Stratospheric tracer transport:  
a modified diabatic circulation model

By C. F. ROGERS* and J. A. PYLE†

Department of Atmospheric Physics, Clarendon Laboratory, University of Oxford

(Received 14 March 1983; revised 9 August 1983)

SUMMARY

We describe a model for stratospheric tracers in which transport consists of advection by the mean diabatic circulation and chemical eddy transport arising from longitudinal variations in in situ sources and sinks. The ozone distribution is reproduced well by the model and all species show interesting variations with longitude. The limitations of the model are discussed; we speculate that the most important of these is the neglect of transient contributions.

1. INTRODUCTION

The concern that the ozone layer may be affected adversely as a result of man's activities has prompted considerable research. In recent years there has been a valuable increase in kinetic and photochemical data, as well as significant advances in the understanding of transport processes in the stratosphere. This paper describes work, which takes advantage of these latter advances, using a two-dimensional numerical model of the atmosphere.

Traditionally, in two-dimensional models the tracer continuity equation is written:

\[ \frac{\partial \overline{R}}{\partial t} + \overline{v} \frac{\partial \overline{R}}{\partial y} + \overline{w} \frac{\partial \overline{R}}{\partial z} = \overline{S} - \left( \frac{1}{\cos \phi} \right) \frac{\partial (\overline{v'} R \cos \phi)}{\partial y} - \rho^{-1} \frac{\partial (\rho \overline{w'} R)}{\partial z} \]

(1)

where overbar represents a zonal mean and prime a departure therefrom, and thus, for example, \( R = \overline{R} + R' \) with \( R \) a volume mixing ratio. \( v \) and \( w \) represent meridional velocities in the \( y \) and \( z \) directions and \( S \) is the net zonal mean source of \( R \).

A problem with Eq. (1) arises with the treatment of the eddy terms involving departures from the zonal mean. This is usually solved by relating the fluxes to the mean gradients of the tracer, using a tensor of transport coefficients (Reed and German 1965). Thus, for example,

\[ \overline{v' R'} = -K_{yy}(\partial \overline{R}/\partial y) - K_{yz}(\partial \overline{R}/\partial z). \]

(2)

The problem then becomes one of finding the appropriate \( K \)s.

Recent ideas, stemming from the work on Lagrangian circulations by Andrews and McIntyre (1976), have suggested simplifications to Eq. (1). In particular, Dunkerton (1978) demonstrated that the equation could be rewritten as follows:

\[ \frac{\partial \overline{R}^L}{\partial t} + \overline{v^L}(\partial \overline{R}^L/\partial y) + \overline{w^L}(\partial \overline{R}^L/\partial z) = \overline{S^L} \]

(3)

where superscript 'L' represents a Lagrangian mean. (In a simple case, this could be an average following an air parcel.) The continuity equation is now particularly simple; no eddy terms arise.

A problem with applying Eq. (3) arises in the determination of the Lagrangian mean (McIntyre 1980). However, an equation similar to (3) can be obtained if \( \overline{v^L} \) and \( \overline{w^L} \) are replaced by the residual mean meridional circulation (Andrews and McIntyre 1976), if \( \overline{R}^L \) is replaced by \( \overline{R} \) and if the waves are steady and adiabatic. In this case, the disappearance of the eddy terms is well understood in terms of the so-called 'non-acceleration theorem' (see Andrews and McIntyre 1976). In the absence of transience or damping of the wave, a circulation is driven by the wave which exactly cancels the effect of the wave on the zonal mean. Thus, the residual circulation arises following the cancellation of the eddy and the

*Present address: Institute of Oceanographic Sciences, Wrotham, Kent 5
†Present address: Rutherford Appleton Laboratory, Chilton, Didcot, Oxon
secondary eddy-driven circulation (Palmer 1981; Holton 1981). It can be shown, furthermore, that this circulation is related to the diabatic heating (Dunkerton 1978).

Pyle and Rogers (1980b) were the first to use the diabatic circulation as the residual circulation in a numerical model of the ozone layer, with subsequent models by Holton (1981), Miller et al. (1981) and Garcia and Solomon (1983). Prabhakara (1963) had used a diabatic circulation, based on that calculated by Murgatroyd and Singleton (1961), to calculate the distribution of ozone but it seems that he regarded this as the total Eulerian circulation.

It is a consequence of the non-acceleration theorem that the eddy terms disappear, when Eq. (3) is recast as above in terms of the residual circulation, only when the wave is steady and undamped. Furthermore, Matsuno (1980), Hartmann and Garcia (1979), Plumb (1979), Pyle and Rogers (1980a), Danielsen (1981) and Tung (1982) have all shown that steady waves can also produce a net transport if the tracer is not inert. Longitudinal variations in sources and sinks, if correlated in some manner with planetary-scale waves, can produce meridional transport of the tracer. By considering the case of a steady planetary wave and a reactive tracer, Pyle and Rogers (1980a) derived expressions for the transport coefficients which depend on the meridional wind perturbations and the lifetime of the tracer. The Ks can be separated into two components (Matsuno 1980; Pyle and Rogers 1980a): an antisymmetric tensor which depends only on the properties of the planetary wave; and a symmetric tensor which depends also on the tracer lifetime.

Thus

$$
\begin{pmatrix}
0 & K'_{xz} \\
-K'_{yz} & 0
\end{pmatrix}
$$

and

$$
\begin{pmatrix}
K''_{yy} & K''_{yz} \\
K''_{zy} & K''_{zz}
\end{pmatrix}
$$

are the two components. The latter models the net transport accomplished by a wave when the tracer is reactive while the former models that transport which is exactly cancelled by the induced mean circulation.

The model described below uses the two main ideas outlined above. We use, for our mean circulation, the circulation driven by the diabatic heating. However, we also include the wave transport of non-conservative tracers by using the symmetric component of the K tensor.

In the next section we describe in more detail the model, including the derivation of the diabatic circulation, the Ks and a description of our photochemical scheme. Subsequently we describe the model performance and suggest further areas of improvement.

2. THE MODEL

Our model consists of two separate elements, for the calculation of the zonal mean and eddy terms respectively. The zonal mean transport and chemistry are calculated using a version of the two-dimensional model described by Harwood and Pyle (1975). In this version the temperature and zonal wind are not computed but are specified using values, stored on magnetic tape, calculated in a previous model run. The mean meridional circulation is computed, but with the eddy forcing by heat and momentum fluxes ignored.

The diabatic heating is calculated, using the prescribed temperatures but with model-dependent ozone amounts.

For the eddy calculation the Fourier amplitudes for wavenumbers 1 and 2 of \( u', w' \) and \( R' \) are found using the same model grid as in the mean calculation. The wave amplitudes are found by solving the quasi-geostrophic potential vorticity equation with observed forcing at 100 mb and using the same background fields of temperature and zonal wind as used in the calculation of zonal mean quantities. Likewise the same chemical scheme is used to calculate the zonal mean sources and sinks, and to find the eddy sources used in the determination of the K coefficients (see section 2(b)).

(a) The mean circulation

The time-dependent, two-dimensional, zonal mean model of the atmosphere devel-
oped by Harwood and Pyle (1975) (hereafter HP) is used as a framework for the present calculation. However, there are a number of significant changes from previously published versions of the model.

The model extends from pole to pole and from the ground to approximately 90 km, although the chemical calculations described here are taken up to only about 60 km. The dependent zonal mean variables, tracer mixing ratios and meridional streamfunction are held as functions of time, height and latitude with a spatial resolution of π/19 in latitude and approximately 3.5 km in height (0.5 pressure scale heights). Fourier amplitudes of the planetary wave or eddy fields are also held on the same spatial grid. These are calculated every ten days, less frequently than the one hour timestep adopted for the zonal mean dependent variables.

In the present calculations the standard formulation of the two-dimensional model, as described by HP, is modified. We use a residual mean circulation as discussed above. In this formulation a mean meridional circulation, which is the difference between the Eulerian mean meridional circulation and the convergence of the horizontal eddy heat flux, is introduced.

Consider a (y, ζ) coordinate system with y = distance northwards and ζ = log(p₀/p), with p = pressure and p₀ = 1000 mb and with velocity components v and w. Let overbar denote the zonal mean (e.g. \( \bar{R} = (1/2\pi) \int Rd\lambda \) integrated from 0 to 2\( \pi \); \( \lambda \) = longitude) and prime a departure therefrom (i.e. \( R = \bar{R} + \varphi \)). A residual mean meridional circulation may be defined as (Andrews and McIntyre 1976; Palmer 1981)

\[
\bar{V}^R = \bar{V} - \frac{\partial}{\partial \xi} \left( \frac{V'\theta'}{\theta'} \right) = \\
\bar{W}^R = \bar{W} + \frac{\partial}{\partial \xi} \left( \frac{V'\theta'}{\theta'} \right)
\]  

(4)

where the definitions, following the notation of HP, are made: \( W = we^{-\xi} \cos \phi \), \( V = ve^{-\xi} \cos \phi \), \( \theta \) is the potential temperature and \( \phi \) is latitude. The model dynamical equations retain the same form as in HP. The thermodynamic equation becomes

\[
\frac{\partial}{\partial t} \{ \theta (\cos \phi)e^{-\xi} \} + \frac{\partial}{\partial y} (\bar{V}^R \theta) + \frac{\partial}{\partial \xi} (\bar{W}^R \theta) = \bar{q} (\cos \phi)e^{-\xi} + Q
\]

(5)

where

\[
Q = -\frac{\partial}{\partial \xi} \left( \frac{V'\theta'\varphi}{\theta'} \right).
\]

It can be shown (e.g. Plumb 1979; Holton 1981) that \( Q \) (and incidentally the Eliassen–Palm flux divergence in the accompanying momentum equation) disappears for steady, adiabatic waves.

In this case the rate of change of \( \theta \) following the residual circulation is just equal to the diabatic heating and \( (\bar{V}^R, \bar{W}^R) \) may be interpreted as the diabatic circulation.

To find the diabatic circulation the full set of dynamical equations in HP could be solved with the eddy terms set to zero. In this way, apart from \( V^R \) and \( W^R \), the temperature and zonal wind fields would also be calculated. We have chosen instead to specify time-varying temperature and zonal wind fields and to solve for the meridional diabatic stream function. Thus the momentum and thermodynamic equations (Eqs. 2.13 and 2.14 in HP) are not used prognostically but the second-order partial differential equation for the streamfunction (Eq. 2.17 in HP) is used to diagnose the diabatic circulation. Specifying the temperature and zonal fields is done for convenience, but it does introduce an inconsistency: there is no guarantee that, for example, using \( \bar{V}^R \) and \( \bar{W}^R \) in the thermodynamic equation would produce the tendency in the temperature fields which we impose.

Two points can be advanced in favour of the procedure which we adopt. Firstly, the
tendency which we impose is realistic. Any difference between this and that implied by the calculated $\mathcal{F}^R$ and $\mathcal{W}^R$ would be due to the approximations made (e.g. the neglect of $Q$ and the divergence of the Eliassen–Palm flux). In a crude way, we may thus be thought to be allowing for $Q$ and the EP flux divergence.

Secondly, experience suggests that using our best radiation schemes to calculate both the diabatic circulation and the temperature fields produces a particularly poor temperature structure in polar latitudes. Wehrbein and Leovy (1982) have discussed the sensitivity of the modelled polar night jet to radiation schemes. They point out that improving the radiation calculation leads to a deterioration in the representation of the jet. We believe that simple Newtonian cooling schemes, which have built-in some preference for an observed or realistic temperature structure, can do more than model simply radiation; they can imply some extra physical processes by compensating for inadequacies in the dynamical representation. Our specification of the temperature structure should, therefore, be no worse than the use of these simple radiation schemes.

In practice, the mean diabatic circulation is found diagnostically, using zonal winds and temperatures from a previous model run. In the transformed formulation, the streamfunction is found by solving a linear, second-order partial differential equation:

$$\mathcal{L}(\tau, \theta, \psi^R) = \mathcal{R}_1(H) + \mathcal{R}_2(Q) + \mathcal{R}_3(\bar{q}(\cos \phi)e^{-\xi})$$  \hspace{1cm} (6)

where $H$ is the divergence of the EP flux and $\mathcal{R}_1, \mathcal{R}_2$ and $\mathcal{R}_3$ are differential operators. $L$ is an operator whose coefficients depend on the specified zonal mean wind and temperature structure. We have applied the same boundary condition for $\psi^R$ as to $\psi$ in HP (i.e. $\psi = 0$ at the boundaries). While recognizing that this introduces an extra inconsistency at the bottom boundary, a rigorous treatment would involve the determination of the eddy fluxes in the troposphere, which we have not undertaken. For the stratosphere, our approach should be satisfactory.

By neglecting $H$ and $Q$, prescribing $\bar{u}$ and $\bar{T}$, and calculating $\bar{q}$ (which depends on $\bar{T}$ as well as the model-dependent ozone mixing ratios), $\psi^R$ (and hence $\mathcal{F}^R$ and $\mathcal{W}^R$) can be calculated. $\bar{u}$ and $\bar{T}$ are taken from a previous run of the model. They are regarded as a (model-generated) climatology which shows qualitative agreement with the observed atmosphere. The calculation of $\bar{q}$ follows one of the treatments described by Harwood and Pyle (1980) in which rather than treating the lower stratosphere as being in radiative equilibrium, we have used the net heating rates calculated by Rodgers (1967). In this way, the diabatic circulation is recalculated every five days. The use of the above diagnostic equation simplifies our present calculations considerably. Notice that if our procedure was entirely consistent there would be no acceleration of the mean flow by planetary-scale waves. Consistent with this, there was a strong (but not complete) cancellation between mean and eddy motions in our original model.

(b) Tracer continuity equations

The coupled photochemistry and transport of four constituents or groups of constituents ($O_x$, $NO_x$, $H_2O_2$, and $HNO_3$) is treated. It is convenient to assemble these constituents into the constituent vector $\mathbf{R}$, such that $\mathbf{R} = ([O_x], [NO_x], [HNO_3], [H_2O_2])^T$, where $O_x$ is the odd oxygen family ($O_3, O$ and $O(1D)$) and $NO_x$ is the odd nitrogen family ($N, NO$ and $NO_2$).

With this notation the zonally averaged continuity equation for the vector volume mixing ratio is written

$$\frac{\partial}{\partial t} (\bar{\mathbf{R}} e^{-\xi} \cos \phi) + \frac{\partial}{\partial y} (\bar{\mathcal{F}}^R \bar{\mathbf{R}}) + \frac{\partial}{\partial \xi} (\bar{\mathcal{W}}^R \bar{\mathbf{R}}) = \bar{S} e^{-\xi} \cos \phi + \mathbf{F}$$  \hspace{1cm} (7)

where $\bar{S}$ is the zonal mean net rate of production of $\bar{\mathbf{R}}$ and

$$\mathbf{F} = -\{\partial (\mathbf{F}_y)/\partial y\} - \{\partial (\mathbf{F}_\xi)/\partial \xi\}$$

with
\[ F_y = \nabla' \mathbf{R} - (\nabla' \theta / \theta_z) \mathbf{R}_z \quad \text{and} \quad F_z = \nabla' \mathbf{R} + (\nabla' \theta / \theta_z) \mathbf{R}_y. \]

\( S \) is assumed to depend only on products of zonal mean mixing ratios. We have, therefore, ignored the eddy contribution discussed by Tuck (1979).

A determination of the eddy contributions contained in \( \mathbf{F} \) may be based on the linear perturbation continuity equation for the constituent volume mixing ratio \( \mathbf{R}' \) (Pyle and Rogers 1980a). To first order in Rossby number

\[ \{ (\partial / \partial t) + \mathbf{a} (\partial / \partial x) \} \mathbf{R}' - A \mathbf{R}' = -v' (\partial \mathbf{R}/\partial y) - w' (\partial \mathbf{R}/\partial \zeta) \]  

where the coupling matrix \( A \) is related to the perturbation net source

\[ S' = -A \mathbf{R}' + \mathcal{O}(R^2). \]

In general \( A \) depends on rate constants or zonal mean volume mixing ratios. The appearance of the coupling matrix \( A \) (which, in general, is non-diagonal) in the eddy equation is simply a reflection of the coupled nature of chemical processes in the atmosphere. The use of families of constituents, however, may to some extent remove some of this complication. We wish to examine the coupling contributions in a future calculation. However, we proceed in the present calculation with the neglect of the off-diagonal elements of \( A \).

Restricting our treatment to stationary, planetary perturbations in \( \mathbf{R} \), the perturbation continuity equation for each zonal wavenumber, \( m \), may be solved as

\[ r_m = -(A + im\tilde{w})^{-1} \{ q_m (\partial \mathbf{R}/\partial y) + p_m (\partial \mathbf{R}/\partial \zeta) \} \]

where \( r_m, q_m \) and \( p_m \) are the Fourier components of \( \mathbf{R}' \), \( v' \) and \( w' \) respectively and \( \tilde{w} \) is the angular velocity of the basic state. The \( v' \) and \( w' \) may be readily derived from geopotential wave perturbations calculated from the planetary wave equation described in the appendix. Consistently the same zonal wind and temperature state is used to determine the planetary wave perturbations as was used to determine the diabatic circulation.

The above equation describes the planetary wave structure at a given height of any of the constituents. By summing in the vertical, we are able to determine the longitudinal variations in the column totals of \( \mathbf{R} \).

For stationary planetary waves the eddy transports which contribute to \( \mathbf{F} \) may be written

\[ \begin{pmatrix} V' \mathbf{R}' \\ W' \mathbf{R}' \end{pmatrix} = - \begin{pmatrix} K''_{yy} & K''_{y\zeta} \\ K''_{\zeta y} & K''_{\zeta\zeta} \end{pmatrix} \begin{pmatrix} \partial \mathbf{R}/\partial y \\ \partial \mathbf{R}/\partial \zeta \end{pmatrix} - \begin{pmatrix} 0 & K'_{y\zeta} \\ K'_{\zeta y} & 0 \end{pmatrix} \begin{pmatrix} \partial \mathbf{R}/\partial y \\ \partial \mathbf{R}/\partial \zeta \end{pmatrix}. \]

Double prime indicates dependence on chemistry. In contrast \( K' \) contains no dependence on chemical processes. The antisymmetry of the inert \( K \) field and its relationship to the Stokes correction to the Eulerian mean meridional velocities has been noted by a number of authors (e.g. Matsuno 1980). It should be emphasized that the limitation to stationary planetary waves neglects transient contributions to the eddy fluxes which are expected to provide additional contributions to the transport.

It should be noted that Eq. (11), although derived for a chemical constituent, is equally valid for potential temperature. Our use of a diabatic circulation had involved the neglect of the perturbation source \( q' \) and hence under the same approximation

\[ \begin{pmatrix} V' \theta' \\ W' \theta' \end{pmatrix} = - \begin{pmatrix} 0 & K'_{y\zeta} \\ K'_{\zeta y} & 0 \end{pmatrix} \begin{pmatrix} \partial \theta/\partial y \\ \partial \theta/\partial \zeta \end{pmatrix}. \]

We see at once that in Eq. (7) the eddy contribution \( \mathbf{F} \) can be written in terms of the chemical \( K \) fields only, demonstrating explicitly the cancellation inherent in the non-acceleration theorem, i.e.

\[ \begin{pmatrix} F_y \\ F_z \end{pmatrix} = - \begin{pmatrix} K''_{yy} & K''_{y\zeta} \\ K''_{\zeta y} & K''_{\zeta\zeta} \end{pmatrix} \begin{pmatrix} \partial \mathbf{R}/\partial y \\ \partial \mathbf{R}/\partial \zeta \end{pmatrix}. \]
The chemical transport tensor above is not generally symmetric, but it may be treated as approximately symmetric for the present calculation. For completeness the expressions for the \( K \) fields are given below:

\[
\begin{align*}
K''_{(\xi\xi)} &= \frac{1}{2} \sum \frac{A}{A^2 + (\partial m)^2} \left| \begin{pmatrix} q_m \\ p_m \end{pmatrix} \right|^2 \\
K'_{yz} &= K'^{*}_{zy} = \frac{1}{2} \sum \frac{A}{A^2 + (\partial m)^2} \text{Re} \left\{ p_m q_m^* \right\}
\end{align*}
\]

(14)

when the summation is over all wavenumbers. The calculation of the planetary wave structure is confined to regions with pressures less than 100 mb. Thus \( p_m, q_m \) are not calculated in the troposphere, where in practice they would anyway be dominated by synoptic-scale waves. The simple expedient of assuming \( p_m, q_m \) to be constant in the troposphere has been adopted. While this procedure is clearly unsatisfactory, our main concern is with the distribution of tracers in the stratosphere where the impact of the approximation is generally small, although in high latitudes the stratosphere does extend to pressures greater than 100 mb. The tropospheric \( K' \)s are still allowed to vary with the lifetime of the tracer and the zonal wind speed.

(c) The chemical scheme

The photochemical scheme used in the calculation of \( S \) and \( A \) is that described by Pyle (1980). \( \mathrm{H}, \mathrm{OH} \) and \( \mathrm{HO}_2 \) are assumed to be in photochemical steady state as are the individual species within the odd oxygen and nitrogen families. For other gases, e.g. \( \mathrm{H}_2\mathrm{O}, \mathrm{CH}_4 \) and \( \mathrm{N}_2\mathrm{O} \), fixed profiles, constant with latitude, are employed.

The scheme is quite adequate for our present purpose, which is to test recent ideas of tracer transport within a model framework.

(d) Some computational details

The tracer continuity equation (Eq. (7)) is solved for the four constituents by the Adams–Bashforth method using a one-hour timestep. This is shorter than in our previous calculations, necessitated by somewhat larger \( K \) values.

The diabatic circulation in Eq. (7) is recomputed every five days, as discussed above.

The \( K \) values used in the calculations of \( F \) are calculated every timestep using Eq. (14). The meridional wind perturbations, \( q_m \) and \( p_m \), are computed only every ten days, for \( m = 1, 2 \), using the quasi-geostrophic potential vorticity equation. The method is described in the appendix.

The calculation of \( F \) encounters two difficulties both concerned with the treatment of a nearly inert tracer (\( A \) small). For such a constituent the chemical eddy contribution, like the net zonal mean source, is small and transport is brought about almost entirely by advection. It becomes possible in this case for negative mixing ratios to develop in certain grid boxes after continued advection out of the box. The situation arises with development of unrealistically large gradients between boxes and hence unrealistically large fluxes. It is possible to employ a filling scheme (see e.g. Mahlman and Moxim 1978) to correct for the negative mixing ratios such that all values are zero or positive. Despite such a scheme in our model, and in the absence of any other transport mechanism except advection, the rate of accumulation of negative values can be severe. It was found that the introduction of a sub-grid-scale diffusion scheme had the effect of controlling the occurrence of negative values by smoothing the variability between boxes. The scheme is introduced to attempt to simulate the effects of transfers involving scales below the chosen grid resolution. Since we are interested in the effect of large-scale motion on transport, a desirable scheme for sub-grid-scale transfers would be one which was scale selective, leaving larger resolved scales virtually unaffected, but acting to reduce the build-up of scales near the grid scale itself. Such a scheme was used by Mahlman and Moxim in a
general circulation model study. We have used a similar but simpler scheme by supplementing the horizontal $K_{yy}$ with a sub-grid-scale diffusion coefficient of the form

$$D = 5.0 \times 10^{5} \{[(\bar{R}_{i,j} - \bar{R}_{i,j+1})/2]/[(\bar{R}_{i,j} + \bar{R}_{i,j+1})/2]\}^{2} \text{m}^{2}\text{s}^{-1}$$

where $i$ and $j$ represent vertical and horizontal boxes respectively.

The quadratic factor rapidly decreases $D$ when neighbouring boxes are of comparable size. The optimum value was determined from a number of experiments using different constants, the chosen value being the smallest consistent with effectively controlling the occurrence of negative mixing ratios for nearly inert tracers.

A further problem arises from the stationary approximation to the perturbation continuity equation. The expressions for $K$ contain the factor $A/[A^{2} + (\vec{\omega} m)^{2}]$, which can become large if $A$ and $\vec{\omega} m$ are small simultaneously. A completely satisfactory approach to this problem does not appear possible owing to the neglect of transient phenomena (which would introduce a non-zero contribution in the denominator (see for example Hartmann and Garcia 1979)), and non-linear processes.

As a practical solution, we have set $\vec{\omega} m = 1.6 \times 10^{-6} \text{s}^{-1}$ whenever the magnitude of the wind falls below this value. This is invoked only for nearly inert tracers ($A^{-1} < 7$ days) near a zero wind line.

Notice that for a completely inert tracer the chemical eddy $K_{s}$ can be written

$$\lim_{A \rightarrow 0} K_{yy} = \frac{1}{2} n \Sigma \delta(\vec{\omega} m) |\omega m|^{2}$$

which is zero except at a critical line. (As shown by Dickinson (1969) the nature of statistically stationary eddies would modify this result, ensuring a finite answer.)

3. SOME MODEL RESULTS

(a) Diabatic circulation

There are a number of limitations on the calculated diabatic circulation and its use as a residual circulation. For example, the effects of planetary wave transience and dissipation have been ignored. We have used model zonal mean wind and temperature fields which will be different to some extent from those found in the atmosphere. Thirdly, our calculations will be limited by the accuracy of our radiation schemes.

The calculation of $q'$ follows the treatment described by Harwood and Pyle (1980) in which rather than treating the lower stratosphere as being in radiative equilibrium, we have used the net heating rates calculated by Rodgers (1967). In Harwood and Pyle the sensitivity of the model, and especially the distribution of ozone, to lower stratosphere heating rates is discussed. We believe this sensitivity will apply equally to the calculations described here.

The wind and temperature structure used in the calculations was taken from a model run which excluded small-scale frictional dissipation. In consequence, the mesospheric zonal wind jets do not close and are larger than observed. However, the agreement is better in the stratosphere, although the strength of the jets is still somewhat exaggerated (see Haigh and Pyle 1982).

Figure 1 shows cross-sections of the meridional circulation during March. In the stratosphere there is a thermally direct cell with rising motion in the tropics and sinking in higher latitudes. Consistent with this is poleward flow in both hemispheres in the stratosphere. In the mesosphere, there is a flow from the spring hemisphere.

The meridional circulation agrees qualitatively with the residual circulation calculated by Holton and Wehrbein (1980) using a truncated semispectral model, including some transience and dissipation. The circulations calculated here are weaker than those reported by Holton and Wehrbein.

In the troposphere, our neglect of transient phenomena should be particularly serious. However, we are dealing with tracers which are mainly confined to the strato-
sphere and mesosphere. Our poor representation of tropospheric dynamics, while clearly being unsatisfactory, is probably not crucial.

(b) $K$ fields

Since the stratospheric zonal mean temperature and wind structure are satisfactory, the stationary planetary wave structure can be expected to be reasonably realistic. Indeed this is the case. For example, in the winter hemisphere, the planetary wave amplitude maxima lie close to the core of the polar night jet attaining their largest values of $\sim 1000$ m at $\sim 50$ km. The phase variation is consistent with the northward transport of sensible heat and momentum. (The planetary wave amplitudes were discussed in some detail for an unrealistic zonal wind structure in Pyle and Rogers (1980a).) Consequently our use of the calculated wave fields to determine the chemical contribution to the eddy transports may be regarded with some confidence.

In Fig. 2 are shown cross-sections of $K_{yz}$ calculated for $O_3$ and NO$_x$. The differences between the two arise because of their different chemical lifetimes, as discussed in detail by Pyle and Rogers (1980a).
The calculated $K$ fields show a number of differences from the observationally derived coefficients (e.g. Luther 1973) used in previous two-dimensional model studies. Indeed, since our approach is to include explicitly only the chemical contribution to the eddy fluxes, we should not expect the $K$s to be the same.

A striking difference between the calculated $K$ fields and those determined from observations is the contrast between winter and summer. In Fig. 2 there is a difference in the lower stratosphere of more than two orders of magnitude between summer and winter $K$ fields compared with a factor of about four in Luther's tabulations. Figure 2 clearly depicts the lack of vertical penetration of the planetary waves into the easterly jet in the summer hemisphere, as expected from the work of Charney and Drazin (1961). Two explanations may be offered for the much reduced hemispheric differences in the observational $K$s. Firstly, it is to be expected that transient planetary wave activity would play some role in the summer hemisphere, thus increasing the $K$s there. (Of course, these transient eddies would also be active in the winter hemisphere.) Secondly, an appreciable
contribution at low altitudes may be expected from the shorter wavelength baroclinic waves in both hemispheres. The inclusion of these two factors should reduce the summer to winter differences.

We do not find a very dramatic hemispheric difference in the $K_s$. In a GCM study, Manabe and Mahlman (1976) showed that at 10mb the eddy kinetic energy is a factor of ten greater in the northern winter compared with the southern winter. We might, therefore, expect a similar difference in the $K$ fields. That we see only small, non-systematic differences is possibly due to the zonal wind used. These do not mirror the observed hemispheric differences (Haigh and Pyle 1982). Manabe and Mahlman also indicate that the neglect of transient waves in our calculations will be more serious in the southern hemisphere.

(c) Chemical constituents

The latitude–time section of total ozone from the run is shown in Fig. 3. The gross features of the observed distribution are reproduced, with an equatorial minimum and

spring high latitude maxima in both hemispheres. There are two noticeable improvements over previous runs with the Eulerian model and similar photochemical schemes (e.g. Pyle 1980; Haigh and Pyle 1982). The equatorial minimum is reduced in these runs to about 260 matm-cm, in very good agreement with observations. Secondly, the seasonal behaviour in high latitudes is good, with a peak-to-peak variation of more than 80 matm-cm at 70°N. Previous model runs (and some other two-dimensional models) show much smaller seasonal variation in ozone column amounts. The ozone budget comprises a complex
interaction of photochemistry and transport and it is probable that these improvements are to some extent fortuitous. Previous calculations, for example, have shown how sensitive the low latitude ozone column is to the lower stratospheric net radiative heating, a quantity which is difficult to calculate.

Preliminary investigations suggest that the improvement is due to the smaller eddy transports in this model. In previous runs, the compensation between mean and eddy transports was strong in low latitudes and also in the high latitude summer. Our planetary wave model predicts very little eddy activity in the summer hemisphere and in low latitudes throughout the year. It appears that the removal of ozone by the diabatic circulation from the equatorial low latitudes throughout the year, and from the summer hemisphere, is not compensated by a chemical eddy convergence. The inclusion of some time-dependence might be expected to change this picture. In fact, transient eddies in summer in the middle latitudes could reduce the ozone column amounts shown; in this region the seasonal variation is much less than observed. The ozone budget in the model will be described in detail in a paper in preparation.

In an early model experiment (Pyle and Rogers 1980b) only advection by the diabatic circulation was considered. Chemical eddies were ignored. This resulted in very poor high latitude behaviour with maximum ozone amounts occurring instead in middle latitudes. Even though the $K_s$s we calculate are often smaller than typical values used previously, it is clear that the eddies do still play an important role.

Figure 4 shows a cross-section of the ozone concentration from a day in December. The main observational features are reproduced with a decrease in the height of the maximum with latitude. However, there is too much ozone in the equatorial middle and upper stratosphere. Although this would be reduced somewhat by the inclusion of chlorine chemistry, the over-estimation is an unsatisfactory feature of the model.

In Figure 5, ozone profiles for 30 April at northern hemisphere latitudes are plotted. The profiles intersect between 20 and 30 mb. This cross-over point has been used as an indication of the height which separates the dynamically controlled region below from the photochemically controlled region above. The observed cross-over is fairly constant with latitude, up to about 60°N, at 26 mb (Dütsch 1964). The cross-over has been modelled quite well and suggests that the diabatic formulation models the relative importance of dynamics and photochemistry in a realistic fashion. Figure 5 shows again the rather poor equatorial behaviour. Although, as suggested above, a more comprehensive chemical
Figure 5. Profiles of the ozone concentration \((10^{12} \text{ mols cm}^{-2})\) for various latitudes, 30 April.

Figure 6. Latitude-longitude section of total ozone (matm-cm) above approximately 100 mb for December.

scheme should improve things it appears clear that vertical transport also plays a major role here.

In Fig. 6 is shown a plot of the latitude-longitude section of total ozone above
approximately 100 mb for December. There is reasonable agreement with the data of Prabhakara et al. (1976) in the northern hemisphere. There is a predominantly wavenumber-one pattern in the winter hemisphere with a high, which in the model is displaced some distance from the Aleutians. The amplitude of the wave is about 100 m atm cm and is in good agreement with satellite observations. The structure in equatorial latitudes should be treated with some caution since the eddy calculation employs the geostrophic approximation for the planetary wave winds.

![Graph showing NO₂ profile comparison](image)

Figure 7. A mid-latitude model NO₂ profile versus observations.

Figure 7 shows a comparison of modelled NO₂ mixing ratios for August with the September balloon measurements of Roscoe et al. (1981). The agreement is excellent. On the other hand, the modelled values are lower than many of the sunset absorption measurements, although the shapes of modelled and observed profiles are still in good agreement. The present model computes day-average values for the constituents. Given the diurnal behaviour of NO₂ it is thus not surprising that better agreement is obtained with Roscoe's midday observations than sunset observations.

Similarly the NO mixing ratios in the model appear to be lower than observed in the lower stratosphere with mid-latitude mixing ratios of 0·15 p.p.b.v. and 1 p.p.b.v. at 20 and 30 km, respectively. At 40 km the value is about 9 p.p.b.v. in agreement with observations.

The latitudinal variation of the NO₂ column has attracted interest recently with the identification by Noxon (1979) of a steep 'cliff' beyond which the NO₂ column amount is low. In Fig. 8 is plotted the latitudinal variation of the modelled NO₂ amount above about 14·5 km in January. Three modelled plots are shown representing zonal mean values and the values appropriate to longitudes 60°W and 180°W. Also plotted are the winter-time measurements of Coffey et al. (1981), which for convenience we have plotted on a reduced scale. The measurements were made from an aircraft at about 11 km and should therefore be expected to be a little larger than the model numbers. The discrepancy suggests that the model NO₂ column amount is too low in low latitudes. The interesting feature to emerge is the significant variation of the NO₂ column amount with longitude for latitudes polewards of 40°. The behaviour at 180°W appears to be more nearly consistent with the observations made over the USA, although it does not show as dramatic a cliff as found by Noxon. On the other hand, the model zonal mean and values around 60°W continue to increase with latitude.

We do not present these results as an explanation of the Noxon cliff. Indeed, Noxon
finds lowest NO$_2$ column amounts when the flow is from the polar night, where this model predicts largest column amounts. Solomon and Garcia (1983) have pointed out the role of N$_2$O$_5$ in producing the cliff. The neglect of N$_2$O$_5$ will clearly be important in our study. Nevertheless, our point is that comparison of model and observations can be rendered quite unsatisfactory without longitudinal information. Attempts by purely zonal mean models to reproduce a cliff in NO$_2$ are likely to be misleading. Figure 8 demonstrates that planetary-scale dynamics play a major role. Indeed, this could be inferred from Noxon’s suggestion that the appearance of the cliff is connected intimately with the position of the polar vortex. However, the implications of our result are wider than this. They suggest the need for even greater caution in comparing models with observations and point to the need for detailed concurrent meteorological observations.

Figure 9 shows the model mid-latitude profile for HNO$_3$ compared with various observations. There is generally good agreement: the model HNO$_3$ is a little on the high side of the observations in the upper stratosphere but other models show a larger discrep-
ancy here (see e.g. Fig. 1-119, WMO 1982). The agreement here is due to the model OH, which agrees well with observations, and the lower NO\textsubscript{2} mixing ratios discussed above.

The model predicts column amounts of HNO\textsubscript{3} which are much larger than measured by Muehle et al. (1978) and Coffey et al. (1981). We find no evidence for a decrease in the column amount at high latitudes, either in the zonal mean or at individual longitudes, as compared with the results of Muehle et al., who found a decrease northwards of about 60°N in the spring. Again, the inclusion of N\textsubscript{2}O\textsubscript{5} in our photochemical scheme would be expected to have considerable influence on the nitrogen budget in high latitudes during winter and spring.

It is interesting that a longitude–latitude plot of HNO\textsubscript{3} column amounts (Fig. 10)

![Figure 10. Latitude–longitude section of total HNO\textsubscript{3} (10\textsuperscript{-1}matm-cm) above approximately 100 mb for March.](image)

shows a wavenumber-two pattern, as compared with the column amounts of O\textsubscript{3} (see Fig. 6) and NO and NO\textsubscript{2}, which all are dominated in the model by wavenumber one. The contribution to the HNO\textsubscript{3} column amount is confined to low altitudes where higher wavenumbers are still significant.

4. CONCLUSION

The motivation for the present work springs from recent theoretical advances in our understanding of the factors leading to net transport in the stratosphere and this study represents a practical attempt to use some of these ideas in a realistic simulation of the ozone distribution. The model comprises the diabatic circulation plus a contribution to eddy transport which arises when the tracer considered is not inert. Otherwise eddies are ignored and the diabatic circulation is our approximation to the residual circulation, defined as the difference between the Eulerian mean circulation and the circulation driven by steady, dissipationless waves.

It is important to appreciate that the study is not attempting to obtain as perfect a simulation as possible but rather our concern is understanding the various processes contributing to the simulated tracer distribution. Thus, the present study, being preliminary, contains a number of approximations which it is hoped to remove as progress is made. It must, of course, be acknowledged that many of the approximations are forced simply due to the two-dimensional formulation.

Probably the single most important neglect in the present simulation is that associated with transient contributions to the eddy fluxes. These contributions would be of importance in the determination of the residual circulation as well as providing extra contributions to the constituent continuity equation.
Despite these limitations, the model results are encouraging. The stationary chemical eddy contribution together with the diabatic circulation produce a reasonable simulation of the ozone distribution. The variation of the total column amount is good, with an equatorial minimum and high latitude spring maxima (which it was not possible to model with the diabatic circulation alone (Pyle and Rogers 1980b)). We find improvements over previous models in the strength of the equatorial minimum and the seasonal variation in high latitudes. The low latitude behaviour we attribute to the diabatic circulation (although the details of the ozone profile suggest that some improvement in the calculation of the radiative heating rate and the diabatic circulation is probably still necessary). The very low $K_s$ calculated for the summer hemisphere appear to be a reason for the improved seasonal behaviour. The eddies, though, still play an important role in the high altitude winter and spring hemispheres.

Notice that the stationary chemical eddy contributions, as well as being consistent with the zonal mean wind, also include a wave–mean flow interaction through the chemical time constant, which is determined from the model mean state. This is an element of chemical/dynamical coupling which has been ignored in previous two-dimensional models.

A further advantage of our approach in determining some aspects of the planetary wave structure is that statements concerning the longitudinal behaviour can now be made. For example, in the northern hemisphere winter we find a wavenumber-one pattern in the total ozone column with a maximum near the Aleutians in fair agreement with observations. The variation of the NO$_3$ column amount with longitude is very interesting and possibly sheds some light on the observations made by Noxon (1979). We find at some longitudes a decrease of NO$_3$ towards the pole whereas at other longitudes the gradient is opposite. More generally, this result points to the problem of making comparisons between simplified models and limited data sets.

Finally, we believe that the results of the calculations described here are sufficiently encouraging to commend this approach to other modellers.

**APPENDIX**

The geopotential wave fields above 100 mb and extending to about 90 km are determined by solving a Matsuno-type (Matsuno 1970) wave equation for the planetary wave. The generalization incorporates a height-dependent Newtonian cooling and Rayleigh friction parametrization. It should be noted that the use of dissipating planetary waves introduces an inconsistency in our residual circulation. For such waves the divergence of the EP flux as well as $Q$ will be non-zero, in contradiction with our assumed neglect. The profiles of the cooling and friction parameters are shown in Fig. 11.

The stationary geopotential height perturbation satisfies:

$$
\frac{\sin^2 \phi}{\cos \phi} \frac{\partial}{\partial \phi} \left( \frac{\cos \phi}{\sin^2 \phi} \frac{\partial \Phi_m}{\partial \phi} \right) + \frac{v_1}{v_0} (\sin^2 \phi) e^\xi \frac{\partial}{\partial \xi} \left( e^{-\xi} \frac{\partial \Phi_m}{\partial \xi} \right) - \\
- \frac{1}{S v_0} \sin^2 \phi \frac{\partial \alpha_N}{\partial \xi} \frac{\partial \Phi_m}{\partial \xi} + \left( \frac{m}{v_0} \frac{1}{\cos \phi} \frac{\partial \tilde{q}}{\partial \phi} - \frac{m^2}{\cos \phi} \right) \Phi_m = 0
$$

where

$$
\frac{\partial \tilde{q}}{\partial \phi} = 2(\Omega + \tilde{\omega}) - \frac{\partial^2 \tilde{\omega}}{\partial \phi^2} + 3 \tan \phi \frac{\partial \tilde{\omega}}{\partial \phi} - (\sin^2 \phi) e^\xi \frac{\partial}{\partial \xi} \left( e^{-\xi} \frac{\partial \tilde{\omega}}{\partial \xi} \right),
$$

the meridional gradient of the basic state potential vorticity; and $\tilde{\omega} = \tilde{u}/(a \cos \phi)$, the angular velocity of the basic state.

$v_0 = \tilde{\omega} m - i \alpha_R$ with $\alpha_R = \text{Rayleigh friction coefficient};$

$v_1 = \tilde{\omega} m - i \alpha_N$ with $\alpha_N = \text{Newtonian cooling coefficient};$
$S = \frac{R/(2\Omega a)^2}{(\kappa \bar{T} + \partial T/\partial \xi)}$, the stability parameter, and $m =$ zonal wavenumber. A detailed derivation may be found in Schoeberl and Geller (1977), or following Matsuno (1970).

The above equation is transformed into canonical form by the change of dependent variable, $\Psi_m = S^{-1/2} \exp(-\frac{1}{4} \xi) \Phi_m$, and solved with a zero top boundary condition at about 95 km. It is noted that the geopotential eddy fields are used only up to 60 km, sufficiently distant from the top boundary to eliminate spurious effects.

The presence of the zero wind lines in the mean zonal wind requires a further comment. To ensure complete absorption of wave energy at the zero wind lines, the Rayleigh friction parameter is increased from its value in Fig. 11 to $5 \times 10^{-5}$ near the critical line. The coefficient increases, depending on the local zonal wind speed, up to a maximum value corresponding to typical values in the upper mesosphere.

Solutions are obtained for the first two zonal wavenumbers. The boundary conditions, the amplitude and phase of the 100 mb geopotential height field, were kindly supplied by the Freie Universitaet der Berlin. Global, monthly mean values were used.
ACKNOWLEDGMENT

This work was supported by NERC.

REFERENCES


Coffey, M. T., Mankin, W. G. and Goldman, A. 1981 Simultaneous spectroscopic determination of the latitudinal, seasonal, and diurnal variability of stratospheric N₂O, NO, NO₂ and HNO₃. ibid., 86, 7331–7341.


<table>
<thead>
<tr>
<th>Author(s)</th>
<th>Year</th>
<th>Title/Description</th>
</tr>
</thead>
</table>