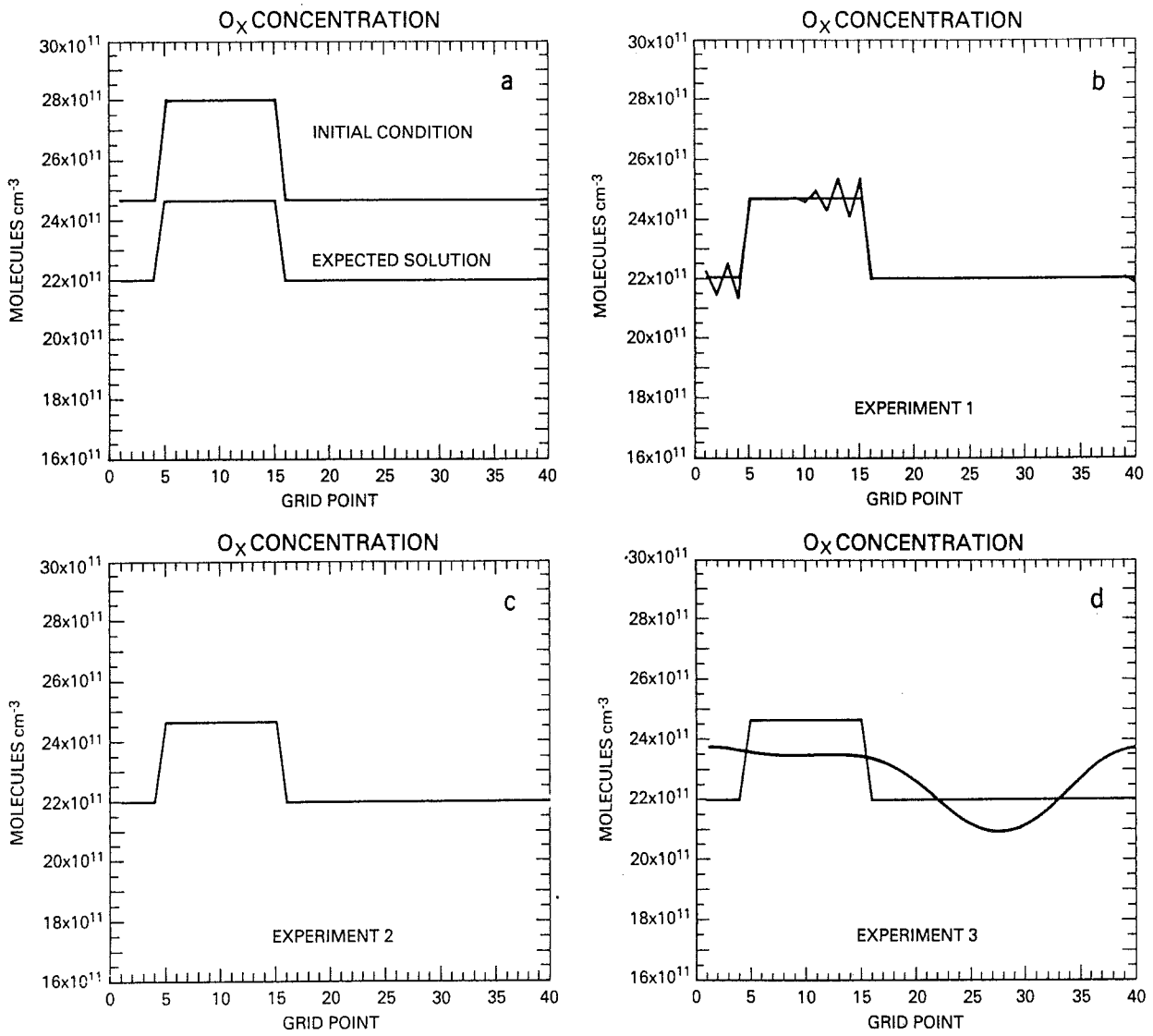

Fig. 12. Odd oxygen concentration for combined chemistry and transport experiments. (*a*) The initial condition and the expected solution. The expected solution is reproduced in Figures 12*b* through 12*d*. (*b*) Exact transport. Errors are formed by calculating the chemistry and the advection terms at the same time. (*c*) Exact transport. Exact results are obtained by calculating the chemistry with "advected" constituent densities. (*d*) Transport not exact. The diffusion and dispersion errors of the transport scheme overwhelm the errors seen in Figure 12*b*.

treatment of the combination of the transport and chemistry terms that produces these errors. For this experiment the oscillations become so large in N_2O_5 that negative mixing ratios are generated. The second experiment, equation (24), shows that for this particular problem the process split method produces exact results (Figure 12*c*). In the third experiment ($\varepsilon = 0.5$; transport is not exact) the errors associated with the transport routine are seen to dominate the errors associated with the combination of chemistry and transport (compare to Figure 12*b*). The details of combining chemistry and transport calculations are deferred to a later paper, in preparation by this author.

6. Summary

Of the multitude of schemes that are available, or that can be effortlessly developed by permutating various methodologies, the following general classification can be made. A few schemes are bad enough that their use would certainly invalidate any model results. A vast majority of transport schemes fall into a category where it is difficult to judge one scheme to be better than another. There are a select few schemes that offer very accurate results. As a general conclusion, there is a certain level of accuracy that can be obtained by the judicious use of simple finite difference algorithms, and any additional increase in accuracy can require great computational and human effort. This section will highlight the most promising schemes.

The question of computational time and memory is of some interest. Many researchers argue that advection calculations are cheap in comparison to the overall cost of running a model. This is a valid statement when the transport of a single quantity is compared to the cost of an atmospheric general circulation model. It is also generally true that the calculation of the transport of a single constituent is small in comparison to the cost of computing the chemistry production and loss. Therefore the conclusion might be made that the cost of making a super accurate transport scheme is small in comparison to the total cost of the model.

There is, however, a point of diminishing returns. A stratospheric constituent model might be expected to have 40 or more continuity equations, depending on the method used to integrate the chemistry. The cost of transport is very expensive and makes up a large fraction of the calculation. Therefore an economic transport routine is very important. A scheme that spends much of its extra computational effort in assuring that step discontinuities are calculated accurately is not appropriate for global atmospheric applications.

The question of efficiency of computer storage is more obvious. If it is desired to transport even 20 constituents on a (72, 36, and 30; grid points in longitude, latitude, and height, which is a medium resolution troposphere/stratosphere general circulation model) grid, then the difference between a two- and three-level time scheme is 1.6×10^6 words. To advect the first and second moments of the constituent provides an even larger expense. Constituents that are not transported also take up considerable storage. Therefore a profligate attitude toward computer time and storage can easily lead to a model that cannot be run on any computer.

It is difficult to recommend any particular scheme for use in all situations. *Thompson* [1984] offers a long list of general recommendations. Aside from recommending odd-order schemes (either third or fifth), Thompson recommends explicit, second-order accurate time stepping with ε well below unity, an upwind bias, and a strong sharp filter on the shortest wavelengths. The convergence of the meridians at the pole might require such short time steps that implicit schemes become attractive. With implicit schemes, dispersion errors become more prominent. An interesting conclusion of *Smolarkiewicz* [1984] is that both space and time truncation errors should be at least equal to the dimensionality of the problem.

Thompson [1984] recommends odd-order schemes, and several recent studies investigate the virtues of odd-order schemes [*Schlesinger*, 1985; *Takacs*, 1985]. The preference for odd-order schemes largely arises in the attempt to reduce dispersion errors. As is shown by *Takacs* [1985], going from an odd-order scheme to the next higher even-order scheme does not reduce the dispersion error but does require more multiplications. The even-order scheme, however, does reduce dissipation errors. Many previous studies emphasize the problems of modeling regions of sharp gradients; hence the reduction of dispersion errors is most important. It has been argued in this review that in particular, for middle atmospheric applications, it is best to reduce dissipation errors. By reducing numerical dissipation errors to a minimum, the modeler obtains maximum control over adding physical diffusion, an essential mechanism in any transport model.

Therefore for straightforward finite difference applications, reasonable minimum requirements are second-order accurate time differences and fourth-order spatial differences. Leapfrog time differences with fourth-order centered spatial differences can be viewed as the minimum effort scheme. LF4 is not positive definite, and a filling algorithm is a likely requirement. The three time levels required with the leapfrog scheme may be unattractive both from the point of view of computer storage and the incorporation of chemistry. *Smolarkiewicz*'s [1984] scheme is a positive definite finite difference scheme that offers a good mix of accuracy and cost.

The recommendation from the most complete, up to date, published intercomparison of transport algorithms by *Chock* [1985] and *Chock and Dunker* [1983] is to use the chapeau function finite element method with the Forester filter to remedy dispersion errors (sections 3.2.4 and 3.2.5). This scheme is not the most accurate that was tested, but, weighing cost versus accuracy, it was chosen as the best. *Chock* [1985] suggests forward Euler stabilized with diffusion (sections 3.1.1–3.1.3) as a good time-stepping method. However, if the user wants to maintain control over the model diffusion, the implicit method discussed by *Chock and Dunker* [1983] is more appropriate for middle atmospheric models. Petrov-Galerkin finite element techniques (section 3.2.4) have the potential for producing very accurate results.

For absolute accuracy, though at the expense of short time steps to reduce the phase errors associated with time differencing, the pseudospectral (or spectral) technique is the best. High accuracy requires that a large number of basis functions be carried. Pseudospectral methods are most useful if the basis functions identically meet the boundary conditions.

In practice, global applications of spectral or pseudospectral methods generally involve modeling the horizontal transport with expansion functions and the vertical transport with a finite difference technique. The biggest source of negative mixing ratios in such a model is generally due to the vertical differencing. However, there are difficulties associated with Gibb's phenomena near regions of sharp gradients. The pseudospectral technique does not offer all of the advantages of the spectral technique at the poles [*Merilees and Orszag*, 1979].

Perhaps the most accurate scheme developed to date is the pseudospectral flux-corrected transport algorithm of *Zalesak* [1981*b*]. The flux-corrected transport procedure provides a method for making any scheme monotonic. However, the production of a scheme that does not square off peaks is a difficult task that requires as much art as science. The adaptation of pseudospectral flux-corrected transport to spherical geometry is not straightforward (P. Rasch, personal communication, 1986), and the combined cost of the pseudospectral technique and the flux limiting make this a very expensive method.

From the discussion in section 5, local upstream volume schemes (section 3.2.6) have many positive attributes: they are monotonic, the time steps can be large, boundary conditions are easy to apply, and absolute mass conservation is easy to code. These schemes can have unusual dissipation characteristics. *Prather* [1986] reports his scheme to be accurate and stable in three dimensions. The method of moments can be efficiently coded in three dimensions [*Pepper and Cooper*, 1983]. Coding difficulties and storage requirements prohibit a wholehearted recommendation of these schemes.

Many adequate advection algorithms have been developed. Many of these algorithms have not been tested or generalized to the conditions necessary for atmospheric applications. The choice of a particular algorithm for a model will depend on personal preferences and model constraints. Even the most accurate algorithms described will leave a numerical effect on the computation. The most important consideration in choosing an advection algorithm is to assure that numerical constituent models are reflecting the physics and chemistry of the system rather than the inaccuracies of the numerical methods.

NOTATION

CF	chapeau function.
FCT	flux-corrected transport.
FED	Euler forward stabilized with diffusion.

i (subscript)	space increment index.
LF4	leapfrog time differences with fourth-order centered space differences.
t (superscript)	time index.
u	velocity.
ε	Courant-Freidrichs-Lewy number, $u\Delta t/\Delta x$.
μ	mixing ratio.
Δt	time step.
Δx	space increment.

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REFERENCES

Ames, W. F., *Numerical Methods for Partial Differential Equations*, 2nd ed., 356 pp., Academic, New York, 1977.

Anderson, D., and B. Fattahi, A comparison of numerical solutions of the advective equations, *J. Atmos. Sci.*, *31*, 1500–1506, 1974.

Arakawa, A., Computational design for long term integration of the equations of fluid motion: Two-dimensional incompressible flow, part 1, *J. Comput. Phys.*, *1*, 119–143, 1966.

Arakawa, A., and V. R. Lamb, Computational design of the basic dynamical processes of the UCLA general circulation model, in *Methods in Computational Physics*, vol. 17, pp. 173–265, Academic, New York, 1977.

Asselin, R., Frequency filter for time integrations, *Mon. Weather Rev.*, *100*, 487–490, 1972.

Augenbaum, J. M., A Lagrangian method for the shallow-water equations on a Voronoi mesh, *J. Comput. Phys.*, *53*, 240–265, 1984.

Bates, J. R., and A. McDonald, Multiply-upstream, semi-Lagrangian advective schemes: Analysis and application to a multilevel primitive equation model, *Mon. Weather Rev.*, *110*, 1831–1842, 1982.

Bates, J. R., and A. McDonald, Comments on "Some properties and comparative performance of the semi-Lagrangian method of Robert in the solution of the advection-diffusion equation," *Atmos. Oceans*, *23*, 193–194, 1985.

Book, D. L. (ed.), *Finite-Difference Techniques for Vectorized Fluid Dynamics Calculations*, 226 pp., Springer-Verlag, New York, 1981.

Book, D. L., J. P. Boris, and K. Hain, Flux-corrected transort II: Generalizations of the method, *J. Comput. Phys.*, *18*, 248–283, 1975.

Boris, J. P., and D. L. Book, Flux-corrected transport, I, SHASTA: A fluid transport algorithm that works, *J. Comput. Phys.*, *11*, 38–69, 1973.

Boris, J. P., and D. L. Book, Flux-corrected transport, III, Minimal-error FCT algorithms, *J. Comput. Phys.*, *20*, 397–431, 1976.

Burstein, S. Z., and A. A. Mirin, Third order difference methods for hyperbolic equations, *J. Comput. Phys.*, *5*, 547–571, 1970.

Carnahan, B., H. A. Luther, and J. O. Wilkes, *Applied Numerical Methods*, 604 pp., John Wiley, New York, 1969.

Chao, W. C., Formulation of an explicit-multiple-time-step time integration method for use by a global primitive equation grid model, *Mon. Weather Rev.*, *110*, 1603–1617, 1982.

Chapman, M., FRAM—Nonlinear damping algorithms for the continuity equation, *J. Comput. Phys.*, *44*, 84–103, 1981.

Chock, D. P., A comparison of numerical methods for solving the advection equation, II, *Atmos. Environ.*, *19*, 571–586, 1985.

Chock, D. P., and A. M. Dunker, A comparison of numerical methods for solving the advection equation, *Atmos. Environ.*, *17*, 11–24, 1983.

Christensen, O., and L. P. Prahm, A pseudospectral model for dispersion of atmospheric pollutants, *J. Appl. Meteorol.*, *15*, 1284–1294, 1976.

Clancy, R. M., A note on finite differencing of the advection-diffusion equation, *Mon. Weather Rev.*, *109*, 1807–1809, 1981.

Clark, T. L., Numerical simulations with a three-dimensional cloud model: Lateral boundary condition experiments and multicellular severe storm simulations, *J. Atmos. Sci.*, *36*, 2191–2215, 1979.

Clark, T. L., and W. D. Hall, A numerical experiment on stochastic condensation theory, *J. Atmos. Sci.*, *36*, 470–483, 1979.

Clough, S. A., N. S. Grahame, and A. O'Neill, Potential vorticity in the stratosphere derived using data from satellites, *Q. J. R. Meteorol. Soc.*, *111*, 335–358, 1985.

Cloutman, L. D., and L. W. Fullerton, Automated computation of modified equations (NOTE), *J. Comput. Phys.*, *29*, 141–144, 1978.

Colella, P., A direct Eulerian MUSCL scheme for gas dynamics, *Rep. LBL-14104*, Lawrence Berkeley Lab., Berkeley, Calif., 1982.

Colella, P., and H. M. Glaz, Efficient solution algorithms for the Riemann problem for real gases, *J. Comput. Phys.*, *59*, 264–289, 1985.

Colella, P., and P. R. Woodward, The piecewise parabolic method (PPM) for gas-dynamical simulations, *J. Comput. Phys.*, *54*, 174–201, 1984.

Courant, R., and D. Hilbert, *Methods of Mathematical Physics*, vol. 2, *Partial Differential Equations*, p. 830, Interscience, New York, 1962.

Courant, R. E., E. Isaacson, and M. Rees, On the solution of nonlinear hyperbolic differential equations by finite differences, *Commun. Pure Appl. Math.*, *5*, 243–255, 1952.

Crowley, W. P., Second-order numerical advection, *J. Comput. Phys.*, *1*, 471–484, 1967.

Crowley, W. P., Numerical advection experiments, *Mon. Weather Rev.*, *96*, 1–11, 1968.

Deque, M., and D. Cariolle, Some destabilizing properties of the Asselin time filter, *Mon. Weather Rev.*, *114*, 880–884, 1986.

Dryden, H. L., F. D. Murnaghan, and H. Bateman, *Hydrodynamics*, 634 pp., Dover, New York, 1956.

Egan, B. A., and J. R. Mahoney, Numerical modeling of advection and diffusion of urban area source pollutants, *J. Appl. Meteorol.*, *11*, 312–322, 1972.

Emery, A. F., An evaluation of several differencing methods for inviscid fluid flow problems, *J. Comput. Phys.*, *2*, 306–331, 1968.

Fleischer, M. T., and F. L. Worley, Jr., Orthogonal collocation—Application to diffusion from point sources, *Atmos. Environ.*, *12*, 1349–1357, 1978.

Forester, C. K., High order monotonic convective difference schemes, *J. Comput. Phys.*, *23*, 1–22, 1977.

Fromm, J. E., A method for reducing dispersion in convective difference schemes, *J. Comput. Phys.*, *3*, 176–189, 1968.

Gadd, A. J., A split explicit integration scheme for numerical weather prediction, *Q. J. R. Meteorol. Soc.*, *104*, 569–582, 1978*a*.

Gadd, A. J., A numerical advection scheme with small phase speed errors, *Q. J. R. Meteorol. Soc.*, *104*, 583–594, 1978*b*.

Gadd, A. J., Two refinements of the split explicit integration scheme, *Q. J. R. Meteorol. Soc.*, *106*, 215–220, 1980.

Garcia, R. R., and S. Solomon, A numerical model of the zonally averaged dynamical and chemical structure of the middle atmosphere, *J. Geophys. Res.*, *88*, 1379–1400, 1983.

Gary, J., Nonlinear instability, in *Numerical Methods Used in Atmospheric Models*, vol. 2, GARP *Publ. Ser.* 17, pp. 476–499, World Meteorological Organization, Geneva, 1979.

Gelinas, R. J., S. K. Doss, and K. Miller, The moving finite element method: Applications to general partial differential equations with multiple large gradients, *J. Comput. Phys.*, *40*, 202–249, 1981.

Gerald, C. F., *Applied Numerical Analysis*, 2nd ed., 557 pp., Addison-Wesley, Reading, Mass., 1978.

Gidel, L. T., P. J. Crutzen, and J. Fishman, A two-dimensional photochemical model of the atmosphere, 1, Chlorocarbon emissions and their effect on stratospheric ozone, *J. Geophys. Res.*, *88*, 6622–6640, 1983.

Gill, A. E., *Atmosphere-Ocean Dynamics*, 662 pp., Academic, New York, 1982.

Godunov, S. K., Finite difference method for numerical computation of discontinuous solutions of the equations of fluid dynamics, *Mat. Sb.*, *47*, 271, 1959.

Gordon, H. B., A flux formulation of the spectral atmospheric equations suitable for use in long-term climate modeling, *Mon. Weather Rev.*, *109*, 56–64, 1981.

Gottlieb, D., and S. A. Orszag, *Numerical Analysis of Spectral Meth-*

ods: Theory and Applications, 172 pp., Society for Industrial and Applied Mathematics, Philadelphia, Pa., 1977.

Gresho, P. M., and R. L. Lee, Don't suppress the wiggles—They're telling you something, *Comput. Fluids*, *9*, 223–253, 1981.

Grotjahn, R., and J. J. O'Brien, Some inaccuracies in finite differencing hyperbolic equations, *Mon. Weather Rev.*, *104*, 180–194, 1976.

Hunt, K., *The Partial Donor Cell Method*, *Memo. Rep. 3713*, Nav. Res. Lab., Washington, D. C., 1978.

Haltiner, G. J., and R. T. Williams, *Numerical Prediction and Dynamic Meteorology*, 477 pp., John Wiley, New York, 1980.

Harten, A., The artificial compression method for computation of shocks and contact discontinuities, I, Single conservation laws, *Commun. Pure Appl. Math.*, *30*, 611–638, 1977.

Harten, A., The artificial compression method for computation of shocks and contact discontinuities, III, Self-adjusting hybrid schemes, *Math. Comput.*, *32*, 363–389, 1978.

Harten, A., and G. Zwas, Self-adjusting hybrid schemes for shock computations, *J. Comput. Phys.*, *9*, 568–583, 1972.

Hasbani, Y., E. Livne, and M. Bercovier, Finite elements and characteristics applied to advection-diffusion equations, *Comput. Fluids*, *2*, 71–83, 1983.

Hirt, C. W., Heuristic stability theory for finite-difference equations, *J. Comput. Phys.*, *2*, 339–355, 1968.

Holton, J. R., An advective model for two-dimensional transport of stratospheric trace species, *J. Geophys. Res.*, *86*, 11,989–11,994, 1981.

Hsu, C.-P. F., Air parcel motions during a numerically simulated sudden stratospheric warming, *J. Atmos. Sci.*, *37*, 2768–2792, 1980.

Hughes, T. J. R. (Ed.), *Finite Element Methods for Convection Dominated Flows*, American Society of Mechanical Engineers, New York, 1979.

Hughes, T. J. R., and A. Brooks, A theoretical framework for Petrov-Galerkin methods with discontinuous weighting functions: Application to the streamline-upwind procedure, in *Finite Elements in Fluids*, vol. 4, edited R. H. Gallagher, D. H. Norrie, J. T. Oden, and O. C. Zienkiewicz, 647 pp., John Wiley, New York, 1982.

Kreiss, H. O., and J. Oliger, Comparison of accurate methods for the integration of hyperbolic equations, *Tellus*, *24*, 199–215, 1972.

Krishnamurti, T. N., Numerical integration of primative equations by a quasi-Lagrangian advective scheme, *J. Appl. Meteorol.*, *1*, 508–521, 1962.

Kurihara, Y., On the use of implicit and iterative methods for the time intergration of the wave equation, *Mon. Weather Rev.*, *93*, 33–46, 1965.

Kutler, P., H. Lomax, and R. F. Warming, Computation of space shuttle flow fields using noncentered finite-difference schemes, *AIAA Pap. 72-193*, 1972.

Lamb, H. L., *Hydrodynamics*, 738 pp., Dover, New York, 1945.

Lapidus, L., and G. F. Pinder, *Numerical Solution of Partial Differential Equations in Science and Engineering*, 677 pp., John Wiley, New York, 1982.

Lax, P., and B. Wendroff, Systems of conservation laws, *Commun. Pure Appl. Math.*, *13*, 217–237, 1960.

Leonard, B. P., A survey of finite differences of opinion on numerical muddling of the incomprehensible defective confusion equation, in *Finite Element Methods for Convection Dominated Flows*, edited by T. J. R. Hughes, American Society of Mechanical Engineers, New York, 1979.

Leonard, B. P., Note on the von Neumann stability of the explicit FTCS convective diffusion equation, *Appl. Math. Modelling*, *4*, 401–402, 1980.

Leovy, C. B., C. R. Sun, M. H. Hitchman, E. E. Remsberg, J. M. Russell III, L. L. Gordley, J. C. Gille, and L. V. Lyjak, Transport of ozone in the middle atmosphere: Evidence for planetary wave breaking, *J. Atmos. Sci.*, *42*, 230–244, 1985.

Lilly, D. K., On the computational stability of numerical solutions of time dependent nonlinear geophysical fluid dynamics problems, *Mon. Weather Rev.*, *93*, 11–26, 1965.

Long, P. E., and D. W. Pepper, An examination of some simple numerical schemes for calculating scalar advection, *J. Appl. Meteorol.*, *20*, 146–156, 1981.

MacCormack, R. W., The effect of viscosity in hypervelocity impact cratering, *AIAA Pap. 69-354*, 1969.

Machenhauer, B., The spectral method, in *Numerical Methods Used in Atmospheric Models*, vol. 2, *GARP Publ. Ser. 17*, pp. 124–277, World Meteorological Organization, Geneva, 1979.

Mahlman, J. D., Mechanistic interpretation of stratospheric tracer transport, *Adv. Geophys.*, *28A*, 301–323, 1985.

Mahlman, J. D., and W. J. Moxim, Tracer simulation using a global general circulation model: Results from a midlatitude instanteous source experiment, *J. Atmos. Sci.*, *35*, 1340–1374, 1978.

Mahlman, J. D., and R. W. Sinclair, Tests of various numerical algorithms applied to a simple trace constituent air transport problem, in *Fate of Pollutants in the Air and Water Environments*, vol. 8, part 1, edited by I.H. Suffet, John Wiley, New York, 1977.

Marchuk, G. I., *Numerical Methods in Weather Prediction*, 277 pp., Academic, New York, 1974.

McDonald, A., A semi-Lagrangian and semi-implicit two time-level integration scheme, *Mon. Weather Rev.*, *114*, 824–830, 1986.

McRae, G. J., W. R. Goodin, and J. H. Seinfeld, Numerical solution of the atmospheric diffusion equation for chemically reacting flows, *J. Comput. Phys.*, *45*, 1–42, 1982.

Merilees, P. E., and S. A. Orszag, The psuedospectral method, in *Numerical Methods Used in Atmospheric Models*, vol. 2, *GARP Publ. Ser. 17*, pp. 278–301, World Meteorological Organization, Geneva, 1979.

Mesinger, F., and A. Arakawa, *Numerical Methods Used in Atmospheric Models*, vol. 1, *GARP Publ. Ser. 17*, pp. 1–64, World Meteorlogical Organization, Geneva, 1976.

Mied, R. P., and G. J. Lindemann, Mass transfer between Gulf Stream rings, *J. Geophys. Res.*, *89*, 6365–6372, 1984.

Molenkamp, C. R., Accuracy of finite-difference methods applied to the advection equation, *J. Appl. Meteorol.*, *7*, 160–167, 1968.

Morton, K. W., Stability and convergence in fluid flow problems, *Proc. R. Soc. London, Ser. A*, *323*, 237–253, 1971.

Nastrom, G. D., W. H. Jasperson, and K. S. Gage, Horizontal spectra of atmospheric tracers measured during the Global Atmospheric Sampling Program, *J. Geophys. Res.*, *91*, 13,201–13,209, 1986.

O'Brien, J. J. (Ed.), *Advanced Physical Oceanographic Numerical Modeling*, 608 pp., D. Reidel, Hingham, Mass., 1986.

Oran, E. S., and J. P. Boris, Detailed modelling of combustion systems, *Prog. Energy Combust. Sci.*, *7*, 1–72, 1981.

Orszag, S. A., Numerical simulation of incompressible flows within simple boundaries, I, Galerkin (spectral) representations, *Stud. Appl. Math.*, *50*, 293–327, 1971*a*.

Orszag, S. A., Numerical simulation of incompressible flow within simple boundaries: Accuracy, *J. Fluid Mech.*, *49*, part 1, 75–112, 1971*b*.

Orszag, S. A., Comparison of pseudospectral and spectral approximation, *Stud. Appl. Math.*, *51*, 253–259, 1972.

Orszag, S. A., and L. W. Jayne, Local errors of difference approximations to hyperbolic equations, *J. Comput. Phys.*, *14*, 93–103, 1974.

Paolucci, S., and D. R. Chenoweth, Stability of the explicit finite differenced transport equation, *J. Comput. Phys.*, *47*, 489–496, 1982.

Pedersen, L. B., and L. P. Prahm, A method for numerical solution of the advection equation, *Tellus*, *26*, 594–602, 1974.

Pepper, D. W., and A. J. Baker, A high order accurate numerical algorithm for three-dimensional transport prediction, *Comput. Fluids*, *8*, 371–390, 1980.

Pepper, D. W., and R. E. Cooper, Preliminary analysis of four numerical models for calculating the mesoscale transport of Kr-85, *Atmos. Environ.*, *17*, 1881–1895, 1983.

Pepper, D. W., and P. E. Long, A comparison of results using second-order moments with and without width correction to solve the advection equation, *J. Appl. Meteorol.*, *17*, 228–233, 1978.

Pepper, D. W., C. D. Kern, and P. E. Long, Jr., Modeling the dispersion of atmospheric pollution using cubic splines and chapeau functions, *Atmos. Environ.*, *13*, 223–237, 1979.

Peyret, R., and T. D. Taylor, *Computational Methods for Fluid Flow*, 358 pp., Springer-Verlag, New York, 1983.

Phillips, N. A., An example of nonlinear computational instability, in *The Atmosphere and Sea in Motion*, pp. 501–504, Rockefeller Institute Press, New York, 1959.

Piacsek, S. A., and G. P. Williams, Conservation properties of convection difference schemes, *J. Comput. Phys.*, *6*, 392–405, 1970.

Piva, R., A. Di Carlo, and G. Guj, Finite element MAC scheme in general curvilinear coordinates, *Comput. Fluids*, *8*, 225–241, 1980.

Plumb, R. A., and J. D. Mahlman, Transport characteristics of the GFDL general circulation/transport model, *J. Atmos. Sci.*, in press, 1987.

Prather, M. J., Numerical advection by conservation of second-order moments, *J. Geophys. Res.*, *91*, 6671–6681, 1986.

Pudykiewicz, J., and A. Staniforth, Some properties and comparative performance of the semi-Lagrangian method of Robert in the solution of the advection-diffusion equation, *Atmos. Ocean*, *22*, 283–308, 1984.

Richtmyer, R. D., *Principles of Advanced Mathematical Physics*, vol. 1, 422 pp., Springer-Verlag, New York, 1978.

Richtmyer, R. D., and K. W. Morton, *Difference Methods for Initial Value Problems*, 2nd ed., 405 pp., John Wiley, New York, 1967.

Ritchie, H., Eliminating the interpolation associated with the semi-Lagrangian scheme, *Mon. Weather Rev.*, *114*, 135–146, 1986.

Roache, P. J., *Computational Fluid Dynamics*, 446 pp., Hermosa, Albuquerque, N. M., 1976.

Robert, A., A stable numerical integration scheme for the primitive meteorlogical equations, *Atmos. Oceans*, *19*, 35–46, 1981.

Robert, A., A semi-Lagrangian and semi-implicit numerical integration scheme for the primitive meteorlogical equations, *J. Meteorol. Soc. Jpn.*, *60*, 319–325, 1982.

Robert, A., T. L. Yee, and H. Ritchie, A semi-Lagrangian and semi-implicit numerical integration scheme for multilevel atmospheric models, *Mon. Weather Rev.*, *113*, 388–394, 1985.

Roberts, K. V., and N. O. Weiss, Convective difference schemes, *Math. Comput.*, *20*, 272–299, 1966.

Roe, P. L., The use of the Riemann problem in finite difference schemes, *Lect. Notes Phys.*, *141*, 354–359, 1981.

Rubin, E. L., and S. Z. Burstein, Difference methods for the inviscid and viscous equations of a compressible gas, *J. Comput. Phys.*, *2*, 178–196, 1967.

Runca, E., P. Melli, and F. Sardei, An analysis of a finite difference and a Galerkin technique applied to the simulation of advection and diffusion of air pollutates from a line source, *J. Comput. Phys.*, *59*, 152–166, 1985.

Rusanov, V. V., On difference schemes of third order accuracy for nonlinear hyperbolic systems, *J. Comput. Phys.*, *5*, 507–516, 1970.

Russell, G. L., and J. A. Lerner, A new finite-differencing scheme for the tracer transport equation, *J. Appl. Meteorol.*, *20*, 1483–1498, 1981.

Schere, K. L., An evaluation of several numerical advection schemes, *Atmos. Environ.*, *17*, 1897–1907, 1983.

Schlesinger, R. E., Effects of upstream-biased third order space correction terms on multidimensional Crowley advection schemes, *Mon. Weather Rev.*, *113*, 1109–1130, 1985.

Schneider, H. R., A numerical transport scheme that avoids negative mixing ratios, *Mon. Weather Rev.*, *112*, 1206–1217, 1984.

Sklarew, R. C., A. J. Fabrick, and J. E. Prager, A particle-cell-method for numerical solution of the atmospheric diffusion equation, and applications to air pollution problems, vol. 1, *Rep. 3SR-844*, Syst. Sci. and Software, La Jolla, Calif., 1971.

Smolarkiewicz, P. K., The multidimensional Crowley advection scheme, *Mon. Weather Rev.*, *110*, 1968–1983, 1982.

Smolarkiewicz, P. K., A simple positive definite advection scheme with small implicit diffusion, *Mon. Weather Rev.*, *111*, 479–486, 1983.

Smolarkiewicz, P. K., A fully multidimensional positive definite advection transport algorithm with small implicit diffusion, *J. Comput. Phys.*, *54*, 325–362, 1984.

Smolarkiewicz, P. K., On the accuracy of the Crowley advection scheme, *Mon. Weather Rev.*, *113*, 1425–1429, 1985.

Sod, G. A., A survey of several finite difference methods for systems of nonlinear hyperbolic conservation laws, *J. Comput. Phys.*, *27*, 1–31, 1978.

Staniforth, A., and J. Pudykiewicz, Reply to comments and addenda to "Some properties and comparative performance of the semi-Lagrangian method of Robert in the solution of the advection-diffusion equation," *Atmos. Ocean*, *23*, 195–200, 1985.

Staniforth, A., and C. Temperton, Semi-implicit semi-Lagrangian integration schemes for a barotropic finite-element regional model, *Mon. Weather Rev.*, *114*, 2078–2090, 1986.

Stordal, F., I. S. A. Isaksen, and K. Horntveth, A diabatic circulation two-dimensional model with photochemistry: Simulations of ozone and long-lived tracers with surface sources, *J. Geophys. Res.*, *90*, 5757–5776, 1985.

Strang, G., On the construction and comparison of difference schemes, *SIAM J. Numer. Anal.*, *5*, 506–517, 1968.

Strobel, D. F., Parameterization of linear wave chemical transport in planetary atmospheres by eddy diffusion, *J. Geophys. Res.*, *86*, 9806–9810, 1981.

Takacs, L. L., A two-step scheme for the advection equation with minimized dissipation and dispersion errors *Mon. Weather Rev.*, *113*, 1050–1065, 1985.

Takacs, L. L., and R. C. Balgovind, High latitude filtering in global grid-point models, *Mon. Weather Rev.*, *111*, 2005–2015, 1983.

Taylor, C., and P. Hood, A numerical solution of the Navier-Stokes equations using the finite element technique, *Comput. Fluids*, *1*, 73–100, 1973.

Taylor, T. D., E. Ndefo, and B. S. Masson, A study of numerical solutions for solving viscous and invisid flow problems, *J. Comput. Phys.*, *9*, 99–119, 1972.

Tennekes, H., Turbulent flow in two and three dimensions, *Bull. Am. Meteorl. Soc.*, *59*, 22–28, 1978.

Thompson, J. F., Convection schemes for use with curvilinear coordinate systems—A survey, *Misc. Pap. E-84-4*, 262 pp., U. S. Army Corps of Eng., Dep. of the Army, Washington, D. C., 1984.

van Leer, B., Towards the ultimate conservative difference schemes, I. The quest of monotonicity, *Lect. Notes Phys.*, *18*, 164–168, 1973.

van Leer, B., Towards the ultimate conservative difference scheme, II. Monotonicity and conservation combined in a second-order scheme, *J. Comput. Phys.*, *14*, 361–370, 1974.

van Leer, B., Towards the ultimate conservative difference scheme, III, Upstream-centered finite-difference schemes for ideal incompressible flow, *J. Comput. Phys.*, *23*, 263–275, 1977*a*.

van Leer, B., Towards the ultimate conservative difference scheme, IV, A new approach to numerical convection, *J. Comput. Phys.*, *23*, 276–299, 1977*b*.

van Leer, B., Towards the ultimate conservative difference scheme, V, A second-order sequel to Godunov's method, *J. Comput. Phys.*, *32*, 101–136, 1979.

Welander, P., Studies on the general development of motion in a two-dimensional, ideal fluid, *Tellus*, *7*, 141–156, 1955.

Wengle, H., and J. H. Seinfeld, Pseudospectral solution of atmospheric diffusion problems, *J. Comput. Phys.*, *26*, 87–106, 1978.

Wengle, H., B. van den Bosch, and J. H. Seinfeld, Solution of atmospheric diffusion problems by pseudo-spectral and orthogonal collocation methods, *Atmos. Environ.*, *12*, 1021–1032, 1978.

Wesseling, P., On the construction of accurate difference schemes for hyperbolic partial differential equations, *J. Eng. Math.*, *7*, 19–31, 1973.

Woodward, P. R., and P. Colella, High resolution difference schemes for compressible gas dynamics, *Lect. Notes Phys.*, *141*, 434–441, 1981.

Woodward, P. R., and P. Colella, The numerical simulation of two-dimensional fluid flow with strong shocks, *J. Comput. Phys.*, *54*, 115–123, 1984.

Yanenko, N. N., *The Method of Fractional Steps*, p. 160, Springer-Verlag, New York, 1971.

Young, J. A., Comparative properties of some time differencing schemes for linear and nonlinear oscillations, *Mon. Weather Rev.*, *96*, 357–364, 1968.

Zalesak, S. T., Fully multidimensional flux-corrected transport algorithms for fluids, *J. Comput. Phys.*, *31*, 335–362, 1979.

Zalesak, S. T., High order "ZIP" differencing of convective terms, *J. Comput. Phys.*, *40*, 497–508, 1981*a*.

Zalesak, S. T., Very high order and pseudospectral flux-correct transport (FCT) algorithms for conservation laws, in *Advances in Computer Methods for Partial Differential Equations IV*, edited by R. Vichnevetsky and R. S. Steplman, International Association for Mathematics and Computers in Simulation, Rutgers University, New Brunswick, N. J., 1981*b*.

Zalesak, S. T., A physical interpretation of the Richtmyer two-step Lax-Wendroff scheme, and its generalization to higher spatial order, in *Advances in Computer Methods for Partial Differential Equations V*, edited by R. Vichnevetsky and R. S. Steplman, International Association for Mathematics and Computers in Simulation, Rutgers University, New Brunswick, N. J., 1984.

Zienkiewicz, O. C., and K. Morgan, *Finite Elements and Approximation*, 328 pp., John Wiley, New York, 1983.

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