An isentropic two-dimensional model with an interactive parametrization of dynamical and chemical planetary-wave fluxes

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SUMMARY

An interactive chemical–dynamical isentropic two-dimensional model is described, and its behaviour analysed when a parametrization of the three longest Rossby waves is included in the model. Eddy fluxes of chemicals and of Ertel's potential vorticity are all calculated from the modelled waves, and are therefore consistent with each other. The chemical fluxes arise from dissipation of zonal asymmetries, both by photo-chemistry ('chemical eddy fluxes') and by 'planetary wave breaking'. The chemical eddy fluxes for ozone and NO, are much larger than the wave-breaking ones, and thus the diffusion matrix (which has only one non-zero element) is far from being independent of chemical species. The waves have a large immediate effect on the ozone distribution, but the effect persists throughout the year only when the wave fluxes induce a persistent change in the photochemical equilibrium state for ozone (mainly by changing NO,).

1. INTRODUCTION

When two-dimensional (2D) (zonally averaged) models first appeared, they were formulated in isobaric coordinates and used an Eulerian-mean (EM) circulation (e.g. Rao 1973; Harwood and Pyle 1975). Investigations into the Lagrangian motion of air parcels revealed shortcomings in using the EM circulation, and potential advantages in the transformed EM (TEM) circulation (see, for example, Andrews and McIntyre 1976; Matsuno 1980). In the TEM circulation the part of the EM circulation that arises from, and whose effect is cancelled by, the eddy heat fluxes due to adiabatic, small, steady, quasi-geostrophic planetary waves is removed. It is thus a clearer indication of net transport. Eddy fluxes (whose parametrization constitutes one of the major problems facing 2D models) should be smaller when the TEM formalism is used, and should also have a more diffusive nature (as opposed to the advective nature of fluxes due to steady, small, adiabatic waves). This clearer separation between advection and diffusion can simplify interpretation of model results and real data. The separation becomes even clearer in isentropic coordinates, where adiabatic planetary waves (even if large and non-steady) can result in transport only along isentropic surfaces.

The work of Tung (1982, 1986) and Andrews (1983) has revealed further advantages of isentropic coordinates over the TEM formalism, mainly due to the fact that the vertical velocity across isentropic surfaces is proportional to the diabatic heating. Tung (1986) showed that the eddy forcing of the zonal-momentum equation by nonlinear, non-geostrophic waves is the sum of the horizontal eddy flux of Ertel's potential vorticity (PV) and the vertical eddy flux of zonal momentum. Use of isentropic coordinates can simplify the parametrization of the eddy fluxes due to adiabatic (or almost adiabatic) stratospheric planetary waves (Tung 1982). Vertical eddy fluxes are neglected, so three members of the diffusion tensor $K$ vanish leaving only $K_{yy}$. Observational support for neglecting the vertical eddy flux of ozone in comparison with the advective flux due to the mean vertical velocity was provided by Pawson and Harwood (1989).

$K_{yy}$ can be divided into two parts. One part is due to the breaking of planetary waves, which is independent of the quantity being diffused since it involves the physical dispersion of air parcels. The other part is the 'chemical eddy' $K_{yy}$ due to quasi-stationary

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waves, which is in general different for each quantity since it depends on the lifetime of zonal asymmetries of that quantity. In many studies it has been assumed that the same $K$ can be used for all chemical and dynamical quantities, mainly, it seems, for simplicity and because of a lack of a simple parametrization. Use of the same $K$ for all species involves the implicit assumption that either (1) parcel dispersion is the main source of $K$ or (2) the lifetime of zonal asymmetries is the same for all chemical and dynamical quantities. Pyle and Rogers (1980) and Smith et al. (1988) estimated chemical eddy $K_{yp}$ for ozone and NO$_x$ and found them to be large (about $30 \times 10^5$ms$^{-1}$) so that (1) cannot be valid, and since (2) is also in general not true, use of a single $K$ seems unjustifiable, as has been emphasized in several previous studies (e.g. Pyle and Rogers 1980).

Fairly strong criticism has been levelled at the use of a constant eddy diffusivity to represent the effect of homogeneous turbulence in cases where the scale of the mean variations is comparable with the scale of the turbulent regions. In particular, McIntyre (1990) noted that the eddy flux of PV is greatest in the ‘surf zone’ where the large-scale PV gradient is smallest, and seems to be inhibited by the strong ‘large-scale’ gradients on the edge of the vortex. Also, the rate of dissipation of a blob of tracer, which is scale-independent for homogeneous turbulence, is strongly scale-dependent if the eddy flux is proportional to the mean tracer gradient (as it is for eddy diffusion). His arguments do not appear to rule out, however, the practical effectiveness of a diffusion coefficient which varies over the model domain and depends on the mean state, and he concedes that this approach may yield benefits, the justification for which would be provided by their ability to represent the real atmospheric processes. One such example is given by the work of Garcia (1991) where a linearized wave equation is used, in conjunction with a 2D model, to parametrize the effect of breaking planetary waves in regions where the zonal-mean PV gradient is small. His results compare favourably with those from a nonlinear three-dimensional (3D) model. A similar approach is taken here, with a linearized wave parametrization being used to calculate a spatially varying $K_{yp}$ for each chemical species in a 2D model. One obstacle which would still have to be tackled is that of the ‘PV barrier’ across which there might be little parcel dispersion, since the undulating barrier, spanning a range of latitudes, would be blurred in a zonal-mean picture. It might, however, be simpler to treat if PV were used as the meridional coordinate instead of latitude.

It is worth noting here that if, for a certain quantity (which could be a gas or PV), chemical eddy fluxes are much larger than the fluxes due to breaking planetary waves then the above criticisms become less important for that quantity—within the approximations used in deriving a chemical eddy $K_{yp}$, the eddy flux is indeed down the mean gradient and is proportional to that gradient.

The purpose of this paper is to show how the dynamical, prognostic equations can be solved in a 2D isentropic model, and how a simple, interactive, parametrization of the eddy fluxes due to extra-tropical planetary waves can be incorporated in this model. It is not our intention, in this paper, to prove that a model using isentropic coordinates is significantly ‘better’ than an ‘equivalent’ TEM model—such a comparison would not be straightforward. Rather, we have used the advantages offered by isentropic coordinates to construct a model with a high degree of interaction, whose worth will be evaluated with further use. A number of previous 2D models have incorporated interactive parametrizations of either the wave forcing of the dynamical equations (e.g. Holton and Wehrbein 1980; Hitchman and Brasseur 1988; Garcia 1991) or of chemical eddy fluxes (e.g. Rogers and Pyle 1984; Garcia and Solomon 1983), but this model parametrizes both the wave forcing of the dynamics and the chemical eddy fluxes, so that the effect of waves on the chemistry is consistent with their effect on the dynamics. Although this
is similar in principle to the isobaric-coordinate model of Smith and Brasseur (1990), the use of isentropic coordinates allows the wave fluxes to be parametrized in a simpler (and hopefully more accurate) way than is possible in isobaric coordinates. The effect of these fluxes on the model’s chemistry and dynamics will be described and interpreted.

2. EQUATIONS AND NUMERICAL SCHEME

The model predicts the evolution of the zonal mean, taken along isentropic surfaces, of pressure and zonal wind using the following equations (which are either given by, or are easily derived from, those of Tung (1986)). A subscript denotes differentiation with respect to that variable, except for the diffusion coefficients \( K_{yy} \) and \( K_{zz} \), and an overbar denotes a zonal mean on an isentropic surface.

Continuity:

\[
\bar{\rho} \cos \phi + \bar{V} \phi + \bar{W} \phi = 0
\]  

(1)

where \( t \) is time, \( \rho = - \frac{p}{g} \) (the isentropic density), where \( g \) is the gravitational acceleration, \( p \) is pressure on an isentropic surface, and \( z = \ln(\theta/250) \)—though below the \( \theta = 350 \) K surface hybrid coordinates are used (see below), \( \theta \) is potential temperature, \( \phi \) is latitude and \( (\bar{V}, \bar{W}) = \cos \phi (\bar{v} \rho / a, \bar{w} \rho) \), where \( a \) is the radius of the earth, \( \bar{v} \) is northward velocity, \( w \) is the material rate of change of \( z \).

Momentum:

\[
\cos \phi (\bar{\rho} \tau) \phi + (\bar{V} \tau) \phi + (\bar{W} \tau) \phi = a \cos^2 \phi \bar{\rho} \bar{\tau}
\]  

(2)

where \( \tau = a \cos \phi (\bar{u} + a \Omega \cos \phi) \) is the specific zonally averaged angular momentum and \( \Omega \) is the earth’s rate of rotation, \( \Pi = (\zeta + f)/\rho \) is Ertel’s potential vorticity, \( f \) is the Coriolis parameter, \( \zeta \) is the relative vorticity and \( \bar{\tau} \) is given by

\[
\bar{\tau} = \bar{v}^* \rho \Pi - \frac{w^* \tau}{a \cos \phi}
\]  

(3)

where an asterisk denotes the deviation from the density-weighted zonal mean (i.e. \( v^* = v - \bar{v} \rho / \bar{\rho} \)).

Thermal wind:

\[
2 \tan \phi \bar{x} = -c_p \kappa \frac{\bar{p}}{p_0} \left( \frac{\bar{p}}{p} \right) a^2 \cos^2 \phi
\]  

(4)

where \( p_0 \) is 1000 mb and \( \kappa = R/c_p \), where \( R \) is the gas constant for air and \( c_p \) is the specific heat at constant pressure. \( \bar{W} \) is directly related to the diabatic heating rate, \( Q \), through the thermodynamic equation

\[
\bar{W} = \left( \frac{Q - w^* T^*}{Q + w^* T^*} \right) \rho + w^* T^*
\]  

(5)

where a prime denotes a departure from a zonal average and \( T \) is temperature. In the stratosphere the eddy terms are calculated from the planetary-wave parametrization (see section 3), but in the troposphere, which in the present version is only crudely treated, \( w^* T^* \) is parametrized using \( K_{zz} \), and \( w^* T^* \) is considered to be included in the specification of \( Q \) (see section 7).
These equations are solved in the following manner. Equation (1) is re-written as

\[(\overline{W} - \frac{\cos \phi}{g} \overline{p})_z + \overline{V}_\phi = 0\]

and a stream function \(\psi\) defined such that

\[\psi\phi = \overline{W} - \frac{\cos \phi}{g} \overline{p}, \quad \text{and} \quad \psi_z = -\overline{V}\]

so that (1) is automatically satisfied. In this way, for a given \(\overline{W}\) and \(\overline{F}\), the \(\psi\) (and hence \(\overline{V}\)) required to maintain thermal-wind balance between \(\overline{p}\) and \(\overline{u}\) at each time step can be found—expressions for \(\overline{p}_t\) and \(u_t\) are written in terms of \(\psi\), \(\overline{W}\) and \(\overline{F}\), and these expressions are used to eliminate \(\overline{p}_t\) and \(u_t\), from the time-derivative of (3), resulting in the 2nd order partial differential equation (PDE) for \(\psi\)

\[\psi_{zz} H - \psi_{\phi\phi} I + \psi_{z} H_z - \psi_{\phi} I + \overline{\tau} L_z + I(W + \overline{W}_\phi) = 0\]

where

\[H = \frac{\overline{\tau}_\phi}{\rho \cos \phi}\]
\[I = \frac{g \epsilon \alpha^2 \overline{\tau}_\phi \cos \phi}{2 \tan \phi \rho}\]
\[J = (\kappa - 1) \left(\frac{\overline{p}_\phi}{\overline{p}}\right) + \tan \phi\]
\[L = \frac{1}{\rho} (\alpha \cos^2 \phi \overline{p} \overline{F} - \overline{W} \overline{e}_z)\]

In order that a unique solution to this PDE exists, the PDE must be elliptic. This will be so provided that \(HI < 0\), or equivalently \(\overline{\tau}_\phi \overline{p}_z \phi > 0\). The finite-difference form of this PDE is solved by relaxation, and it turns out that this method converges to a solution provided that the above ellipticity condition is satisfied by the model fields (although strictly speaking the necessary condition for convergence is that the matrix multiplying the vector of discrete \(\psi\) values be diagonally dominant). If the ellipticity inequality comes close to being violated, heat or momentum fluxes are produced by the model to return it to a 'safe' state with a time constant of 2 days. Although this is a somewhat artificial feature it does have a physical basis, since regions where \(\overline{p}_z > 0\) in the real atmosphere are statically unstable. Similarly, \(\overline{\tau} < 0\) and \(\phi \overline{r}_\phi > 0\) indicate inertially unstable regions.

The \(\overline{\tau}\) and \(\overline{p}\) fields are updated using (1) and (2). Although \(\overline{V}\) is chosen to maintain thermal-wind balance, numerical errors in the calculation of \(\overline{V}\) can lead to a drift out of balance. Therefore, at the end of each time step, the horizontal gradient of \(\overline{p}\) is relaxed, with a one-day time constant, towards the value implied by the \(\overline{\tau}\) field. In previous versions of the model the \(\overline{\tau}\) field was updated using (2) at the equator and the ground only, thermal-wind balance being used to fill in the remaining values. Thus the effect of errors in \(\overline{V}\) accumulated at the poles, leading to large values of \(\overline{u}\) in the most poleward boxes. The present method alleviates this problem somewhat, but fairly large polar \(\overline{u}\) values still occur in winter. Too coarse a horizontal resolution might also contribute to this defect.
In the four model layers which lie below the $\theta = 350$ K level (which is near the tropopause) hybrid coordinates similar to those of Tung and Yang (1988) are used to avoid intersection of coordinate layers with the ground, with

$$z = \ln\left(\frac{350}{250}\right) \ln\left(\frac{\theta}{\theta_e}\right)$$

where $\theta_e$ is the surface potential temperature for $\theta < 350$ K and is a constant 250 K above that level. The relevant re-definitions of $\bar{W}$ and the thermal-wind equation are given in their paper. The time-derivative of the thermal-wind equation is straightforward to derive, account being taken of the rate of change of $\theta_e$. In an attempt to retain wholly isentropic coordinates, a model version incorporating the idea of Lorenz (1955) on using ‘underground isentropes’ was experimented with. In the bottom few model layers, whose isentropic surfaces intersected the ground, the low-latitude boxes were either fully or partially empty. Problems were encountered in maintaining thermal-wind balance where the surfaces intersected the ground, and since planetary waves are unlikely to be almost adiabatic in the troposphere, use of the above hybrid coordinates seemed preferable.

The numerical grid used has 19 boxes uniformly spaced from pole to pole, and has a variable vertical resolution that is adjusted at present to give boxes approximately 3.5 km high. $\tau$ and chemical mixing ratios are held at the centres of the boxes, $\bar{p}$ at the middle of their tops and bottoms, and $\psi$ at their corners. Winds and temperatures are modelled from the ground up to about 100 km, while the chemistry is only modelled up to about 60 km. A 4-hour Adams–Bashforth time step is used for both the chemistry and dynamics. Chemical species evolve according to the equation

$$\cos \phi(\bar{\rho}_z \hat{x}) + (\bar{V})_\phi + (\bar{W})_z = \cos \phi \bar{\rho} S + (\cos \phi \bar{\rho} K_{yy} \hat{x})_y + \cos \phi(\bar{\rho} K_{zz} \hat{x})_z$$  \(8\)

where a hat denotes a density-weighted zonal mean (i.e. $\hat{x} = \bar{x} / \bar{p}$), and $\chi$ denotes a mixing ratio for a species and $S$ the chemical source of that species.

If a negative mixing ratio occurs in a box all the advective fluxes out of that box are each reduced by the same fraction $\delta$ required to bring the mixing ratio up to zero. This is equivalent to splitting the 4-hour time step into two time steps, the first of duration (4 hours) $\times \delta$ during which the mixing ratio falls linearly to zero, and the second of duration (4 hours) $\times (1 - \delta)$ during which the mixing ratio is zero. Adjusting the fluxes in this way might make the mixing ratio in a neighbouring box negative, so the procedure is repeated until no box has a negative mixing ratio.

In the bottom box many of the families have their mixing ratios specified. For the model runs described in this paper, bottom boundary conditions corresponding to 1970 values were used; CH$_4$ was 1.42 p.p.m.v. (parts per million by volume) and total chlorine was 1.5 p.p.b.v. (per billion (10$^{-9}$)), and the models were spun-up over 7 years to allow the chemistry to stabilize, and to be independent of the initial conditions. CO$_2$ was specified as a constant 325 p.p.m.v. everywhere. At the top boundary (about 60 km), rather than setting the flux through the boundary to be locally zero (which leads to an unrealistic flux convergence or divergence near the top boundary for certain chemicals), the latitudinal integral of the flux is constrained to be zero. This allows a local flux through the boundary but constrains the net downward flux. Where $\bar{W}$ is negative, the downward flux is defined as $\bar{W}m$, where $m$ is effectively the mixing ratio above the top boundary, given by

$$m = \frac{\int \bar{W} \hat{x} d\phi}_{\text{upward}} - \frac{(\int \bar{W} d\phi)}_{\text{downward}}.$$
$K_{zz}$ is set to $7 \times 10^{-10}$ s$^{-1}$ in the troposphere (corresponding to about 5 m$^2$s$^{-1}$ in geometrical coordinates) and $10^{-10}$ s$^{-1}$ in the stratosphere (equivalent to about 0.07 m$^2$s$^{-1}$). The stratospheric value is much smaller than that used by Garcia and Solomon (1983) in their isobaric model (of 0.35 m$^2$s$^{-1}$), since in isentropic coordinates planetary waves should produce a smaller vertical flux than in isobaric coordinates, assuming that gravity waves are not breaking in the stratosphere and that planetary waves are almost adiabatic. The same $K_{zz}$ is used to parametrize the vertical-eddy-flux terms in (2) and (3). $K_{yy}$ is species-dependent being due to 'chemical eddies' and to breaking planetary waves (see next section).

3. Planetary-wave parametrization

Above the troposphere the $K_{yy}$ and $\Phi$ due to extra-tropical planetary-scale Rossby waves are parametrized in a way which allows a realistic wave mean-flow interaction. The method used is similar to that of Garcia (1991), with a linearized PV equation being used to predict the evolution of the eddy PV. The use of a linearized equation may be justified if the treatment of planetary-wave breaking (see below) represents fairly realistically the effect of large nonlinearities. The PV is inverted at each step to find the eddy winds, which are then used to calculate the change in eddy PV over the next time step. However, while Garcia worked in isobaric coordinates and calculated only the zonal wave-number-one component of quasi-geostrophic PV, we calculate the three gravest components of Ertel's PV (which is the most natural PV to use in isentropic coordinates). The equations used here, then, are

$$\left( \frac{\partial}{\partial t} + iuk \right) \Pi^{(n)} + v^{(n)} \tilde{\Pi}_y = -\left( \alpha + \beta^{(n)} \right) \Pi^{(n)}; \quad n = 1, 2, 3; \quad k = \frac{n}{a \cos \phi} \quad (9)$$

where $\Pi^{(n)}$ is the $n$th spectral component of Ertel's PV, and $\alpha$ is a damping coefficient representing mainly thermal damping in the stratosphere and frictional damping in the mesosphere.

The extent to which PV anomalies are dissipated, and not amplified, is an open question. However, it seems to be a fairly good assumption that thermal anomalies are predominantly dissipated in the stratosphere (see, for example, Pawson et al. 1992). Also, from consideration of thermal-wind balance in isentropic coordinates, if there is a local decrease (increase) in density, then the local relative vorticity increases (decreases), and the two effects each lead to a local increase (decrease) in PV. The eddy term $w^{(n)} \tilde{\Pi}_z$ therefore does not appear explicitly in (9) because it is assumed to be included implicitly in the thermal damping of PV. A similar consideration applies to friction—if gravity-wave drag, say, dissipates a relative-vorticity anomaly, then thermal-wind balance will require a change in density such that the PV anomaly is dissipated. The values used here for $\alpha$ are shown in Table (1), and are a rough fit to the thermal damping rates (including the 'photochemical acceleration') of Pawson et al. (1992) in the mid-latitude stratosphere.

<table>
<thead>
<tr>
<th>Height (km) approx.</th>
<th>Damping rate (days$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0–24.5</td>
<td>0.03</td>
</tr>
<tr>
<td>28</td>
<td>0.05</td>
</tr>
<tr>
<td>31.5</td>
<td>0.08</td>
</tr>
<tr>
<td>42</td>
<td>0.2</td>
</tr>
<tr>
<td>52.5</td>
<td>0.32</td>
</tr>
<tr>
<td>63</td>
<td>0.42</td>
</tr>
<tr>
<td>70</td>
<td>0.46</td>
</tr>
<tr>
<td>77–100</td>
<td>0.5</td>
</tr>
</tbody>
</table>

The $\beta^{(n)}$ are additional damping coefficients which are non-zero only in regions where $|\Pi^{(n)}_y| > |\tilde{\Pi}_y|$ (similar to the criterion used by Garcia (1991), except that Ertel's PV replaces quasi-geostrophic PV). The work of Robinson (1988), who found that
nonlinear effects tended to damp the amplitude of the primary wave, is supportive of this procedure. The size of the $\beta^{(n)}$s is chosen to cancel out any growth of $|\Pi^{(n)}|$ which would occur if $\beta^{(n)}$ was absent—i.e. using (9), $\Pi^{(n)}$ is calculated with $\beta^{(n)}$ set to zero (which we shall denote here as $\epsilon$), and then $\beta^{(n)}$ is set equal to $\operatorname{Re}(\epsilon / \Pi^{(n)})$. However, a problem arises in determining $\beta^{(n)}$ in a breaking region when $|\Pi^{(n)}|$ is small. Large $\beta^{(n)}$s are avoided here by setting $\beta^{(n)}$ to zero if $\rho |\Pi^{(n)}| < 1.5 \times 10^{-5} \text{s}^{-1}$. This allows the waves to grow to a sufficient amplitude for $\beta^{(n)}$ to have a sensible value. The breaking criterion was applied to each wave separately, since it was not obvious how to apply it and the subsequent damping to the sum of the three waves.

An exact expression for $\rho \Pi^*$ is given by Tung (1986), namely,

$$\rho \Pi^* = u' \frac{(u' \cos \phi)}{\cos \phi} - \hat{\Pi} \rho'$$

and using this, $\rho \Pi^{(n)}$ can be written approximately (for small waves) as

$$\rho \Pi^{(n)} = u^{(n)} \frac{(u^{(n)} \cos \phi)}{\cos \phi} - \hat{\Pi} \rho^{(n)}.$$

On replacing $u^{(n)}$ and $\rho^{(n)}$ by their geostrophic expressions, and $\rho^{(n)}$ by an expression which is easily derived from the hydrostatic approximation

$$M_z = c_p T$$

and the definitions of density and potential temperature, and after using Matsuno's (1970) definition of relative vorticity (which incorporates the effect of an isallobaric wind), we obtain

$$\rho \Pi^{(n)} = \frac{1}{f} \left[-k^2 + \frac{\sin^2 \phi \phi}{\cos \phi} \frac{\partial}{\partial y} \frac{\cos \phi \partial M^{(n)}}{\sin^2 \phi} \right] -$$

$$- \rho \hat{\Pi} \left[ \frac{[M^{(n)} + M''^{(n)} \left( \frac{1 - 1}{\kappa} \frac{T_z / T - \frac{1}{\kappa}}{c_p(T_z - T)} \right)]}{c_p(T_z - T)} \right].$$

(11)

These 2nd order PDEs are inverted at the start of each time step to find the eddy Montgomery potential. The boundary conditions imposed on $M^{(n)}$ are $M^{(n)} = 0$ along the top boundary (about 100 km) and at $\phi = \pm \frac{1}{2} \pi$, and $M^{(n)} = 0$ at $\phi = 0$. Matsuno's (1970) radiation condition for the top boundary would probably be more realistic, but the PV damping rate chosen ensures that the waves are very small near the top boundary, so that the boundary condition is immaterial. The equatorial condition was found to be necessary to avoid numerical instabilities near the equator. Since $M^{(n)}$ is not held at the equator (because of the choice of grid) the equatorial boundary condition means that the waves in the two hemispheres are independent. The bottom boundary of the wave-model grid lies on the 350 K isentropic surface, where $M^{(n)}$ is set equal to the monthly-averaged values derived from the Stratospheric Sounding Unit (SSU) satellite data for 1981, multiplied by a factor of 1.4. (For a brief description of the SSU data see, for example, Clough et al. (1985).) This factor (chosen to give a more realistic performance) can be considered as a crude compensation for the averaging-out of transient waves at the bottom boundary. Figure 1 shows $|M^{(n)}|$ at 15 km.

Inversion of the PDEs is performed by relaxation, the ellipticity condition being equivalent to $\phi \tau_0 \rho_z > 0$. This is similar to the ellipticity condition for the PDE for $\psi$ (see section 2) and in fact the heat and momentum fluxes which maintain ellipticity for that
PDE also ensure that these equations remain elliptic. After $M^{(n)}$ is obtained from $\Pi^{(n)}$, (9) is integrated over one time step, using the geostrophic $v^{(n)}$ and an Adams–Bashforth explicit scheme.

The grid used is the same as that used for the zonal-mean quantities, with $\Pi^{(n)}$ and $M^{(n)}$ held at the middle of the box sides. The $\Pi^{(n)}$ are represented in the model by their real and imaginary parts, allowing the real and imaginary parts of (11) to be solved separately. However, $\Pi^{(n)}$ is converted into a magnitude and phase before (9) is integrated. This allows the change in $\Pi^{(n)}$ due to advection by $\bar{u}$ (which changes only the phase of $\Pi^{(n)}$) to be integrated exactly over a finite time step, and thus increases the stability of the solution in regions where $\bar{k}\bar{u}$ is large.

Since the two hemispheres are independent the time step is chosen separately for each hemisphere. Its maximum value is 4 hours, and is reduced by the factor $(1 + 4\text{ hours} \times F)$ rounded down to the nearest integer, where $F$ is the maximum value in the hemisphere of either $2\bar{|u|}k/\pi$ or $8|v'|/\Delta y$. Thus if either the phase change in 4 hours due to $\bar{u}$ is greater than $\pi/2$, or if a wave parcel could cross more than one eighth of a grid box in 4 hours, then the time step is at most 2 hours.

4. Eddy Fluxes

The eddy PV flux, $\bar{\rho}w^{(n)}\Pi^{(n)}$, is calculated using the geostrophic $v^{(n)}$, and the vertical eddy flux in (3) is estimated by assuming $w^{(n)} = -\alpha T^{(n)}/T$ and using (10). The sum of these two terms over the three waves, plus a Rayleigh friction term which is supposed to represent the effect of breaking gravity waves in the upper stratosphere and mesosphere, gives the $F$ used in (2).

The $K_{yy}$ used in (8) is the sum of two parts, one of which ($K_{yy}^h$) depends on the photo-chemical dissipation rate (which is species-dependent) while the other part ($K_{yy}^w$) depends on the dispersion of PV due to wave-breaking. Adding the two $K_{yy}$s in this way is justified, if the $\beta$s are sufficiently small and the waves are sufficiently linear, by the following argument. The linearized equation for the evolution of an eddy mixing ratio, $q'$, can be written as

$$D_t q' + \bar{q}_t D_l \delta = D_l \sigma$$

(12)
where \( D_t = \partial / \partial t + \bar{u} \partial / \partial x \), \( \delta \) is a horizontal displacement defined by \( D_t \delta = \sigma \), and \( D_t \sigma = - \gamma q' \), where \( \gamma \) is the rate of photo-chemical dissipation of \( q' \). If \( D_t \delta_q \) is neglected, this implies that

\[
q' + \delta q_y = \sigma
\]

and hence \( \overline{v'q'} = - D_t \delta q_y + \sigma D_t \delta \). This can be manipulated using the above expressions and definitions, to give

\[
\overline{v'q'} = - \left[ \frac{1}{2} \overline{(\delta^2)_t} + \gamma \overline{\delta^2} \right] q_y + (\alpha \delta)_t + \alpha \sigma \delta.
\]

If \( \sigma \) is small compared with \( \delta q_y \), then the last two terms can be neglected. The two terms in the square brackets are then identified as \( K_{yy}^{br} \) and \( K_{yy}^{ch} \) respectively, and hence the total \( K_{yy} \) is their sum.

However, in Garcia’s parametrization, which is followed here, dispersion is assumed to dissipate the eddy PV (with rate \( \beta (\alpha) \)), and hence \( K_{yy}^{br} \) is given by an expression equivalent to \( \beta \delta^2 \), and not by the dispersive term \( \frac{1}{2} \overline{(\delta^2)}_t \). Nevertheless, since it is assumed to arise from dispersion in a breaking planetary wave, this value for \( K_{yy}^{br} \) is simply added to the \( K_{yy}^{ch} \) for each chemical species to give the total \( K_{yy} \). (An alternative might be to add \( \beta \) to the photo-chemical dissipation rate and hence calculate a purely dissipative \( K_{yy} \), but this would involve the assumption that dispersion acts to dissipate eddies in all quantities, not just PV.)

\( K_{yy}^{ch} \), the ‘chemical eddy’ \( K_{yy} \), does not include the chemical coupling terms considered by Pyle and Rogers (1980), and is due only to the linear dissipation term in the source of the chemical considered. From the above discussion, both \( K_{yy}^{ch} \) and \( K_{yy}^{br} \) are given by

\[
K_{yy} = \sum_{n=1}^{\infty} \frac{\gamma v'^2}{k^2(u - c^{(n)})^2 + \gamma^2}
\]

(13)

where \( \gamma \) is the relevant (i.e. photo-chemical or wave-breaking) dissipation rate (see, for example, Garcia 1991). The photo-chemical dissipation rate is obtained, using the photo-chemical scheme described below, from the term \( - \gamma \hat{x} \) in the zonal-mean source of \( \hat{x} \) (note that for some species \( \gamma = 0 \)). The phase velocity \( c^{(n)} \) is obtained from the rate of change of \( \Pi^{(n)} \). As noted by Rogers and Pyle (1984), when \( \gamma \) is small, \( K_{yy} \) can be very large near a critical line \( (u = c) \). However, from general considerations we may place a rough limit on each term of the sum in (13). On multiplying by \( \chi' \) the equation from which (13) is derived, namely

\[
\chi'_t + \bar{u} \chi'_x + v' \hat{x}_y = - \gamma \chi'
\]

(14)

and taking the zonal average and assuming steady waves, we have

\[
(\overline{v'\chi'}) \hat{x}_y = - \gamma (\overline{\chi'^2}).
\]

If the north-south displacement of the wave is at most \( \pm D \) then, approximately,

\[
|\chi'| \lesssim D |\hat{x}_y|
\]

and so

\[
|\overline{(v'\chi')}| \lesssim \frac{\gamma}{2} D^2 \hat{x}_y.
\]

Therefore we place a limit of \( (\gamma/2)D^2 \) on each term of the sum of (13). \( D \) was chosen, fairly arbitrarily, to be \( a/4n \).
5. Photochemistry

The principal purpose of this paper is to describe the dynamical formulation and behaviour of the present model, but since the chemistry feeds back onto the dynamics in several ways, we shall briefly describe the chemical scheme employed in the runs described here.

The scheme used is essentially that of Pyle (1980). The following chemicals are modelled (family grouping is indicated by square brackets): [O, O1D, N2], [N, NO, NO2, NO3, ClONO2], [H, OH, HO2], [Br, BrO, HBr, HOBr, BrONO2], [I, CI, ClO, ClONO2, Cl2O5, OCIO, HCl, HOCl], [CH4, CH2, CH3OH, CH2O, CH2O, CH2O, HCO], HNO4, HNO3, N2O5, N2O, H2O2, H2O, CO, CH3Br, CCl4, CH2Cl, CH2CCl3, CFC13, CF3Cl2, CHClF2, C2Cl3F3, CBrClF2, CBrF3. The odd hydrogen family is assumed to be in a photochemical steady state.

The model calculates the diurnal average of the family mixing ratios in the following way. First, every 10 days the day-time average photolysis rates are estimated using a five-point Gaussian integral over the day-time segment of a latitude circle. These photolysis rates are used to partition the families, and so a nominal day-time mixing ratio is determined for each member of the family. The 24-hour average rate of change of mixing ratio of a family is the weighted sum of a day-time rate and a night-time rate. The day-time rates are found using the day-time mixing ratios of family members, while most of the night-time rates are taken to be zero on assuming that the following species are negligible at night: O1D, O, OH, H, HO2, NO, N1, CH3, CH2O, HCO and Cl. Non-zero night-time rates come either from rain-out or from reactions involving species which are assumed to have little diurnal variation. Tropospheric rain-out occurs for HNO3, HCl, HBr, HNO4, H2O2, CH2O and CH3OOOH.

Photolysis rates are calculated using the solar flux data from the World Meteorological Organization (WMO) (1986) and the cross-sections from DeMore et al. (1990). The O2 and O3 cross-sections from WMO (1986) are used, and the NO cross-section is taken from Allen and Frederick (1982). The surface albedo is taken to be 0.35, and there is no Rayleigh scattering.

Two heterogeneous reactions, of ClONO2 and N2O5 with H2O on sulphate aerosols, have been included, with a background aerosol surface area of about 0.5×10^-8 cm^-1 specified between 12 and 32 km. A further change made to the scheme is that photolysis rates and heating rates now take into account the height-dependence of the number of daylight hours per day at a certain latitude, which is given by the expression

$$\frac{24}{\pi} \cos^{-1}\left(-\tan \Delta \tan \phi - \frac{(h^2 + 2ah)^{1/2} - (a + h)}{(a + h) \cos \Delta \cos \phi}\right)$$

where \(\Delta\) is the declination of the sun and \(h\) is the height above the surface. Also, the effect of rays from the sun travelling upwards into regions above the surface polar night is estimated. The net effect (due to changes in the heating and photolysis rates) is a general warming of a few degrees throughout the model, though the temperature increases at 50 km at the equinoxes, within about 10 degrees of the poles, are about 15 K. There is also a small reduction in the ozone column, of up to about 6 Dobson units (DU) at mid latitudes.

6. Radiation

The heating due to absorption of solar ultra-violet radiation is calculated every 10 days using the O2, O3 and NO2 cross-sections mentioned above. The scheme (described
in Haigh (1984)) is used to calculate the heating due to absorption of solar energy in the near infrared by H₂O, CO₂, O₂, CH₄ and N₂O. Haigh’s scheme for long-wave cooling due to H₂O, CO₂ and O₃ is also used. The parametrization of CO₂ and O₃ absorptance it uses is known to over-estimate the cooling through its treatment of Doppler broadening (Haigh, personal communication). Modelled mixing ratios are used for all the above calculations, which are performed everywhere above the tropopause.

As with the photochemistry, the variation of daylight with height and the illumination of regions above the surface polar night are taken into account.

7. TROPOSPHERE

The tropospheric physical processes are at present parametrized only crudely, but with the aim of allowing some interaction with the stratosphere.

The total heating is the sum of a convective-type heating (which is supposed to represent both surface fluxes of sensible-heat and latent-heat release) and a specified cooling.

‘Convection’ occurs when the local lapse rate exceeds a certain critical value, and an upwards heat flux is produced which, in the absence of other processes, would relax the lapse rate back to the critical value with a time constant of two days. The critical lapse rate (shown in Table 2) is chosen to confine convection mainly to the moist tropical regions (values being estimated roughly from tropospheric water-vapour data, but slightly tuned to give satisfactory results).

<table>
<thead>
<tr>
<th>TABLE 2. CRITICAL LAPSE RATES USED IN THE MODEL</th>
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</thead>
<tbody>
<tr>
<td>Latitude (°)</td>
</tr>
<tr>
<td>Critical lapse rate (K km⁻¹)</td>
</tr>
</tbody>
</table>

The ground temperature is held at a seasonally varying value (derived from SSU data, extrapolated to 1000 mb) and thus acts as the source of heat which is vertically redistributed by the convection. Because of the relaxational nature of the convection the troposphere is able to respond to dynamical changes in the stratosphere.

The cooling is specified over three latitude bands, values being chosen to give satisfactory results, though being guided by those of Dopplick (1979). Polewards of 20 degrees the cooling varies sinusoidally with season, while equatorwards of 20 degrees it is constant in time. The winter, summer and tropical profiles are shown in Table 3. (The troposphere occupies roughly the four model layers below θ = 350 K, each layer being about 3.5 km high.)

<table>
<thead>
<tr>
<th>TABLE 3. TROPOSPHERIC RADIATIVE COOLING RATES (K DAY⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Level</td>
</tr>
<tr>
<td>-------</td>
</tr>
<tr>
<td>4</td>
</tr>
<tr>
<td>3</td>
</tr>
<tr>
<td>1, 2</td>
</tr>
</tbody>
</table>

Estimates of the Eliassen–Palm flux divergence or \( \mathcal{T} \) in the troposphere (e.g. Yang et al. 1990) show a negative region from about 3 to 10 km, and between 20 and 70 degrees, which is stronger in winter than in summer. Nearer the surface there is a positive region. Therefore, in our model, \( \mathcal{T} \) was parametrized as friction, \( \mathcal{T} = -F \dot{u} \), to which was
added, in the bottom layer only, a specified positive $\mathcal{F}$. A suitable $F$ (shown in Table 4) was found by trial and error.

$K_{zz}$ is set to $7 \times 10^{-10}$ s$^{-1}$ in the troposphere (corresponding to about 5 m$^2$ s$^{-1}$ in geometrical coordinates) and $K_{yy}$ in the troposphere is derived from Luther's (1973) diffusion coefficients in this region by projecting along an isentropic surface, and is the same for all quantities. Strictly speaking this is not a valid procedure, since the model surfaces in the troposphere are sigma coordinate surfaces, not isentropic ones, and also the waves in the troposphere will be much less adiabatic than in the stratosphere, but for our purposes it is sufficient at present.

<table>
<thead>
<tr>
<th>TABLE 4. RA Jury F RICITION COEFFICIENTS (DAYS$^{-1}$)</th>
</tr>
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<tbody>
<tr>
<td>Latitude (degrees)</td>
</tr>
<tr>
<td>Level</td>
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<tr>
<td>-------</td>
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<td>2 to 4</td>
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<td>5</td>
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</tbody>
</table>

8. RESULTS

In this section the modelled winds, temperature and ozone will be compared with observations. The effect of the parametrized eddy fluxes on the model fields will be described, by comparing model runs with and without eddy fluxes of PV and chemicals. The question of whether isentropic coordinates are a significant improvement over the TEM formalism will not be addressed here, but it will be shown that the present eddy flux parametrization is significantly better than one in which $K_{yy}$ was independent of species, and was derived from the ratio of the eddy flux of PV to its mean gradient.

(a) Winds, temperatures and ozone column

The modelled zonal winds for January and July are shown in Fig. 2. In comparison with the observed winds of Barnett and Corney (1985) the summer easterlies in the lower stratosphere are too weak, and the easterly jet maxima are too close to the equator (by about 30 degrees). This is more likely to be due to a deficiency in the heating rates than to one in the wave-driving, since wave amplitudes are very small in the model’s summer easterlies, which extend down to the tropopause.

There is, however, a fairly realistic asymmetry between the modelled winter hemispheres, which is due almost entirely to the asymmetry in the specified wave amplitudes at the tropopause. The only other source of asymmetry in the model is the specified surface temperature, but the effect of this is small, since in a model version which had symmetric surface temperatures the zonal winds differed from those in the above run by at most 5 m s$^{-1}$. The modelled northern hemisphere (NH) stratospheric westerly jet is about 30 m s$^{-1}$ weaker than the modelled southern hemisphere (SH) one. In the lower stratosphere the NH $\vec{u}$ is (unrealistically) close to zero while in the SH $\vec{u}$ is much larger. This feeds back onto the propagation of, and the fluxes produced by, the planetary waves (see section 8(b)).

The reason why $\vec{u}$ is so unrealistically small in the NH winter lower stratosphere is related to the presence of the wave numbers 2 and 3—in a model version with only wave number 1, $\vec{u}$ in the NH winter lower stratosphere is about 25 m s$^{-1}$ more westerly than when the shorter waves are also present. Consistent with linear Rossby wave theory, the shorter waves are trapped in the lower stratosphere by the westerly jet, where they
produce a significant negative PV flux. This PV flux decelerates \( \bar{u} \) and will in turn affect the propagation and dissipation of the wave-number 1 component. The importance of the shorter waves suggests that perhaps more care is needed in their treatment, on account of the scale-dependence of thermal damping (with perhaps different damping rates needed for the different wave components) and because of their larger curvature, and hence greater departure from geostrophy.

The modelled January and July temperatures (Figs. 3(a) and 3(b)) show fairly good agreement with observations (Barnett and Corney 1985) in the summer hemisphere, with the mesopause having a realistic height and temperature, though the lower stratosphere is too cold by up to about 10 K. The modelled winter hemispheres show much larger differences from observations; in the NH the polar temperature at 20 km is close to that observed, with temperatures above being too low (by up to about 40 K at 50 km) and those below being too high (by up to about 20 K). This might be indicative of too strong a negative PV flux at about 20 km (the effect of PV flux on temperature is discussed in section 8(b)), which could also explain the unrealistically small \( \bar{u} \) in the NH winter lower stratosphere (cf. the previous paragraph). Other possible causes of the cold upper stratosphere might be too weak a sink of zonal momentum above 50 km (which could

![Figure 3. Modelled monthly-mean temperatures for (a) January and (b) July. The contour interval is 10 K.](image-url)
be due to an unrealistic parametrization of gravity-wave breaking in terms of Rayleigh friction) or too strong a cooling in the upper stratosphere, possibly due to the Ramanathan parametrization used in the long-wave cooling scheme (Haigh, personal communication). There is also some inter-hemispheric asymmetry in the modelled temperature fields, though not as large as that observed, with the SH winter pole in the model stratosphere being about 10 K cooler than in the NH (compared with an observed difference of over 20 K).

Finally, the modelled ozone column is shown in Fig. 4 (produced using 1970 tropospheric boundary conditions on chlorine loading, as mentioned before). Certain observed inter-hemispheric differences are reproduced, such as the northern winter polar maximum and a SH maximum which lies off the pole and moves polewards in late spring. Values on the whole are reasonable, though the northern maximum is too low and the equatorial value too high by about 20 DU. The inter-hemispheric asymmetry is due almost entirely to the asymmetry in the planetary-wave forcing at the tropopause (the asymmetry in the surface temperature affecting the ozone column by at most 10 DU).

![Figure 4](image)

Figure 4. Modelled ozone column with 1970 chlorine loading. The contour interval is 10 DU.

(b) Nature and effect of PV flux

In this section the structure of the parametrized PV flux will be briefly described, along with its interaction with the zonal-mean state and the effect it has on the modelled winds, dynamics and chemistry.

The monthly-mean parametrized PV flux shows a large inter-hemispheric asymmetry, with the maximum NH flux below 60 km, of about $-7$ m s$^{-1}$ per day, occurring in January, while in the SH the maximum flux descends with time, from 50 km in September/October (when it is about $-9$ m s$^{-1}$ per day) down to 20 km in November. Figure 5(a) shows the PV flux at 30 km. Comparing Fig. 5(b) with Fig. 1 it seems that the NH flux is determined largely by the wave amplitude at 15 km, while in the SH interaction with the zonal-mean state is relatively more important. The approximate relation

$$\overline{\Pi(t)\nu(t)} = -(\alpha + \beta(t))\overline{\Pi(t)^2}/\overline{\Pi}$$

can be derived from (9) with the assumption of steady waves. The PV flux might therefore be expected to be small when $\overline{\Pi}$ is large (noting also that $\beta(t)$ will be zero when $\overline{\Pi}$ is large enough to prevent the wave-breaking criterion from being satisfied). Indeed, it can be seen in Fig. 5(b), which shows $\overline{\rho\Pi}$ at 30 km, that from April till October the large
\( \rho \Pi \), at 60°S causes the PV flux maximum to occur either polewards or equatorwards of 60°S. Then in November the dramatic reduction in \( \rho \Pi \) is accompanied by a large PV flux. Since the SH wave amplitude at 15 km (see Fig. 1) remains almost constant from April till December, it seems reasonable to say that the reduction in \( \rho \Pi \) is initiated by the seasonal cycle, leading to an increased PV flux which in turn leads to a more rapid decrease in \( \rho \Pi \). It is noted that \( \Pi \) should also play an important role in the propagation of planetary waves (see, for example, Matsuno 1970), with the direction of propagation tending to be away from regions of small \( \Pi \), thus tending to enhance the PV flux in regions of large \( \Pi \).

The initial effect of a negative PV flux on the meridional circulation is to induce a polewards \( \bar{V} \) through the region of maximum PV flux, with a return flow above and below to satisfy continuity. This change in \( \bar{V} \) keeps \( T \) in thermal-wind balance with \( \bar{u} \) and spreads vertically the deceleration of \( \bar{u} \). The change in temperature will induce a change in the long-wave cooling which will complete a two-celled circulation.

The effect on the zonal-mean state of a mid-latitude negative PV flux is illustrated schematically in Fig. 6. Note the signs of the temperature change, so that, referring back to section 8(a), it is seen how the anomalous model temperatures in the NH winter above and below 20 km could be explained by an excessively strong negative PV flux at 20 km.

The variability of the tropical tropopause temperature, both observed and modelled, should provide a test of the above idea. The temperature of the observed equatorial tropopause (see Fig. 7), from Barnett and Corney (1985), has an annual cycle of about 5 K, with a maximum in August and a minimum from January till March. The model has a similar but smaller cycle (Fig. 7, dashed line), though the maximum occurs a month later and the minimum is less flat. This cycle, in the model at least, is due mainly to the large negative PV fluxes from about September till February (see Fig. 5(a)) in one or the other hemisphere—a negative PV flux near 30 km at mid or low latitudes in either hemisphere will lower the temperature of the equatorial tropopause (see Fig. 6). This accounts for the falling temperature of the model equatorial tropopause from September till February. No doubt tropospheric processes also play a part in the annual cycle in the real atmosphere, but the modelled cycle indicates that the stratosphere may play an important role in the behaviour of the troposphere.

In order to isolate the effect of the PV flux on the model, two runs were carried out: run A where the PV flux and all the \( K_{ij} \)s above the tropopause were set to zero,
Figure 6. Schematic diagram of the effect of a region of negative PV flux (heavy dashes) on the circulation (solid lines) and rate of change of $\dot{T}$.

Figure 7. Equatorial tropopause temperature—observed (solid) and modelled (dashed).

and run B where the PV flux was included, but the $K_p$s were still set to zero. Subtracting run A from run B then gives the change due to the PV flux. In July the largest reduction in $\bar{u}$ due to the PV flux (run B – run A) occurs at about 30 km and 30$^\circ$S, and is accompanied by the large changes in the horizontal gradient of $\bar{T}$ (see Fig. 8(a)) at 30$^\circ$S, near 20 km and 60 km. The change in temperature affects the ozone distribution both directly through chemistry and indirectly through a change in the long-wave cooling rate, and hence the vertical velocity. (The change in the ozone distribution then feeds back onto the temperature due to its effect on the solar heating rate, so that Fig. 8(a) is the result of a complex interaction, but it can nonetheless be understood, to first order, as the direct response to a negative PV flux.) In the next two paragraphs we will try to interpret the related changes in temperature, heating rate and ozone, due to the PV flux.

The change in the net heating rate (Fig. 8(b)) is well anti-correlated with the change in temperature above 40 km, due to the influence of the long-wave cooling scheme. Below 40 km, however, the change in ultra-violet absorption due to the ozone change (see Fig. 9(a)) becomes important and generally opposes the change in long-wave cooling—below 40 km and polewards of 60 degrees north and south, the temperature
increase leads to increased long-wave cooling and the subsequent increase in subsidence (or decrease in upwelling) raises the ozone mixing ratio (the polar vertical ozone gradient is positive up to 40 km in run A). In the tropics there is net heating below 40 km even though the change in temperature is positive above 30 km. This must be partly due to a positive feedback between ozone and the heating rate—since the equatorial ozone maximum in run A lies at 30 km, any additional upwelling at 30 km will increase the ozone mixing ratio above 30 km (as shown in Fig. 9(a)), leading to an increase in the solar heating, and hence more upwelling. A balance will be achieved since, firstly, the ozone maximum is merely being lifted up and not increased (neglecting possible photochemical effects) and, secondly, the long-wave cooling will tend to oppose the temperature increase. The fall in ozone mixing ratio below 30 km in the tropics is probably due to a combination of two factors—(1) an additional upwelling due to the fall in temperature induced by the PV flux and (2) a reduction in the penetration of sunlight to lower levels due to the increase in ozone above 30 km.
However, the change in ozone can only be partly explained by a change in the advection of ozone, since higher in the stratosphere the ozone photochemical lifetime becomes short in comparison to advective time-scales (see Fig. 10(a)). The changes in ozone should, therefore, be small unless the change in advection also changes the photochemical equilibrium state for ozone. This appears to be the case, since the change in NO$_x$ (Fig. 9(b)) is well anti-correlated with the change in ozone above about 30 km (Fig. 9(a)). Though it is not necessary for our argument to go into details, the change in NO$_x$ seems to be due mainly to the change in circulation, on account of its relatively long photochemical lifetime (see Fig. 10(b)), the induced polewards flow now becoming important because of the strong horizontal gradients in the NO$_x$ (NO$_x$ = N + NO + NO$_2$ + NO$_3$ + ClONO$_2$) of run A (which is similar to that of run B shown in Fig. 15(b)). Diffusion acts directly on the NO$_x$ family, but thereby affects NO$_x$. A detailed discussion would have to consider the change in N$_2$O, the source of NO$_x$, but if advection of an air parcel does not perturb the photochemistry in that parcel significantly (due to a change in insolation) then NO$_x$ can be effectively considered as a tracer. In section 8(c) it will be seen how, above 30 km, a change in NO$_x$ (due to diffusion) of order 0.01 p.p.m.v. led to an ozone change of order 1 p.p.m.v. In Fig. 9, above 30 km, the same order of changes are seen in both NO$_x$ and ozone, and it therefore seems reasonable to say that a major part of the ozone change above 30 km is due to the redistribution of NO$_x$ by a change in the circulation.

![figures](attachment://figures.png)

Figure 10. January photochemical lifetime in days for (a) ozone (contour increment is a factor of about 2) and (b) NO$_x$ (contour increment is a factor of about 1.6).

Finally, Fig. 11(a) shows the net effect of the PV flux on the ozone column, with increases of up to 220 DU at the North Pole in April. In the ozone column of run A (not shown here), which lacks the influence of the PV flux, the maximum of about 340 DU occurs near 40 degrees in summer, with polar values rarely exceeding 200 DU. The change in the ozone column due to the PV flux is dominated by the ozone change between the 350 K and 543 K surfaces (approximately 14 to 24.5 km), which accounts for about 80% of the change in the total column. The change in temperature, due to the PV flux, at 20 km (see Fig. 11(b)) is representative of the temperature change from 14 to 25 km and is seen to be well correlated with the change in the total-ozone column. This correlation, which occurs in the real atmosphere and has been remarked upon by other authors (e.g. Tung and Yang 1988), is probably due mainly to the correlation between
Figure 11. (a) Change in total ozone column (contours every 20 DU) and (b) change in temperature at 20 km (contours every 5 K) due to a stratospheric PV flux (run B – run A). Dashed contours are negative.

temperature, long-wave cooling and down-welling. The fact that, in the model, temperature and ozone increases in the polar lower stratosphere are due to the presence of the negative PV flux is supportive of the claim (of Tung and Yang (1988), amongst others) that a decrease in the wave activity in the lower stratosphere would contribute significantly to the southern ‘ozone hole’.

(c) Diffusion coefficients $K_{yy}$

In this section we shall consider in more detail the nature of the parametrized $K_{yy}$s, and their effect on the distribution of certain trace gases, ozone in particular. In this section, merely for convenience, we shall use the term ‘diffusion’ when referring to the down-gradient flux that the coefficient $K_{yy}$ produces in the model, and it is not to be taken as implying that the ‘chemical eddy’ transport is diffusive or turbulent in nature. A brief discussion of the validity of the $K_{yy}$ approach to the parametrization of eddy transport was given in section 1.

As already stated, the $K_{yy}$ for each chemical family is composed of two parts; $K_{yy}^{br}$ is species-independent, while $K_{yy}^{ch}$ depends on the chemical family’s lifetime, and is in general different for each family. The structure of the SH $K_{yy}^{br}$ throughout the year is similar to that found by Garcia (1991), though the values are smaller by a factor of almost 10, while the NH exhibits a more qualitative difference. The monthly-mean $K_{yy}^{br}$-fields for September and January are shown in Fig. 12. There is, however, a large day-to-day variability in the breaking, with instantaneous values of $K_{yy}^{br}$ reaching five times the monthly-mean value. The general shape of the SH $K_{yy}^{br}$ is the same from June till September, while in October and November the peak moves towards the pole as the westerly jet is broken down. In the NH, Garcia found the wave-breaking to be similar to that of the SH in position and strength, but to cover a larger area. Here, we find that there is very little low-latitude breaking, with the largest $K_{yy}^{br}$ occurring at about 20 km in mid to high latitudes (see Fig. 12(b)) where $\bar{u}$ is close to zero (see Fig. 2(a)).

Since the breaking condition used here is the same as Garcia’s, the difference in the structure of $K_{yy}^{br}$ must be due to the difference in wave propagation (over a zonal-mean state which depends on the physics in the zonal-mean model and the wave-driving) and the determination of $\beta^{(n)}$. Obvious differences between the wave models include the different horizontal and vertical resolutions and the different number of wave
components. Another difference which might be important is the use of Matsuno's definition of relative vorticity in (11). In a version of the model referred to above, in which only the longest wave component was included, because of the change in the zonal-mean state the low-latitude region of wave breaking is broader in the NH in January than in the SH in September. This is in agreement with Garcia's results, though the typical magnitude of $K_{yy}^{br}$ is still much smaller.

The size and strength of the NH low-latitude 20–50 km breaking region has also been found to depend fairly critically on the eddy PV damping rate, $\alpha$, in the lower stratosphere, with a doubling of $\alpha$ tending to reduce the breaking region, and a halving of $\alpha$ increasing $K_{yy}^{br}$ by about 50%. There is also the interaction between the waves and $\tilde{u}$ to consider, both through the dependence of $K_{yy}$ on $\tilde{u}$ in Eq. (13) and through the control that $\tilde{u}$ has over the propagation of the waves. From Fig. 12, where the 0, 10 and 20 m s$^{-1}$ $\tilde{u}$ contours have been overlaid, we see that there is a tendency for $K_{yy}^{br}$ to be large only where $\tilde{u}$ is less than about 15 m s$^{-1}$. In Garcia's model, breaking occurred in regions where $\tilde{u}$ was as much as 40 m s$^{-1}$.

The $K_{yy}^{ch}$s for the odd-oxygen and NO$_x$ families are generally much larger than $K_{yy}^{br}$. This difference can be due only to the difference between the photochemical eddy dissipation rates and the $\beta^{(a)}$s. Figure 13 shows the January-mean total $K_{yy} (=K_{yy}^{br} + K_{yy}^{ch})$ for the ozone and NO$_x$ families. Below about 20 km the lifetimes are not calculated since $K_{yy}$ is derived from Luther's diffusion coefficients in this region (see section 7). From (13), since $K_{yy}^{ch}$ is large when the intrinsic frequency of the wave and the photochemical dissipation rate are comparable (and $v'$ is large), the $K_{yy}$ for ozone is fairly constant with height since the lifetime decreases upwards (see Fig. 10(a)) while $\tilde{u}$ increases. Below about 50 km the $K_{yy}$ for NO$_x$ has a bias towards low altitudes since its lifetime is more constant with height (see Fig. 10(b)).

The $K_{yy}$ for ozone is large in the NH from December till February, December and February being about half the size of January and similar in shape, though biased more towards about 30 km. The SH values are large from May till November, the values from June till August being similar in shape to those of the NH in January, but about half the size. The September values are also similar in shape, but about twice as large as those for the NH in January, while October and November have polar maxima of $85 \times 10^2$ and $50 \times 10^2$ m$^2$s$^{-1}$ at 40 km and 30 km respectively.
These values of $K_{yy}$ for ozone and NO$_x$ are very similar to those derived, using observational data, by Smith et al. (1988) for ozone and HNO$_3$, with peak values of just over $3 \times 10^7$ m$^2$s$^{-1}$ in January in all cases. Also, their ozone $K_{yy}$ appears to peak at a higher altitude than their HNO$_3$ $K_{yy}$, in general agreement with our results. These $K_{yy}$'s affect the ozone distribution in a number of different ways. The most direct is simply by diffusion of ozone down its zonal-mean gradient. However, the other chemicals are also diffused by their own $K_{yy}$'s and the re-distribution of these chemicals, in particular NO$_x$, also has a large effect on ozone. Thirdly, the change in the ozone distribution will change the heating rates (and thus the circulation) which will feed back on the ozone distribution.

In order to separate out the first two effects, two further model runs, C and D, were carried out (for long enough to be roughly annually periodic): run C differs from run B of section 8(b) in that the $K_{yy}$ for ozone is included, so that (run C minus run B) reveals the effect of diffusion of ozone only, and run D includes the $K_{yy}$ for every gas so that (run D minus run B) shows the effect of diffusion of all gases. Figure 14 is the change in the July ozone mixing ratio due to (a) ozone $K_{yy}$ only (i.e. run C minus run B) and (b) all $K_{yy}$'s (i.e. run D minus run B). The January graph had the same general features, so is not shown here.

Figure 14(a) shows clearly the large horizontal diffusion of ozone down the mean gradient in the winter hemisphere. It also shows that the summer hemispheres in runs B and C are very similar, indicating that photochemistry has pulled both models towards very similar equilibrium states, which in turn suggests that the change in ozone has not produced a long-term change in any of the chemicals that determine the ozone equilibrium state large enough to alter that state significantly. This is in fact so, with NO$_x$ changes of the order of 1 p.p.b.v., ClO changes of about 0.05 p.p.b.v. and OH changes of $0.5 \times 10^6$ molecules cm$^{-3}$. Figure 14(b) shows that inclusion of the rest of the $K_{yy}$'s has a large effect on ozone all through the year. The reason for the ozone change can be traced to the change in NO$_x$, shown in Fig. 15(a).

The effect of diffusion on NO$_x$ persists throughout the year, though there is a significant seasonal variation. The large changes in NO$_x$ (about 50% over the equator and even larger over the poles) appear to be a result mainly of down-gradient diffusion of NO$_x$ (the NO$_x$ from run B is shown in Fig. 15(b)), although diffusion of HNO$_4$, HNO$_3$, N$_2$O$_5$, and ClONO$_2$ must all contribute too. The ozone and NO$_x$ changes are well anti-
correlated, except in the polar night where there is no atomic oxygen, and in the tropics below about 25 km. The reason for this tropical, low-altitude ozone increase is probably mainly a combination of two factors—diffusion of ozone (seen also in Fig. 14(a)), and increased solar radiation due to the ozone loss between 25 and 40 km.

There is no chemical eddy $K_{v}$ for Cl$_{y}$ since in the model it has only a zonal-mean source, from the photolysis of chlorofluorocarbons, CH$_{4}$Cl and CCl$_{4}$, and does not contain a term proportional to Cl$_{y}$. The Cl$_{y}$ mixing ratio is, therefore, affected only by changes in the zonal-mean photochemistry and mean circulation. Its net change is small, of the order of 0.1 p.p.b.v., or about 5%. The net change in ClO is in general anticorrelated with NO$_{x}$, since ClO combines with NO$_{x}$ to form ClONOO$_{2}$, reaching a peak of about 0.2 p.p.b.v. over the poles at 35 km, and is about 0.05 p.p.b.v. at 30 km over the equator. The change in ozone due to this change in ClO must be small compared with the effect of a change in NO$_{x}$, since the ClO and ozone changes are in general in
the same direction. The net changes to the ozone column (see Fig. 16) are polar intensifications, with low-latitude increases, of up to 70 DU over the NH winter pole, and small mid-latitude decreases.

For a comparison with different methods of estimating $K_{yy}$, two further model runs were carried out. The first was to see how important it was to use a separate $K_{yy}$ for each chemical species. In this run the $K_{yy}$ for ozone was calculated as in run D, and the $K_{yy}$s for all the other species were then set equal to this $K_{yy}$. The difference between this run and run D was not very significant in terms of the ozone column—compared with run D the polar column increased by about 10 DU while equatorial values fell by about 2 DU. The reason for this change in ozone lies probably in the increased diffusion of Cl$_4$ away from the poles (since in run D the $K_{yy}^{ch}$ for Cl$_4$ was zero), with the Cl$_4$ mixing ratio at polar (low) latitudes decreasing (increasing) by about 0.3 p.p.b.v., from about 20 km to 40 km. This corresponds to changes of from 20% at high latitudes to over 50% at low latitudes.

![Figure 16. Change in ozone column due to all $K_{yy}$s. Dashed contours are negative. Contour interval is 5 DU.](image)

In the second run, $K_{yy}$ was independent of species (as in the run just described) but now it was derived, using the method of Newman et al. (1988), by dividing the eddy flux of PV by its zonal-mean latitudinal gradient. The problem with this method is that $K_{yy}$ can become very large in regions where the latitudinal PV gradient is small (caused perhaps by a down-gradient eddy flux of PV). This was the case in this model run, with $K_{yy}$ exceeding $10^6$ m$^2$s$^{-1}$ in the lower stratosphere NH winter, leading to a polar ozone column of over 1000 DU in January.

9. CONCLUSIONS

Isentropic coordinates provide the natural framework in which to treat eddy fluxes due to adiabatic planetary waves since such waves result in a diffusion matrix $K$ with only one non-zero element, in contrast to the situation in isobaric coordinates where it is not straightforward to calculate the off-diagonal elements of $K$, so that they are often neglected (e.g. Hitchmann and Brasseur 1988; Smith and Brasseur 1990) or estimated from $K_{yy}$ and the slope of isentropic surfaces (e.g. Newman et al. 1988). Isentropic coordinates also offer conceptual advantages stemming from the direct relationship between vertical velocity and diabatic heating rate.
The model described in this paper is in essence a severely truncated, linearized, 3D dynamical model coupled with a 2D chemical model (the eddy fluxes in the chemical model being parametrized with the help of the wave information in the dynamical model) and thus retains the economic benefits of 2D chemical models while incorporating a fairly realistic wave-mean interaction. It should, therefore, be a useful tool for analysing the long-term interactions between waves and zonal-mean chemistry and dynamics, over time-scales where it is too expensive to run a full 3D model.

The planetary-wave parametrization predicts the evolution of Ertel's PV in the three longest waves, and calculates the PV flux (the isentropic equivalent of the Eliassen–Palm flux divergence), and a $K_{yy}$ for each individual chemical family, which is the sum of a wave breaking part, $K_{yy}^{bw}$, and a chemical eddy part, $K_{yy}^{ch}$. The $K_{yy}^{ch}$ for ozone and NO$_3$, with typical winter-time values of $20 \times 10^5$ m$^2$ s$^{-2}$, are in general a factor of 10 times larger than $K_{yy}^{bw}$ and hence the use, as in most other 2D models, of the same diffusion matrix for all chemical families would be unjustified, especially since $K_{yy}^{ch}$ for Cl$_3$ is zero. However, the two runs described at the end of section 8 show:

(i) that use of the ozone $K_{yy}$ for all chemical species, instead of their own $K_{yy}$s, does not significantly affect the ozone column (though it does have a significant effect on Cl$_3$), and

(ii) that use of ‘chemical eddy’ $K_{yy}$s is significantly better than the use of a $K_{yy}$ derived by the PV flux-gradient method.

Diffusion of ozone alone (with no diffusion of other gases) has a large effect mainly in the winter lower stratosphere, where the ozone $K_{yy}$ is large and ozone has a long photochemical lifetime. This effect does not persist throughout the year because the ozone photochemical equilibrium state for ozone has not been significantly affected. A change in ozone which persists throughout the year occurs only when the $K_{yy}$s are included for all the chemical families (NO$_3$ in particular). The ozone change (which is of the order of 1 p.p.m.v. at 30 km) is generally anti-correlated with the change in NO$_3$, since NO$_3$ plays a large part in determining the equilibrium state for ozone. The change in NO$_3$ persists throughout the year because of its longer photochemical lifetime, and hence this is probably the reason why it can be modelled fairly well using a small $K_{yy}$ that is independent of season and latitude (Ko et al. 1985).

The parametrized PV flux affects the ozone column (an increase of over 200 DU at the North Pole during winter) through the change in vertical velocity it induces in the lower stratosphere (14 to 24 km). The long-term effect that the PV flux has on the ozone seems again to be due to a change in the photochemical equilibrium state for ozone.

The troposphere is allowed a limited degree of interaction with the stratosphere. As a result of this, the model tropical tropopause has an annual cycle whose amplitude is about 70% of the observed cycle, and with almost the same phase. The modeled cycle is mainly due to the stratospheric wave-driving, and indicates that stratospheric dynamics might have a considerable impact on the troposphere (though this inference does depend on the degree of realism of the model troposphere).

The eddy fluxes produced by the wave parametrization result in large inter-hemispheric asymmetries in, for example, the ozone column and zonal winds. These model asymmetries are purely a result of the asymmetric wave amplitudes specified at about 15 km from monthly-mean observations.

One aspect in which this model differs from previous 2D models, whose dynamical wave forcing is parametrized in terms of spectral wave components (e.g. Holton and Wehrbein 1980; Hitchmann and Brasseur 1988; Garcia 1991), is that three, rather than one, wave components are represented. The two shorter waves have a large effect on
the PV flux in the lower stratosphere either by a direct contribution or by changing the zonal-mean state and thereby altering the PV flux due to the longest wave. The negative increase in the PV flux results in a decrease in $\ddot{u}$ of on average about 20 m s$^{-1}$ in the lower stratosphere. Also, because the shorter waves affect mainly the lower stratosphere, there are large increases (of up to 100 DU at the North Pole) in the ozone column.

The wave breaking $K_{yy}$ is also affected by the shorter waves, being similar in shape and evolution (though significantly smaller) to that of Garcia (1991) in the absence of the shorter waves. In the presence of all three waves, the wave breaking $K_{yy}$ is in general much smaller than Garcia's and tends to occur in regions where $\ddot{u}$ is less than 20 m s$^{-1}$. Because, in the NH, the winter lower stratospheric $\ddot{u}$ is (unrealistically) close to zero, wave breaking tends to occur in the mid to high latitudes at about 20 km. In the SH $\ddot{u}$ is more westerly and the waves break higher up and closer to the equator.

The wave breaking and PV flux are both sensitive to the rate of dissipation of PV anomalies, which is specified as a height-dependent parameter in the model. This rate is, however, known to be scale-dependent and also might depend on the concentrations of gases like CO$_2$ and H$_2$O. The model behaviour could, therefore, perhaps be improved by including a certain scale-dependence in the dissipation (a different rate for each wave, say). Also, it could be seen whether changes in the damping due to further increases of CO$_2$ could produce a qualitative change in the interaction between waves and the mean state (such as the difference in behaviour between the NH and SH). The influence of resolution on the behaviour of the planetary-wave parametrization might also be worthy of investigation.

This model's main strength is its ability to simulate, over long time-scales, interactions between planetary waves and the zonal-mean chemical and dynamical states, such as would occur during sustained pollution of the atmosphere. (In this respect, it is currently being used to estimate the impact of aircraft on the stratosphere.) One natural phenomenon whose investigation it thus seems suited for is the quasi-biennial oscillation—in particular the connection between the tropical and extra-tropical signals, in which it is possible that planetary waves, interacting with chemistry and volcanic aerosols, may play an important role. Development of the model in this direction is currently under way.

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