Use of a flux-limited scheme for vertical advection in a GCM

By JOHN THUBURN

UK Universities Global Atmospheric Modelling Programme, Department of Meteorology, University of Reading, RG6 2AU

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SUMMARY

A general method of constructing one-dimensional total-variation diminishing advection schemes using flux limiters is presented. A simple scheme that uses the Van Leer limiter is demonstrated in some idealized tests. The scheme is compared with the more usual centred-difference scheme in a global circulation model where the schemes are used to calculate the vertical advection of tracers, moisture, temperature and momentum. In climatic simulations noise is generated by the centred-difference scheme in tracer and temperature profiles near the tropopause, and in the moisture profile near the tropical boundary-layer inversion; this is eliminated when the flux-limited scheme is used. The use of this improved scheme for vertical advection is a cheap and simple way to remove these errors from global circulation models.

1. INTRODUCTION

Over the last 15 years or so ‘spectral’ models have become standard tools for numerical weather prediction and climate study; at the time of writing 19 out of 29 models taking part in the Atmospheric Model Intercomparison Project (AMIP) (organized by the Working Group on Numerical Experimentation (WGNE) sponsored jointly by the World Climate Research Programme and the Commission for Atmospheric Sciences) use a spectral horizontal representation. The spectral transform technique (Orszag 1970; Bourke 1974; Hoskins and Simmons 1975) is formally very accurate, copes well near the poles and allows a straightforward implementation of a semi-implicit time step for resolved gravity waves (Robert et al. 1972). It is usually understood that the scheme used for vertical advection is based on second-order centred differences (e.g. Hoskins and Simmons 1975; Simmons and Burridge 1981).* Centred-difference schemes tend to produce spurious oscillations in the advected quantity upwind of sharp increases of gradient. Some examples are shown in section 5. These errors tend to have been tolerated, or cleaned up, for example by using strong vertical diffusion or by ‘filling’ negative moisture values.

Increasingly, climate models are being used for three-dimensional chemical modelling. Some of the errors associated with the traditional advection schemes, in particular the generation of negative mixing ratios, are a very great problem.

Many schemes have been developed that do not produce spurious oscillations in the advected field; these are variously called ‘monotonicity preserving’, ‘shape preserving’, ‘total variation non-increasing’ or ‘total variation diminishing’ (TVD) schemes. One way to achieve this desirable property is through the technique of ‘flux corrected transport’ (FCT), in which a transport/diffusive step is followed by an antidiffusive correction (Boris and Book 1973; Zalesak 1979). Another, conceptually similar, approach is to use a single step in which the fluxes are carefully constrained using a ‘flux limiter’ (Sweby 1985). (The term FCT is sometimes applied to both the two-step and single-step approaches.) Monotonicity-preserving schemes have been used in ‘offline’ chemical-transport models (e.g. Rood et al. 1991), and similar techniques have been used in smaller-scale dynamical models to obtain positive-definite schemes (Smolarkiewicz and

* Formally, the order of a scheme refers to an asymptotic limit as the grid spacing approaches zero. The scheme referred to is second order on a regularly spaced grid, but the order is ambiguous for an irregular grid unless further conditions are specified.
Clark 1986; Hsu and Arakawa 1990) and fully monotonicity-preserving schemes (Smolarkiewicz and Grabowski 1990). An FCT scheme has been used in an isopycnic ocean model, where it is crucial to avoid negative layer thicknesses (Bleck and Boudra 1986). However, these modern advection schemes have been slow to catch on in atmospheric general circulation models, though the Meteorological Office is considering implementing monotonicity-preserving schemes in their Unified Model (M. Cullen, personal communication).

This paper describes the effects of using a simple flux-limited scheme for vertical advection of tracers, moisture, temperature and momentum in the UK Universities Global Atmospheric Modelling Programme (UGAMP) global circulation model (GCM), which is based on the cycle 27 forecast model of the European Centre for Medium-range Weather Forecasts (ECMWF). In section 2 a general method for constructing TVD schemes using flux limiters is derived and one particular scheme is presented. Its potential advantages are demonstrated in some one-dimensional tests in section 3. GCM simulations using the flux-limited scheme and the centred-difference scheme are compared in sections 4 and 5 and particular aspects of climate simulations most strongly affected by the vertical-advection scheme are highlighted. The flux-limited scheme is shown to offer great improvements over the traditional centred-difference scheme, especially in the vertical distributions of tracers, moisture and temperature, at little extra computational cost.

2. THE NUMERICAL SCHEME

(a) The UGAMP GCM vertical coordinate and the vertical-advection problem

The dynamical component of the UGAMP GCM integrates the primitive equations of atmospheric motion written in terms of an arbitrary vertical coordinate, \( \eta \) (Kasahara 1974). The model levels may be \( \sigma \) levels (Phillips 1957), hybrid \( \sigma-p \) levels (Simmons and Burridge 1981) or hybrid \( \sigma-\theta-p \) levels (Zhu et al. 1992). In the vertical discretization of the UGAMP GCM, advected quantities are defined on model full levels (integer suffixes) while the vertical velocity is defined at the interfaces or ‘half levels’ (half odd integer suffixes). Vertical derivatives are generally expressed in terms of pressure, \( p \), since the model-level pressure and the level spacing, \( \Delta p_k = p_{k+1/2} - p_{k-1/2} \), are easily computed.

We require a numerical scheme to evaluate the term \( \tilde{\omega}(\partial q/\partial p) \) in the equation

\[
\frac{\partial q}{\partial t} + \tilde{\omega} \frac{\partial q}{\partial p} = \text{other terms}
\]  

(2.1)

where \( q \) is a tracer mixing ratio, specific humidity, horizontal velocity or temperature and \( \tilde{\omega} = \eta(\partial p/\partial \eta) \) is the vertical velocity relative to model levels. (A circumflex is used to distinguish \( \tilde{\omega} \) from \( \omega = Dp/Dt \).) Equation (2.1) is in ‘advective form’; the ‘flux form’ is discussed in section 2(f).

(b) Conservation requirement

The total mass of tracer, the potential energy and the angular momentum will be conserved by the vertical-advection scheme provided the finite-difference analogue of

\[
\int_{p_0}^{p^*} \tilde{\omega} \frac{\partial q}{\partial p} dp = -\int_{p_0}^{p^*} q \frac{\partial \tilde{\omega}}{\partial p} dp
\]  

(2.2)
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holds (Simmons and Burridge 1981) where \( p_s \) is the surface pressure. Furthermore, when the finite-difference analogue of

\[
\int_{0}^{p_s} \frac{\partial q}{\partial p} dp = - \int_{0}^{p_s} \frac{1}{2} f \frac{\partial \omega}{\partial p} dp
\]

holds, kinetic energy is conserved by the vertical advection. In the UGAMP GCM the form

\[
\frac{\partial \hat{\omega}}{\partial p} = \frac{1}{\Delta p_k} (\hat{\omega}_{k+1/2} - \hat{\omega}_{k-1/2})
\]

is used in the continuity equation.

(c) A simple TVD scheme

Consider an advection scheme in which the change in the advected quantity is given by the convergence of a flux over a time step,

\[
q_k^{n+1} = q_k^n - (F_{k+1/2} - F_{k-1/2}) \Delta t / \Delta p_k
\]

where the flux is related to some interfacial value of the advected quantity,

\[
F_{k+1/2} = \hat{\omega}_{k+1/2} \cdot q_{k+1/2}
\]

Different numerical schemes prescribe \( q_{k+1/2} \) in different ways in terms of the full-level values, \( q_{k-1}, q_k, q_{k+1}, \ldots \). In the appendix it is shown that when the interfacial value of \( q \) is given by a combination of the corresponding values from a first-order upwind scheme \( q_{k+1/2} = q_{k} \) for \( \hat{\omega} > 0 \) and some other, possibly higher order, scheme \( q_{k+1/2} = q_{k+1/2}^{(H)} \),

\[
q_{k+1/2} = q_k + \phi_+^{(H)} (q_{k+1/2}^{(H)} - q_k) \quad (\hat{\omega} > 0)
\]

the resulting scheme will have the TVD property provided the 'flux limiter', \( \phi^+ \), which may depend on the \( q \)’s, satisfies certain constraints.

It is possible to build a hierarchy of TVD schemes based on high-order schemes of varying complexity and by using more or less strict limiters. For example, such schemes have been tested based on a fourth-order centred-difference scheme and based on a Fourier method using Leonard’s (1988) ‘universal limiter’. From now on we restrict attention to one of the simplest possible TVD schemes where the higher-order scheme uses second-order centred differences,

\[
q_{k+1/2}^{(H)} = \frac{1}{2} (q_k + q_{k+1})
\]

and the limiter is that originally proposed by Van Leer (1974),

\[
\phi_+^{(H)} = \frac{r_k^+ + |r_k^+|}{1 + |r_k^+|}
\]

where \( r_k^+ = \Delta q_{k-1/2} / \Delta q_{k+1/2} \) and \( \Delta q_{k+1/2} = q_{k+1} - q_k \).

This scheme enables us to evaluate \( \frac{\partial (\hat{\omega} q)}{\partial p} \) while Eq. (2.1) requires us to evaluate \( \frac{\partial (\hat{\omega} q)}{\partial p} \), so we must write

\[
\left( \frac{\partial (\hat{\omega} q)}{\partial p} \right)_k = \left( \frac{\partial (\hat{\omega})}{\partial p} \right)_k \left( q \frac{\partial q}{\partial p} \right)_k.
\]
By evaluating
\[
\left( \frac{\partial \mathbf{\omega}}{\partial p} \right)_k = \frac{q_k}{\Delta p_k} (\mathbf{\omega}_k + 1/2 - \mathbf{\omega}_k - 1/2)
\]  
and
\[
\left( \frac{\partial (\mathbf{\omega} q)}{\partial p} \right)_k = \frac{1}{\Delta p_k} (\mathbf{\omega}_k + 1/2 \cdot q_k + 1/2 - \mathbf{\omega}_k - 1/2 \cdot q_k - 1/2)
\]
the finite-difference analogue of (2.2) holds trivially and so the scheme will conserve mass. However, it does not conserve kinetic energy; kinetic energy may increase or decrease, but will tend to be dissipated when there are features of small vertical scale in the horizontal velocity field.

(d) Limiters near boundaries

One column of a GCM can be considered to be a bounded domain of N levels with \( \mathbf{\omega}_1 = \mathbf{\omega}_{N+1/2} = 0 \). It would appear that when \( \mathbf{\omega}_{3/2} > 0 \) the limiter \( \phi^+ \) depends on non-existent data, \( q_0 \), and similarly for \( \phi^- \) when \( \mathbf{\omega}_{N-1/2} < 0 \). Alternative expressions for these limiters are obviously desirable. Simply imposing \( \phi^+ = 0 \) gives a scheme that is rather diffusive, tending to remove gradients near the boundary. \( \phi^- = 1 \), on the other hand, may allow negative mixing ratios to arise near the boundary (see section 4). A better solution is to use the Van Leer limiter, (2.9), using a fictitious value of \( q_0 \), chosen by linearly extrapolating from \( q_1 \) and \( q_2 \), provided the resulting \( q_0 \) has the same sign as \( q_1 \), otherwise \( q_0 \) is set to 0. This may be concisely written:
\[
\Delta q_{1/2} = \begin{cases} \text{MIN}(\Delta q_{3/2}, q_1) & q_1 \geq 0 \\ \text{MAX}(\Delta q_{3/2}, q_1) & q_1 < 0 \end{cases}
\]
with similar expressions for \( \Delta q_{N+1/2} \). The resulting scheme produces no negative mixing ratios near the boundaries, without being too diffusive there.

(e) Time stepping

The derivation in the appendix assumes that a first-order forward time step is used:
\[
q_k^{n+1} = q_k^n + \Delta t \left( \frac{\partial q}{\partial t} \right)_k^n.
\]

With a second-order centred time step (leap-frog),
\[
q_k^{n+1} = q_k^{n-1} + 2\Delta t \left( \frac{\partial q}{\partial t} \right)_k^n
\]
the scheme is no longer TVD and, in fact, is found to be unstable unless both a very short time step and substantial time filtering are used (M. MacVean, personal communication).

A second-order forward time step could be made if we could calculate the second time derivative:
\[
q_k^{n+1} = q_k^n + \left( \frac{\partial q}{\partial t} \right)_k^n \Delta t + \frac{1}{2} \Delta t^2 \left( \frac{\partial^2 q}{\partial t^2} \right)_k^n.
\]
The scheme actually proposed by Van Leer (1974) includes a Courant number dependent term in the antidiffusive flux, making the resulting scheme rather less sensitive to the
Courant number than the scheme described here, though formally it is still only first order in time. When processes other than one-dimensional advection contribute to the tendency of $q$, as they would in a GCM, it becomes non-trivial to build a scheme that is formally second-order accurate in time (see, e.g., Smolarkiewicz 1991). The scheme implemented in the UGAMP GCM uses a first-order forward time step.

Because the UGAMP GCM is designed to use a leap-frog step for the dynamical contributions care must be taken in implementing a forward step for the vertical-advection terms. By analogy with the calculation of the physical parametrization tendencies in the model, the $\partial(\omega q)/\partial p$ term in (2.10) is evaluated using $q$ at step $n - 1$. However, the $\omega^{n-1}$ field is not available so $\omega^n$ must be used. This does not affect the stability of the scheme nor the TVD property. The $q(\partial\omega/\partial p)$ term is evaluated at step $n$ for consistency with the horizontal-advection terms and the continuity equation to ensure mass conservation.

(f) **Flux form of the advection equation**

For tracers and moisture the advective form of the advection equation

$$\frac{\partial q}{\partial t} + \hat{\omega} \frac{\partial q}{\partial p} + v \cdot \nabla q = \text{other terms}$$

(2.17)

may be combined with the mass continuity equation to give the flux form of the advection equation:

$$\frac{\partial Q}{\partial t} + \frac{\partial (\eta Q)}{\partial \eta} + \nabla.(vQ) = \text{other terms}$$

(2.18)

where $Q = q(\partial p/\partial \eta)$. This form has the advantage in that it is generally easier to ensure conservation of the total mass of tracer when the flux form is used. In particular, many spectral models use a horizontal scale-selective dissipation of the form $\nabla^{2n}$, for some integer $n$, applied to the model’s prognostic variables. When $\nabla(\Delta p) \neq 0$, scale-selective dissipation applied to $Q$ conserves mass whereas scale-selective dissipation applied to $q$ does not.

The advection scheme described here may be applied to the flux form of the advection term by noting that $\eta Q = \hat{\omega} q$, so that the vertical-advection term may be evaluated as

$$\left(\frac{\partial (\eta Q)}{\partial \eta}\right)_k = \frac{\hat{\omega}_{k+1/2} \cdot q_{k+1/2} - \hat{\omega}_{k-1/2} \cdot q_{k-1/2}}{\nabla \eta_k}.$$  

(2.19)

When $q_{k+1/2}$ is defined by (2.8) we have the flux form of the second-order centered-difference scheme. The flux form of the flux-limited scheme is obtained by defining $q_{k+1/2}$ using (2.7), (2.8) and (2.9).

3. **ONE-DIMENSIONAL EXAMPLES**

The different behaviour of the second-order centred-difference scheme and the flux-limited scheme described in section 2 can be seen most clearly in simple one-dimensional examples. A simple problem was considered in which a constant wind advects a variety of tracer distributions once around a periodic domain. The results of using the second-order centred-difference scheme are shown in Fig. 1. The sinusoidal tracer profile is treated well, but the sharper profiles are badly distorted and overshoots and undershoots occur.
Figure 1. Four test cases using a second-order centred-difference scheme. In each case an initial profile (indicated by the dashed curves) is advected, left to right, once around a periodic domain of 24 grid points by a constant wind. The Courant number is 0.1.

The corresponding tests using the flux-limited scheme are shown in Fig. 2. The overshoot and undershoot are completely eliminated, as demanded by the theory. The scheme is rather diffusive and at low Courant numbers there is some clipping of extrema, though it is far less diffusive than a first-order upwind scheme (not shown). Note, this diffusive quality is a property of the particular simple scheme studied here and is not necessarily a property of TVD schemes in general. For larger Courant numbers the scheme becomes less diffusive and tends to steepen gradients, though it still retains the TVD property up to $n_c = 0.5$ (including Courant number dependent terms in the antidiffusive flux to give Van Leer’s (1974) scheme reduces this sensitivity). In practice the vertical advection in a GCM probably operates mainly in the low Courant-number range.

To estimate the importance of this diffusive aspect of the scheme in a GCM, note that one revolution in these one-dimensional tests corresponds to something like 6 months of descent across the high-latitude tropopause or in the subtropical troposphere. These are regions of persistent descent in the presence of sharp changes of gradient of tem-
temperature and moisture. However, in regions of tropical convection or in mid-latitude baroclinic waves, vertical velocities resolved by the model can be much greater.

In a GCM there is often a balance between vertical advection and other processes so that the advection acts on a more or less fixed profile of the advected quantity (for example temperature or tracer near the tropopause, moisture near the boundary-layer inversion). To see the effect of different advection schemes it is instructive to run the test cases for one time step. Figure 3 shows the results of using second-order centred-differences and the flux-limited scheme to advect a test profile for one step. The flux-limited scheme preserves the profile well, but the beginning of the distortion process upwind of sharp changes of gradient is clearly visible in the centred-difference case. In a GCM using the centred-difference scheme, undershoot of the temperature and moisture profiles near the boundary-layer inversion spuriously tends to strengthen the inversion.

The flux-limited scheme performs equally well at a variety of resolutions and Courant numbers and also on irregular grids. The scheme has also been tested on a bounded domain, \((p_L, p_R)\), with the non-constant wind profile:
Figure 3. Two test cases using (a) a second-order centred-difference scheme and (b) the flux-limited scheme of section 2. One of the initial profiles from Fig. 1 is advected, left to right, for one time step. The domain is periodic with 24 grid points and the Courant number is 0.2. The dashed curves show solutions calculated by interpolating the tracer mixing ratio from each parcel's initial location—our best estimate of the ‘true’ solution. (In (b) the dashed curve is obscured by the solid curve.)

\[
\hat{\omega}(p) = 4\hat{\omega}_0 \frac{(p_R - p)(p - p_L)}{(p_R - p_L)^2}
\]  

(3.1)

for which an analytic solution can be found. Among other things this enables the effect of different limiters near the boundaries (section 2(d)) to be investigated.

4. Effect on Tracers in a GCM

A pair of climate simulations were performed using the UGAMP GCM at T21 horizontal resolution with 24 levels in the vertical. The hybrid isentropic vertical-coordinate scheme of Zhu et al. (1992) was used. The model was integrated for one annual cycle. Ten passive tracers were included in each integration. Nine of these tracers were released as blobs at a variety of altitudes and latitudes in the northern hemisphere. The tenth tracer was initialized to be zero in the troposphere, with a constant mixing ratio in the stratosphere and a transition region around the tropopause with mixing ratio a function of potential temperature. The tracers were transported only by the model’s resolved winds; there was no representation of transport by unresolved processes such as convection. The first experiment (experiment 1CD) used the second-order centred-difference scheme for vertical advection of tracers and the advective form of the advection equation. The second experiment (experiment 1TVD) used the flux-limited scheme for vertical advection of tracers and the flux form of the advection equation, with horizontal scale-selective dissipation applied to density-weighted tracers, to improve global tracer conservation. Some simple experiments showed that the effects of changing from a centred-difference scheme to a flux-limited scheme for vertical advection are quite distinct from the effects of changing from the advective form to the flux form, so here we will concentrate mainly on the former.

The tracers rapidly disperse in longitude over a time-scale of a few days. Their evolution in the meridional plane is more gradual. Figure 4 shows the zonal mean mixing ratio after 360 days of a tracer that was released near the ground close to the North Pole
Figure 4. Zonal mean mixing ratio after 360 days of a tracer initialized as a blob at low levels over the North Pole in experiment 1CD. (The units are arbitrary.)

in experiment 1CD. The tracer has spread into the tropics, mainly at low levels, and from there it has been carried aloft by the tropical ascent and has spread into both hemispheres, mainly in the upper troposphere. By day 360 the tracer has been distributed throughout both hemispheres in the troposphere. However, little tracer has reached the stratosphere and a sharp gradient has arisen across the tropopause.

Above the tropopause in the northern hemisphere the vertical profile of tracer shows grid-scale oscillations, including negative values. These are a characteristic product of the centred-difference vertical-advection scheme in a region of descent, upwind of a sharp increase of gradient.

Figure 5 shows the zonal mean mixing ratio after 270 days of a tracer released over the North Pole in the lower stratosphere. The tracer has spread over a large part of the

Figure 5. As in Fig. 4 but after 270 days of a tracer initialized as a blob in the lower stratosphere over the North Pole.
northern lower stratosphere, though little has crossed the equator. Also, a significant proportion of the total mass of the tracer has entered the troposphere. Again there are spurious oscillations in the tracer profile in the stratosphere, especially over the North Pole and near the equator. Of 40 zonal mean tracer distributions examined from various stages of this integration, more than one third showed spurious grid-scale oscillations in the vertical.

The profiles from experiment 1TVD corresponding to Figs. 4 and 5 are shown in Figs. 6 and 7. The overall evolution of the tracer fields is rather similar in the two experiments, but the profiles are considerably less noisy in the second experiment. In particular, the spurious grid-scale oscillations do not occur. In Fig. 7 a region of negative tracer mixing ratio has appeared over the North Pole near the top boundary. This is because the simple limiter $\phi^+ = 1$ was used in this experiment (see section 2(d)).

Figure 6. As in Fig. 4 but for the corresponding tracer in experiment 1TVD.

Figure 7. As in Fig. 5 but for the corresponding tracer in experiment 1TVD.
prompted the search that led to the improved limiter given by (2.13). The negative tracer mixing ratios over both poles in Fig. 6 and over the South Pole in Fig. 7 are associated with the spectral horizontal representation.

Counting contours in Fig. 4 and Fig. 6 reveals that the mixing ratio of this tracer is greater at lower levels in the northern hemisphere in the second experiment than in the first. This is because of the improved tracer conservation obtained by applying horizontal scale-selective dissipation to density-weighted tracer rather than tracer mixing ratio. Approximately 15% of the total mass of tracer was lost in the first experiment whereas in the second it was conserved very accurately.

Similar improvements occur when the centred-difference scheme is replaced by the flux-limited scheme in simulations of the distribution of methyl chloroform (CH₃CCl₃) including surface sources and chemical sinks (P. Brown, personal communication).

An important property of the advection term in the continuous equations is that it is linear in the transported quantity. Plumb and McConlogue (1988) show that, for a linear-transport operator, a single species with idealized chemistry will reach a ‘gradient equilibrium’, independent of the absolute strength of its sources, provided the ‘dynamic lifetime’ (defined as the total atmospheric loading divided by the total global source) is large. The centred-difference scheme for advection is linear in the advected quantity, but flux-limited schemes and FCT schemes are generally nonlinear. There is some concern over whether this will lead to systematic errors in long chemistry simulations. The scheme described in section 2, although not linear, has the properties

\[ \mathcal{F}(\alpha q) = \alpha \mathcal{F}(q) \quad \text{for any scalar } \alpha \]  
\[ \nabla q = 0 \Rightarrow \mathcal{F}(q) = 0 \]  

where \( \mathcal{F}(q) \) is the advection operator calculated by the numerical scheme, and, in fact, these properties are sufficient to derive Plumb and McConlogue’s result.

However, this result applies only to a single species. The flux-limited scheme does not satisfy

\[ \mathcal{F}(q_1 + q_2) = \mathcal{F}(q_1) + \mathcal{F}(q_2) \]  

where \( q_1 \) and \( q_2 \) may be the mixing ratios of two different species, and it is conceivable that for several reacting species important correlations may be disrupted by using a nonlinear flux-limited scheme for transport. In simulations of stratospheric ozone, Allen et al. (1991) found that the filling of negative values that is necessary with a spectral advection scheme greatly disrupted correlations between species whereas the nonlinear Van Leer scheme preserved correlations well. Thus, although there may be theoretical qualms concerning the nonlinearity of flux-limited schemes, empirical evidence to date suggests they are a great improvement over linear, non-monotone schemes.

5. Effect on dynamical fields in a GCM

The flux-limited scheme of section 2 has also been used for vertical advection of momentum, temperature and moisture in a GCM. In some initial tests, an adiabatic baroclinic-instability life-cycle simulation (e.g. Hoskins and Simmons 1975) was carried out at T42 horizontal resolution with 15 sigma levels in the vertical. One integration (experiment 2CD) used the original centred-difference scheme for vertical advection of momentum and temperature, the other (experiment 2TVD) used the flux-limited scheme. The zonal mean zonal wind and temperature at day 12, when the life cycle is essentially completed, are almost identical in the two experiments, as are the time-averaged zonal
mean eddy-heat and momentum fluxes. A more sensitive diagnostic is the Rossby–Ertel potential vorticity (PV) viewed on various isentropic surfaces. PV maps from the two experiments are very similar, but close inspection shows that extreme values tend to be slightly reduced in experiment 2TVD. Twice spurious intensification of PV maxima, by about 10% in 24 hours (a sign of imperfect material conservation of PV), was reduced in experiment 2TVD. However, in a preliminary experiment using a higher-order flux-limited scheme, the spurious intensification of the PV maxima is very similar to that in experiment 2CD, suggesting that there may be some fortuitous compensation in experiment 2TVD between dispersion errors in the horizontal advection and the diffusive vertical advection.

A pair of climate simulations were performed using the UGAMP GCM at T42 19 level resolution. They included parametrizations of radiation (Morcrette 1990), convection (a Kuo-type scheme), condensation, vertical mixing, gravity-wave drag and surface processes. The model was integrated for 120 days with ‘perpetual January’ deep-soil and sea-surface boundary conditions and solar forcing. The first experiment (experiment 3CD) used the second-order centred-difference scheme for vertical advection of momentum, temperature and moisture, while the second experiment (experiment 3TVD) used the flux-limited scheme.

The change of vertical-advection scheme had a large effect on the temperature profile above the tropopause, especially at high latitudes. Figure 8 shows the zonal mean temperature averaged over the last 60 days of experiment 3TVD and also the difference between this field and the corresponding field from experiment 3CD. There are strong grid-scale oscillations in the temperature field when the centred-difference scheme is used, similar in nature to the oscillations seen in the tracer experiment described in section 4. Radiative processes would be expected to remove features in the temperature profile that had a small vertical scale. However, the particular numerical implementation of the radiation scheme used in these experiments is unable to damp grid-scale temperature fluctuations. (A modification to the radiation scheme enabling it to damp grid-scale features in the temperature profile has recently been implemented (D. Li, personal communication).)

The moisture distribution is also affected by using a different vertical-advection scheme. The changes are most clearly visible when relative humidity is examined. Figure 9 shows the zonal mean relative humidity averaged over the last 60 days of the two experiments. The relative humidity in experiment 3TVD is rather less noisy than in experiment 3CD. Experiment 3CD shows a double minimum in relative humidity above the tropical boundary-layer inversion in each hemisphere at about 500 hPa and 650 hPa, possibly a spurious product of the centred-difference scheme, whereas experiment 3TVD has a single minimum in each hemisphere. In experiment 3TVD the moisture gradient at the tropopause is rather less sharp than in experiment 3CD at all latitudes, and also the relative humidity in the upper tropical troposphere is larger. Perhaps these features reflect the more diffusive nature of the flux-limited scheme in regions where, although the absolute humidity is small, there are relatively sharp changes in its gradient.

The UGAMP GCM includes a scheme to detect regions of negative humidity and to correct these by ‘borrowing’ moisture from lower levels in the same column. The moisture tendency due to this scheme is one indicator of how badly the advection schemes are performing. Figure 10 shows the accumulated tendencies due to correction of negative moisture values, zonally averaged over sea points, in experiment 3CD. The centred-difference scheme generates negative values above the tropical boundary-layer inversion, typically at an average rate of up to 0.1 g kg\(^{-1}\) d\(^{-1}\), which are filled by taking moisture from lower levels. The tendencies due to this filling scheme are almost invisible in
Figure 8. (a) Zonal mean temperature averaged over days 60 to 120 of experiment 3TVD. The contour interval is 5 degC and the zero contour is dotted. (b) Zonal mean temperature in experiment 3CD minus the zonal mean temperature in experiment 3TVD, averaged over days 60 to 120. The contour interval is 2 degC, the zero contour is dotted and negative contours are dashed.

experiment 3TVD when the same contour interval is used. Similar, but less extensive, errors occur over land points in experiment 3CD. However, in both experiment 3CD and 3TVD the largest tendencies over land due to filling of negatives (about 0.13 g kg\(^{-1}\) d\(^{-1}\)) occur near the ground at the edge of Antarctica. Presumably these negative moisture values are due to limitations of the spectral horizontal representation.

The effects of applying the flux-limited scheme to vertical advection of momentum are more difficult to assess. The zonal mean zonal velocities in the two experiments are very similar. There are differences of perhaps 10% between the two experiments in second-order diagnostics such as zonal mean eddy-heat and momentum fluxes averaged over the last 60 days of the experiments, but these are well within the natural variability of the simulated climate.
Despite the slightly dissipative nature of the flux-limited scheme, which does not conserve kinetic energy, the baroclinic instability experiments 2CD and 2TVD have almost identical global average kinetic energies. Similarly, there is no clear evidence for a systematic change in the average kinetic energy between experiments 3CD and 3TVD.

Integrations 3CD and 3TVD presented here include a parametrization of vertical mixing, which is represented as a vertical diffusion with a diffusion coefficient which depends on the local Richardson number, the vertical shear and a height-dependent mixing length. It is now believed that the diffusivities used in the model's free atmosphere are generally far stronger than can be justified by observations. The ECMWF now use much reduced values (by a factor of about 10) in their operational forecast model. The original strong vertical diffusion may have helped to remove noise generated by the centred-difference vertical-advection scheme. Climate simulations similar to experiments
3CD and 3TVD, in which the vertical diffusion is removed above about 600 hPa, do show a systematic reduction in global average kinetic energy of the order of 5% when the flux-limited scheme is used rather than the centred-difference scheme (M. Blackburn, J. Slingo, personal communication), though it is not clear whether useful information is being lost or whether noise is being reduced. The sensitivity of simulated tropospheric eddies and jet structure to different vertical-advection schemes, vertical diffusion and horizontal scale-selective dissipation is the subject of ongoing research.

6. DISCUSSION AND CONCLUSIONS

In this paper a derivation of a flux-limited advection scheme has been presented and its superiority over a second-order centred-difference scheme has been demonstrated in some one-dimensional tests. This simple flux-limited scheme is a little diffusive, though more sophisticated, less diffusive, schemes are possible.

In the context of a GCM, the use of the centred-difference scheme for vertical advection gives characteristic overshoot and undershoot errors where there are sharp changes of vertical gradient of an advected quantity, for example, in tracers near the tropopause, in temperature around the tropopause, and in moisture near the boundary-layer inversion. Using the flux-limited scheme for vertical advection eliminates these errors. The more diffusive nature of the flux-limited scheme is apparent in reduced vertical moisture gradients at the tropopause and the boundary-layer inversion and, in some integrations, in reduced global average kinetic energy.

When there are no sharp changes in vertical gradient of advected quantities, for example, in adiabatic baroclinic-instability life-cycle simulations, there is little difference between integrations using the centred-difference scheme and the flux-limited scheme.

The implementation of the flux-limited scheme for vertical advection as an option in the UGAMP GCM was straightforward. Also, the scheme is not particularly expensive. Using the flux-limited scheme rather than the centred-difference scheme on ten tracer fields in the experiment described in section 4 increased the computational cost of the
integration by approximately 2%. Therefore, this is a relatively cheap and effective way to improve this GCM, and possibly other similar GCMs, giving large benefits with no major drawbacks.

However, there are also errors associated with using the standard spectral-transform technique for horizontal advection; for example, in the moisture field at high latitudes near the surface, and in distributions of chemical species with sharp horizontal gradients, such as NO₂, near the terminator in the stratosphere (the ‘Noxon cliff’) (D. J. Lary, personal communication). These errors are partly due to calculating diabatic or chemical sources and sinks on the ‘quadratic’ transform grid, giving rise to features that the spectral representation cannot resolve, and hence to Gibbs phenomena. Improving the vertical-advection scheme can do nothing to alleviate these errors; alternative schemes for horizontal advection are needed. For example, monotonicity-preserving schemes have been used in ‘offline’ tracer-transport models (Rood et al. 1991), and semi-Lagrangian schemes with shape-preserving interpolation have been used in GCMs (Rasch and Williamson 1990, also the ECMWF operational forecast model since 1991). As mentioned in section 2(c), a one-dimensional flux-limited scheme based on a Fourier method has been successfully tested. It may be possible to extend this to a fully two-dimensional spectral-based scheme in spherical geometry, though there are several outstanding technical difficulties.

In the immediate future a more accurate flux-limited scheme for vertical advection, based on a fourth-order scheme, will be tested in the UGAMP GCM, to investigate whether reducing the diffusive character of the flux-limited scheme may lead to further improvements in climate and tracer-transport simulations.

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APPENDIX

The FCT schemes of Boris and Book (1973) and Zalesak (1979) use a two-step approach in which a transport/diffusive step is followed by an ‘antidiffusive’ correction. Here we follow more closely, and extend, the approach of Sweby (1985) in which a flux limiter is used to obtain a single-step scheme satisfying the TVD property.

The ‘total variation’ of a function, \( q \), on a set of grid points, \( k \), at time step \( n \) is defined to be

\[
TV(q^n) = \sum_k |\Delta q^n_{k+1/2}|
\]

where \( \Delta q^n_{k+1/2} = q^{n+1}_k - q^n_k \). A scheme is total variation diminishing (TVD), or, more precisely, total variation non-increasing (Harten 1983), if

\[
TV(q^{n+1}) \leq TV(q^n).
\]

Consider a general scheme written in the form

\[
q^{n+1}_k = q^n_k - C_{k-1/2} \cdot \Delta q^n_{k-1/2} + D_{k+1/2} \cdot \Delta q^n_{k+1/2}
\]

where the \( C \)'s and \( D \)'s may depend on the \( q \)'s. The domain may be periodic with
\( q_0 = q_N \), or may be bounded, in which case assume \( q_k = q_1 \) for \( k < 1 \) and \( q_k = q_N \) for \( k > N \). A little algebra (Harten 1983) establishes that the conditions
\[
0 \leq C_{k+1/2}, \quad 0 \leq D_{k+1/2}, \quad C_{k+1/2} + D_{k+1/2} \leq 1 \tag{A.4}
\]
are sufficient to ensure that the scheme (A.3) is TVD.

Now consider a scheme defined by writing the change of the advected quantity as the convergence of a flux:
\[
q_k^{n+1} = q_k^n - (F_{k+1/2} - F_{k-1/2}) \Delta t / \Delta p_k. \tag{A.5}
\]
Comparing this with (A.3) for the case \( D = 0 \), a sufficient condition for the scheme to be TVD is
\[
0 \leq \frac{(F_{k+1/2} - F_{k-1/2})}{\Delta q_{k-1/2}} \frac{\Delta t}{\Delta p_k} \leq 1. \tag{A.6}
\]
The interfacial values of \( q \) corresponding to these fluxes satisfy
\[
F_{k+1/2} = \hat{\omega}_{k+1/2} \cdot q_{k+1/2}. \tag{A.7}
\]
Conditions on \( q_{k+1/2} \) for a scheme to be TVD in the case of \( \hat{\omega} > 0 \) and constant are derived below. The case of \( \hat{\omega} < 0 \) follows in an analogous manner. It is then hoped that any good behaviour of such a scheme carries over to the case of non-constant \( \hat{\omega} \).

In terms of the Courant number, \( n_c = \hat{\omega} \Delta t / \Delta p_k \), the conditions (A.6) become
\[
0 \leq \frac{\Delta q_k}{\Delta q_{k-1/2}} \leq \frac{1}{n_c}. \tag{A.8}
\]
The problem is how to choose the interfacial values, \( q_{k+1/2} \), to give an accurate scheme, subject to these conditions. A scheme may be constructed in which the fluxes are given by a linear combination of fluxes from a first-order upwind or ‘donor cell’ scheme (superscript (L)) and fluxes from another, high order, scheme (superscript (H)).
\[
F_{k+1/2} = F_{k+1/2}^{(L)} + \phi_k (F_{k+1/2}^{(H)} - F_{k+1/2}^{(L)}). \tag{A.9}
\]
(Superscript ‘+’ indicates \( \hat{\omega} > 0 \).) In the first-order upwind scheme the fluxes are given by
\[
F_{k+1/2}^{(L)} = \hat{\omega}_{k+1/2} \cdot q_k \tag{A.10}
\]
when \( \hat{\omega} > 0 \). Incidentally, the first-order upwind scheme automatically satisfies the TVD property, so we are guaranteed to be able to build a TVD scheme by setting \( \phi = 0 \). However, it is very diffusive. For this reason the term in parentheses in (A.9) is sometimes called the ‘antidiffusive flux’, and when multiplied by \( \phi \) may be called the ‘limited antidiffusive flux’. \( \phi \) is called the ‘flux limiter’. If \( \phi_k^+ = 1 \) in (A.9) the scheme reduces to the basic high-order scheme, while if \( \phi_k^+ = 0 \) the scheme becomes a first-order upwind scheme. In general \( \phi_k^+ \) may take different values depending on the values of the field being advected. Removing a factor \( \hat{\omega}_{k+1/2} \) from (A.9) gives
\[
q_{k+1/2} = q_k + \phi_k (q_{k+1/2}^{(H)} - q_k) \tag{A.11}
\]
* \( q_k \) could be incremented using the advective form of the discrete advection equation, \( q_k^{n+1} = q_k^n + \hat{\omega}_k (q_{k+1/2}^n - q_{k-1/2}^n) \Delta t / \Delta p_k \), if a suitable full level \( \hat{\omega} \) were defined. This scheme would be TVD even for non-constant \( \hat{\omega} \), but it would not, in general, conserve mass. Instead we use the flux form, (A.5), with a correction to retrieve the advective form if required, (2.10)–(2.12), which does conserve mass. The flux form of the scheme on its own is not, and should not be, TVD, since, for example, a tracer may accumulate in a convergent flow.
so that
\[ \Delta q_k = \Delta q_{k-1/2} + \phi^+_k (q_{k+1/2}^{\text{H}} - q_k) - \phi^+_{k-1} (q_{k-1/2}^{\text{H}} - q_{k-1}). \]  
(A.12)

Substituting this in (A.8) gives the sufficient condition for the scheme to be TVD:
\[ 0 \leq 1 + \phi^+_k s^+_k / r^+_k - \phi^+_{k-1} s^+_{k-1} \leq 1/n_c \]  
(A.13)

where
\[ s^+_k = (q_{k+1/2}^{\text{H}} - q_k)/\Delta q_{k+1/2} \]  
(A.14)
\[ r^+_k = \Delta q_{k-1/2}/\Delta q_{k+1/2}. \]  
(A.15)

We may allow \( \phi^+_k \) to depend on \( r^+_k \) and \( s^+_k \), so that \( \phi^+_k = \phi^+(s^+_k, r^+_k) \). Equation (A.13) will certainly be satisfied if
\[ 0 \leq \phi^+(s, r)s/r \leq 1/n_c - 1 \]  
(A.16)
\[ 0 \leq \phi^+(s, r)s \leq 1 \]  
(A.17)

for all \( r \) and \( s \). Condition (A.16) limits the antidiffusive flux at the outflow side of the grid cell while condition (A.17) limits the antidiffusive flux at the inflow side of the grid cell. Within these constraints we are free to choose the \( \phi \)’s to give the resulting scheme other desirable properties.

A scheme will be subject to a minimal amount of flux limiting when \( \phi \) is chosen to be as close as possible to unity, subject to the constraints (A.16) and (A.17). It can be shown that a limiter chosen in this fashion is equivalent to the ‘universal limiter’ of Leonard (1988).

The TVD property, (A.2), is a single global constraint on a scheme whereas (A.16) and (A.17) constitute a set of constraints at each grid box. In fact (A.16) and (A.17) imply no: only the global TVD property but also that, locally, extrema cannot grow and no new extrema can appear, so that the solution is free from spurious oscillations. This may be verified using the ‘normalized variable’ approach of Leonard (1988).

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