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Abstract

This report gives a description of a new two-dimensional atmospheric transport model, suitable for studying atmospheric tracers with relatively long lifetimes. The numerical conventions and input requirements are outlined and a detailed description of the numerical processes is given.

1. Introduction

This report describes a two-dimensional atmospheric transport model that has been developed within the Division of Atmospheric Research of CSIRO, Australia. It describes the characteristics of the computer implementation of the transport model and in particular it covers:

(i) numerical schemes;

(ii) sign and unit conventions;

(iii) the way in which different source terms can be included, but no details of the ways in which specific sources are modelled;

(iv) the way in which the transport coefficients are represented, but not the way in which these fields can be tuned as part of the model calibration procedure.

This modelling project at DAR grew out of earlier work in this Division (formerly the Division of Atmospheric Physics). A two-dimensional model was described by Hyson et al. (1980) and applied to modelling the seasonal cycle of CO_2 by Pearman and Hyson (1980, 1981). Further studies of CO_2 distributions using that model have been described by Pearman et al. (1983). The earlier model has also been used for a number of other studies involving constituents such as CO_2, ^{13}C and chlorofluorocarbons, (Fraser et al. (1983), Pearman and Hyson (1986), Fraser et al. (1985)).

The present report defines a new model. The objects of the development of the model are:

(i) to improve the numerical techniques involved in the finite difference scheme of the model;

(ii) to restructure the model so as to give more flexibility in its possible uses, allowing for convenient changes in choice of tracers, choice of transport fields, resolution and mode of operation.

The transport model is defined by a transport equation and a set of transport coefficients. In order to implement the model on a computer, a finite representation of the transport equation is required. This report is mainly concerned with a finite difference representation of the model although a spectral form of the model is also possible. For the purposes of defining particular cases, the transport fields are always defined in spectral form. In the finite difference representations of the model, these spectral expansions are used to define the coefficients on the appropriate spatial grid. This

provides a systematic way of changing the resolution of the finite difference scheme without involving ad hoc interpolations of transport fields.

The layout of the remainder of this report is as follows. Section 2 gives the general specifications that apply to all versions of the model. Section 3 gives the basic transport equation and describes the co-ordinate transformations that are involved in expressing this equation in the standard dimensionless form used in the computer routines. Section 4 defines the standard spectral representation of the transport fields and in particular it gives the symmetries that are appropriate given the boundary conditions. Section 5 gives the standard finite difference scheme that is used and analyses the stability and accuracy of the numerical schemes that are considered. Section 6 discusses some of the different ways in which the numerical forms of the transport equation can be used in particular calculations and describes how sources are represented. Section 7 compares this model to the older two-dimensional model.

2. Specification of the computer model

The computer model is designed to be a finite difference representation of the two-dimensional transport equations including source and sink terms. The main features are

(i)   Calculations within the model use dimensionless variables (see Section 3).

(ii)   The horizontal and vertical grids are equally spaced in terms of their respective co-ordinates.

(iii)   The vertical co-ordinate may be either reduced pressure p or a height co-ordinate given by $-\ln(p)$.

(iv)   The transport equation also allows the horizontal co-ordinate to be either the latitude (in radians), or $y=\sin(\text{latitude})$, but at the time of writing the routines to input the relevant transport coefficients have only been implemented for the latter case.

(v)   All routines are written so as to be independent of the resolution. The actual resolution is defined in a single common block which is initialised by a data statement in a BLOCK DATA subprogram. (The same subprogram must allocate sufficient storage for the concentration, derivative and transport fields.)

(vi)   The tracer variables are formally described in terms of their concentrations at relevant grid points rather than the mass of tracer in each 'cell'. While the distinction is not

significant for an equal pressure and sine (latitude) grid it is very important for all other grids.

(vii)   A spectral representation of the transport fields is used as the standard input. The grid values required by the finite difference form are obtained by expanding the spectral form onto the grid. This provides a systematic way of redefining the transport coefficients when the model resolution is changed.

(viii)   The transport equation is set up so that the transport fields can be effectively changed at each time step according to the spectral representation. This provides a smooth variation in derived quantities. (Section 4 describes the structures that are used in allowing the 'continuous' change of transport fields.) The changes may be made less frequently if required.

(ix)   The model is implemented as a library of routines that can be linked together in different ways for different problems. In particular, the calculation of the transports is entirely separate from the source-sink calculations so that the same transport routines can be used with any tracer, and with any number of tracers, subject to the limitations of the computer.

(x)   The time-stepping routines are provided with a standard 'interupt' facility to allow for abnormal actions (e.g. additional output) at particular times.

(xi)   The standard ordering of co-ordinates in the computer code is: vertical, horizontal, time, regardless of whether real space-time, or Fourier or mixed representations are involved.

3. The transport equation

In the model, the transport equation is expressed in terms of reduced quantities that are obtained by scaling the more general physical quantities.

The quantities that define the reduced units are

a   the radius of the earth (6.371×10^6 m)

H   the scale height of the atmosphere (8×10^3 m)

P_o the surface pressure (1012.5 mb)

M   the mass of the atmosphere (5.137×10^{18} kg)

T   the period of seasonal variation (1 year = 3.15576 x 10^7 sec)

These quantities are used to construct the dimensionless quantities:

$p = P_z/P_o$ (pressure in atmospheres),   (3.1a)

$t = $ time$/T$ (time in years),   (3.1b)

$z = x_3/H$ (height in scale heights),   (3.1c)

$\phi = x_2/a$ (horizontal distance in earth radii
                      $\equiv$ latitude in radians).   (3.1d)

The 'two-dimensional densities' are expressed in terms of zonally integrated mass per unit square

$$m_{\phi z} = (2\pi a^2 H \rho(x_3) \cos\phi)/M, \quad\quad\quad (3.2)$$

where x_2 and x_3 are the horizontal and vertical co-ordinates in general units (e.g. metres) and $\rho(z)$ is the atmospheric density at height z.

The isothermal assumption corresponds to

$$\rho(x_3) = \rho(0) \exp(-x_3/H) = \rho_o p, \quad\quad\quad (3.3)$$

so

$$M = 4\pi a^2 \int_0^\infty \rho(x_3) \, dx_3 = 4\pi a^2 \rho_o H \quad\quad\quad (3.4)$$

and

$$m_{\phi z} = \frac{1}{2} p \cos\phi . \quad\quad\quad (3.5)$$

In the vertical there is a choice of p or z co-ordinates, the p co-ordinate giving an 'equal mass' division of the atmosphere. In the horizontal direction the reduced equal mass co-ordinate is denoted y where

$$y = \sin\phi . \quad\quad\quad (3.6)$$

(In more general units, $a\sin\phi$ gives an equal mass co-ordinate).

In terms of other combinations of co-ordinates the two-dimensional densities are:

$$m_{yp} = \tfrac{1}{2} \quad , \tag{3.7a}$$

$$m_{yz} = \tfrac{1}{2}p \quad , \tag{3.7b}$$

$$m_{\phi p} = \tfrac{1}{2}\cos\phi \quad , \tag{3.7c}$$

and are related by

$$\int_0^\infty \int_{-\pi/2}^{\pi/2} m_{\phi z}\, d\phi dz = \int_0^\infty \int_{-1}^1 m_{yz}\, dydz$$

$$= \int_0^1 \int_{-\pi/2}^{\pi/2} m_{\phi p}\, d\phi dp$$

$$= \int_0^1 \int_{-1}^1 m_{yp}\, dydp = 1 \quad . \tag{3.8}$$

The advective flow conserves atmospheric mass, a property that can be written in general vector notation as

$$\mathrm{div}(m\underline{v}) = 0 \quad . \tag{3.9}$$

This implies that we can write

$$m\underline{v} = \mathrm{curl}\ \underline{\psi} \quad . \tag{3.10}$$

For two-dimensional flows ψ can be regarded as a pseudoscalar and

$$mv_y = -\frac{\partial\psi}{\partial z} \quad , \tag{3.11a}$$

$$mv_z = +\frac{\partial\psi}{\partial y} \quad . \tag{3.11b}$$

More generally,

$$m_{yz}v_y = m_{\phi z}v_\phi = -\frac{\partial\psi}{\partial z} \quad . \tag{3.12a}$$

Multiplying by $\frac{\partial z}{\partial p} = \frac{-1}{p}$ and using (3.5) and (3.7a-c) shows that (3.12a) is equivalent to

$$m_{yp}v_y = m_{\phi p}v_\phi = \frac{\partial\psi}{\partial p} \quad . \tag{3.12b}$$

In the vertical direction

$$m_{yz}v_z = -m_{yp}v_p = \frac{\partial\psi}{\partial y} \quad . \tag{3.12c}$$

Multiplying by $\frac{\partial y}{\partial \phi} = \cos\phi$ gives

$$m_{\phi z} v_z = -m_{\phi p} v_p = \frac{\partial \psi}{\partial \phi} \quad . \tag{3.12d}$$

These relations occur because

$$v_y = v_\phi \cos\phi \quad , \tag{3.13a}$$

$$v_p = -p \, v_z \quad . \tag{3.13b}$$

The velocity v_ϕ is the conventional mean meridional velocity and v_z is the mean vertical velocity. The quantity v_p is (in reduced units) the vertical 'pressure velocity' ω used by Oort (1983).

Since m_{yz} is proportional to ρ, the divergence equation becomes

$$-\frac{\partial^2 \psi}{\partial \phi \partial z} + \frac{\partial^2 \psi}{\partial z \partial \phi}$$

$$= \frac{\partial}{\partial \phi} \, m_{\phi z} v_\phi + \frac{\partial}{\partial z} \, m_{\phi z} v_z$$

$$= \frac{1}{2\rho_o} \left[\frac{\partial}{\partial \phi} \, \rho \cos\phi \, v_\phi + \cos\phi \frac{\partial}{\partial z} \, \rho \, v_z \right]$$

$$= \frac{\cos\phi}{2\rho_o} \quad \text{x [div } \rho\underline{v} \text{ in spherical co-ordinates, ignoring radial divergence].} \tag{3.14}$$

In looking at the advection of tracers we use the relations (based on 3.13 a-b),

$$v_y \frac{\partial c}{\partial y} = v_\phi \cos\phi \frac{\partial c}{\partial y} = v_\phi \frac{dy}{d\phi} \frac{\partial c}{\partial y} = v_\phi \frac{\partial c}{\partial \phi} \quad , \tag{3.15a}$$

$$v_p \frac{\partial c}{\partial p} = -p \, v_z \frac{\partial c}{\partial p} = v_z \frac{dp}{dz} \frac{\partial c}{\partial p} = v_z \frac{\partial c}{\partial z} \quad . \tag{3.15b}$$

The general derivative which represents the rate of change of ρc in a moving fluid parcel is

$$\frac{D}{Dt} (\rho c) = \frac{\partial}{\partial t} (\rho c) + \text{div}(\rho \underline{v} c) \quad .$$

$$= \rho \frac{\partial c}{\partial t} + \rho \, \underline{v}.\text{grad}(c) \quad , \tag{3.16}$$

8

using $\frac{\partial \rho}{\partial t} = 0$ and div$(\rho \underline{v}) = 0$. Equations (3.15a-b) show that the $\underline{v}$.grad(c) can be expressed in any of the four co-ordinate systems using the appropriate v.

The lowest order closure of the zonal averaging process equates $\frac{D}{Dt}(\rho c)$ to the divergence of a flux that is linearly related to the concentration gradient through a diffusion tensor $\underline{K}$.

Thus the full transport equation can be written in y-p co-ordinates as

$$m_{yp}\left(\frac{\partial c}{\partial t} + \underline{v}.grad\ c\right) = \frac{\partial}{\partial y}\left(m_{yp}\ K_{yy}\ \frac{\partial c}{\partial y} + m_{yp}\ K_{yp}\ \frac{\partial c}{\partial p}\right)$$

$$+ \frac{\partial}{\partial p}\left(m_{yp}\ K_{py}\ \frac{\partial c}{\partial y} + m_{yp}\ K_{pp}\ \frac{\partial c}{\partial p}\right)\ . \quad (3.17a)$$

Multiplying by p gives

$$m_{yz}\left(\frac{\partial c}{\partial t} + \underline{v}.grad\ c\right) = \frac{\partial}{\partial y}\left(m_{yz}\ K_{yy}\ \frac{\partial c}{\partial y} + m_{yz}\ K_{yz}\ \frac{\partial c}{\partial z}\right)$$

$$+ \frac{\partial}{\partial z}\left(m_{yz}\ K_{zy}\ \frac{\partial c}{\partial y} + m_{yz}\ K_{zz}\ \frac{\partial c}{\partial z}\right)\ , \quad (3.17b)$$

taking

$$K_{yp} = -p\ K_{yz}\ , \quad\quad\quad\quad\quad\quad\quad\quad\quad (3.18a)$$

$$K_{py} = -p\ K_{zy}\ , \quad\quad\quad\quad\quad\quad\quad\quad\quad (3.18b)$$

$$K_{pp} = p^2\ K_{zz}\ . \quad\quad\quad\quad\quad\quad\quad\quad\quad (3.18c)$$

Multiplying by $\cos\phi$ gives

$$m_{\phi p}\left(\frac{\partial c}{\partial t} + v.grad\ c\right) = \frac{\partial}{\partial \phi}\left(m_{\phi p}\ K_{\phi\phi}\ \frac{\partial c}{\partial \phi} + m_{\phi p}\ K_{\phi p}\ \frac{\partial c}{\partial p}\right)$$

$$+ \frac{\partial}{\partial p}\left(m_{\phi p}\ K_{p\phi}\ \frac{\partial c}{\partial \phi} + m_{\phi p}\ K_{pp}\ \frac{\partial c}{\partial p}\right), \quad (3.18d)$$

taking

$$K_{yy} = \cos^2\phi\ K_{\phi\phi}\ , \quad\quad\quad\quad\quad\quad\quad\quad (3.18e)$$

$$K_{yp} = \cos\phi\ K_{\phi p}\ , \quad\quad\quad\quad\quad\quad\quad\quad (3.18f)$$

$$K_{py} = \cos\phi\ K_{p\phi}\ , \quad\quad\quad\quad\quad\quad\quad\quad (3.18g)$$

and finally, multiplying to both p and $\cos\phi$ gives

$$m_{\phi z} \left[\frac{\partial c}{\partial t} + \underline{v}.\text{grad } c \right] = \frac{\partial}{\partial \phi} \left[m_{\phi z} \; K_{\phi \phi} \; \frac{\partial c}{\partial \phi} + m_{\phi z} \; K_{\phi z} \; \frac{\partial c}{\partial z} \right]$$

$$+ \frac{\partial}{\partial z} \left[m_{\phi z} \; K_{z\phi} \; \frac{\partial c}{\partial \phi} + m_{\phi z} \; K_{zz} \; \frac{\partial c}{\partial z} \right] \quad , \text{(3.18h)}$$

taking

$$K_{yp} = p \, \cos\phi \; K_{\phi z} \quad , \tag{3.18i}$$

$$K_{py} = p \, \cos\phi \; K_{z\phi} \quad , \tag{3.18j}$$

in addition to the relations (3.18a-d).

The relations can be summarised in a general tensor notation as

$$m_{\alpha\beta} \left[\frac{\partial c}{\partial t} + v_\alpha \frac{\partial c}{\partial \alpha} + v_\beta \frac{\partial c}{\partial \beta} \right]$$

$$= \frac{\partial}{\partial \alpha} \left[m_{\alpha\beta} \; K_{\alpha\alpha} \; \frac{\partial c}{\partial \alpha} + m_{\alpha\beta} \; K_{\alpha\beta} \; \frac{\partial c}{\partial \beta} \right]$$

$$+ \frac{\partial}{\partial \beta} \left[m_{\alpha\beta} \; K_{\beta\alpha} \; \frac{\partial c}{\partial \alpha} + m_{\alpha\beta} \; K_{\beta\beta} \; \frac{\partial c}{\partial \beta} \right] \quad , \tag{3.19}$$

and relations (3.12) reduce to

$$m_{\alpha\beta} \, v_\beta = + \frac{\partial \psi}{\partial \alpha} \quad , \tag{3.20a}$$

$$m_{\alpha\beta} \, v_\alpha = - \frac{\partial \psi}{\partial \beta} \quad , \tag{3.20b}$$

so long as (α,β) define a right handed co-ordinate system e.g. (y,z), (ϕ,z), (p,ϕ), (p,y).

(For convenience of coding the numerical model actually uses $\alpha = \ln p$ $= -z$ or p and $\beta = y$ or ϕ. Hence α always increases downwards and β always increases northwards.)

Combining eqs. (3.20 a,b) and (3.19) gives

$$m_{\alpha\beta} \; \frac{\partial c}{\partial t} = \frac{\partial}{\partial \alpha} \left[m_{\alpha\beta} \; K_{\alpha\alpha} \; \frac{\partial c}{\partial \alpha} + (m_{\alpha\beta} \; K_{\alpha\beta} - \psi) \; \frac{\partial c}{\partial \beta} \right]$$

$$+ \frac{\partial}{\partial \beta} \left[m_{\alpha\beta} \; K_{\beta\beta} \; \frac{\partial c}{\partial \beta} + (m_{\alpha\beta} \; K_{\beta\alpha} + \psi) \; \frac{\partial c}{\partial \alpha} \right] \quad . \tag{3.21}$$

10

Clearly, any anti-symmetric contribution to the diffusion tensor will influence the transport in precisely the same way as the streamfunction ψ. Therefore we define

$$K_s = (K_{\alpha\beta} + K_{\beta\alpha})/2 \quad , \tag{3.22}$$

and

$$\psi^* = \psi + m_{\alpha\beta} (K_{\beta\alpha} - K_{\alpha\beta})/2 \quad , \tag{3.23}$$

so that eq. (3.21) simplifies to

$$m_{\alpha\beta} \frac{\partial c}{\partial t} = \frac{\partial}{\partial \alpha} \left[m_{\alpha\beta} K_{\alpha\alpha} \frac{\partial c}{\partial \alpha} + (m_{\alpha\beta} K_s - \psi^*) \frac{\partial c}{\partial \beta} \right]$$

$$+ \frac{\partial}{\partial \beta} \left[m_{\alpha\beta} K_{\beta\beta} \frac{\partial c}{\partial \beta} + (m_{\alpha\beta} K_s + \psi^*) \frac{\partial c}{\partial \alpha} \right] \quad . \tag{3.24}$$

It is this equation which will be numerically integrated.

4. Transport fields; spectral specification and boundary conditions

The four transport fields (the streamfunction and the three diffusion coefficients) are expanded as a multiple Fourier series, viz.,

$$F(p,y,t) = \sum_{k,m,n} f_{kmn} \, g_k(p) \, g_m(y^*) \, g_n(2t) \quad , \tag{4.1}$$

where $y^* = \tfrac{1}{2}(y+1)$, (4.2a)

and $g_n(x) = \begin{cases} \cos(n_\pi x) & n \geqq 0 \\ \sin(n_\pi x) & n < 0 \end{cases}$ (4.2b)

This can be regarded as a triple Fourier expansion on the range

$$-1 \leqq y^* \leqq 1 \tag{4.3a}$$
$$-1 \leqq p \leqq 1 \tag{4.3b}$$
$$0 \leqq t \leqq 1 \quad . \tag{4.3c}$$

The extended range of y^* and p (see eqs. 4.3) has been chosen so that each of the transport fields will be an odd or even function of the space variables. This enables some of the boundary conditions to be satisfied automatically.

Although each co-ordinate system uses one particular set of transport coefficients (e.g. a constant pressure and sine (latitude)

model uses ψ, K_{yy}, K_{yp} and K_{pp}) the computer code is written more generally. Fourier coefficients of different types of co-ordinate systems are read, the fields are projected onto the appropriate grid, and then these grid values are multiplied by scaling factors to convert them to the relevant co-ordinate systems. Thus at each grid point we have a set of Fourier coefficients describing the temporal variation of the transport coefficients. These spectral representations are summed at regular intervals in order to obtain the coefficients required in the transport routine. After the evaluation of the coefficients for a particular time, additional constraints such as the positivity constraints (4.6 a-c) are applied.

In practice the coefficients are derived from K_{yy}, K_{zz} and K_s (in p-y space). These have been chosen because they vary more slowly in space than the other possibilities. Hence, a desired accuracy can be achieved with the smallest possible number of fourier coefficients.

Both mass and velocity streamfunctions have been tested in the initial Fourier decomposition. For further discussion of the differences and the physical applicability of this formalism, see Enting and Mansbridge (1986).

We have obtained sets of spectral coefficients by taking least squares fits to various sets of transport coefficients from other sources. The choices of expansions are as follows:

(i) The streamfunction, ψ, is odd in p and y. Thus there is no flow through the boundaries as $\psi=0$ for p=0 or 1 and y*=0 or 1.

(ii) The cross-diffusion term, K_s, is odd in p and y, and so $K_s=0$ on the boundaries. At y*=0 and 1 this boundary condition is a necessary consequence of the geometry of a zonally averaged model. At p=0 and 1 the condition ensures that no tracer cross-diffuses through these boundaries.

(iii) The horizontal diffusion, K_{yy}, is even in p. This choice is made because K_{yy} is observed to be fairly constant over height with no tendency towards zero at the horizontal boundaries. However, the geometry of the model indicates that $K_{yy} \to 0$ quadratically when y* → 0 and 1 (see eqn 3.18e). This behaviour has been reproduced in two different ways. One method is to express K_{yy} as an even series in y but to chose the Fourier coefficients so that $K_{yy} = 0$ at y* = 0 and 1; this then ensures quadratic convergence. The second method is to use a sine series expansion. Although this only ensures a linear convergence to zero it does not require any arbitrary modification of a least squares fit. The former approach has been used in dealing with the K_{yy}'s of Hyson et al. (1980) and the latter in dealing with those of Plumb and Mahlman (1985). Neither approach was clearly superior.

(iv) The vertical diffusion, K_{zz}, is also handled differently for the Hyson and the Plumb fields. The Hyson fields were derived without assuming any boundary conditions on the K_{zz}'s. (The condition of no tracer flux through the vertical boundaries is met by enforcing $\partial c/\partial p = 0$ at those boundaries.) Accordingly, they were fitted by cosines in p and y*. Because we are using an enlarged spatial domain these series will fit the Hyson field smoothly. However, the Plumb fields have $K_{zz} \rightarrow 0$ at y* = 0 or 1 and p = 0. Hence it was appropriate to expand these in sine series in both directions.

Using symmetric expansions, as above, also ensures continuity of the transport fields and their first derivatives. This improves the rate of convergence of the Fourier expansion (see Acton, 1970, pp 225-227).

Having found a spectral expansion of the transport fields it is then easy to represent these fields at the appropriate points in the grid used by the numerical scheme. However, the scheme will be unstable if the tracer is transported counter-gradient. This is demonstrated by the stability analysis in Section 5. Alternatively, from physical grounds, it must be very difficult to describe the "unmixing" process as tracer gradients are strengthened.

Values of the diffusion coefficients which imply up-gradient transfer can occur for many reasons. Firstly, they may result from errors involved in observing or modelling the real atmosphere. A second source of error is the least squares spectral analysis described earlier in this section. Also, up-gradient fluxes may actually occur in some regions of the atmosphere. Wallace (1978) describes, and offers an explanation for, this phenomenon.

The diffusive flux of a tracer is given in eq. (3.19) and so the condition of no up-gradient flux is that

$$-[m_{\alpha\beta}K_{\alpha\alpha}\frac{\partial c}{\partial \alpha} + m_{\alpha\beta}K_{\alpha\beta}\frac{\partial c}{\partial \beta}]\frac{\partial c}{\partial \alpha} - [m_{\alpha\beta}K_{\beta\beta}\frac{\partial c}{\partial \beta} + m_{\alpha\beta}K_{\beta\alpha}\frac{\partial c}{\partial \alpha}]\frac{\partial c}{\partial \beta} \leq 0.$$

$$(4.4)$$

After some manipulation eq. (4.4) becomes

$$K_{\alpha\alpha}\left(\frac{\partial c}{\partial \alpha}\right)^2 + 2K_s\frac{\partial c}{\partial \alpha}\frac{\partial c}{\partial \beta} + K_{\beta\beta}\left(\frac{\partial c}{\partial \beta}\right)^2 \geq 0 \qquad . \qquad (4.5)$$

Note that the antisymmetric part of the diffusion tensor (which contributes to streamfunction $\psi*$) has disappeared and is therefore unrestricted. It is easily shown that eq. (4.5) is true for any $\partial c/\partial \alpha$ and $\partial c/\partial \beta$ if and only if

$$K_{\alpha\alpha} \geq 0 \quad , \qquad (4.6a)$$

$$K_{\beta\beta} \geq 0 \quad , \qquad (4.6b)$$

$$|K_s| \leq K_{\alpha\alpha}^{\frac{1}{2}} K_{\beta\beta}^{\frac{1}{2}} \quad . \qquad (4.6c)$$

These conditions are always applied to the gridded values of the diffusion coefficients. In fact, as explained in Section 5, positive lower bounds are sometimes put on the $K_{\alpha\alpha}$ and $K_{\beta\beta}$.

5. Numerical implementation and stability

In the general coordinates of Section 3 the tracer equation to be solved is

$$m_{\alpha\beta} \frac{\partial c}{\partial t} = \frac{\partial}{\partial \alpha} \left[m_{\alpha\beta} K_{\alpha\alpha} \frac{\partial c}{\partial \alpha} + (m_{\alpha\beta} K_s - \psi^*) \frac{\partial c}{\partial \beta} \right]$$

$$+ \frac{\partial}{\partial \beta} \left[m_{\alpha\beta} K_{\beta\beta} \frac{\partial c}{\partial \beta} + (m_{\alpha\beta} K_s + \psi^*) \frac{\partial c}{\partial \alpha} \right] + m_{\alpha\beta} R, \quad (5.1)$$

where R represents the combined source and sink terms.

In eq.(5.1) the transport terms can be arranged as the divergence of a flux vector. This flux through the boundaries of a cell can be approximated by a centred-space differencing scheme as described by Miller et al. (1981). The resultant, mass conserving, finite difference equation is

$m(I,J) \, \partial/\partial t \, [c(I,J)] - m(I,J) \, R(I,J) =$

$[c(I-1,J) - c(I,J)] \, Q_{\alpha\alpha}(I-1,J) + [c(I+1,J) - c(I,J)] \, Q_{\alpha\alpha}(I,J)$

$+ [c(I,J+1) - c(I,J)] \, Q_{\beta\beta}(I,J) + [c(I,J-1) - c(I,J)] \, Q_{\beta\beta}(I,J-1)$

$+ [c(I-1,J-1) - c(I,J)] \, Q_s(I-1,J-1) - [c(I+1,J-1) - c(I,J)] \, Q_s(I,J-1)$

$- [c(I-1,J+1) - c(I,J)] \, Q_s(I-1,J) + [c(I+1,J+1) - c(I,J)] \, Q_s(I,J)$

$+ [c(I+1,J) - c(I,J+1)] \, \psi(I,J) + [c(I,J+1) - c(I-1,J)] \, \psi(I-1,J)$

$+ [c(I-1,J) - c(I,J-1)] \, \psi(I-1,J-1) + [c(I,J-1) - c(I+1,J)] \, \psi(I,J-1) .$

$$(5.2)$$

Here

$$Q_{\alpha\alpha}(I,J) \quad = \quad m \, K_{\alpha\alpha}/(\Delta\alpha)^2 \quad , \qquad (5.3a)$$

$$Q_{\beta\beta}(I,J) \quad = \quad m \, K_{\beta\beta}/(\Delta\beta)^2 \quad , \qquad (5.3b)$$

$$Q_s(I,J) \quad = \quad m \, K_s/(2\Delta\alpha\Delta\beta) \quad , \qquad (5.3c)$$

$$\psi(I,J) \quad = \quad \psi^*/(2\Delta\alpha\Delta\beta) \qquad , \qquad (5.3d)$$

and the terms on the right-hand side of eqs.(5.3) are evaluated at the

positions shown in Fig.1. Note that the index I increases downwards (increasing pressure or decreasing height) and the index J increases northwards.
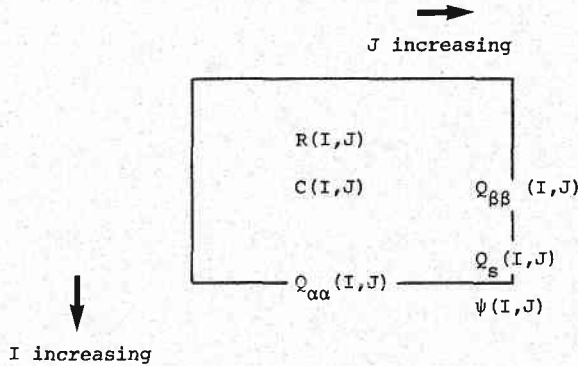
J increasing

R(I,J)

C(I,J) $Q_{\beta\beta}$ (I,J)

Q_s (I,J)

$Q_{\alpha\alpha}$ (I,J) ———— ψ (I,J)

I increasing

Figure 1. The positions of C(I,J), $Q_{\alpha\alpha}$(I,J), $Q_{\beta\beta}$(I,J), Q_s(I,J),
R(I,J) and ψ(I,J) in the (I,J) cell.

The use of a centred space differencing scheme ensures that the errors introduced by the transport terms are $O(\Delta\alpha^2, \Delta\beta^2)$. These small errors are most noticeable when the value of c changes greatly from one cell to the next, such as when radioactive tracer has just been released in a simulated nuclear explosion. Of course, every grid point method assumes that all fields only vary slowly and so will handle such conditions poorly.

However, these errors will be much smaller than those in an alternative scheme such as upwind differencing. There the $O(\Delta\alpha, \Delta\beta)$ errors are manifested as numerical diffusion (see Noye, 1982, p.87).

For the time integration of eq.(5.1) a predictor-corrector method was chosen. This has $O(\Delta t)^2$ errors and so is more accurate than a simple forward time differencing scheme; it also has better numerical stability properties which will be discussed later. The predictor-corrector method was chosen ahead of fully implicit methods, which have greater accuracy and are unconditionally stable, for two reasons. Firstly an explicit scheme uses less computer time (per step) and less space. Secondly, a fully implicit method is impractical once source terms are included.

The predictor-corrector method is best described by using the following notation. Let the sets of transport co-efficients and concentrations be denoted by $\{\phi_k(t), k=1,K\}$ and $\{c_i, i=1,N\}$. Then eq.(5.2) can be rewritten as

$$\frac{\partial c_i}{\partial t} = \sum_{j=1}^{N} L(\underline{\phi})_{ij} \, c_j + R_i(t) \qquad (5.4a)$$

$$= \sum_{j=1}^{N} \sum_{k=1}^{K} L_{ijk} \, c_j \, \phi_k(t) + R_i(t) \quad . \qquad (5.4b)$$

The form (5.4b) emphasises that the transport operator L is linear and independent of t.

The predictor-corrector method has two steps. The first, the predictor, is a forward time step giving

$$c_i^*(t+\Delta t) = c_i(t) + \Delta t \left[\sum_j L[\underline{\phi}(t)]_{ij} \, c_j(t) + R_i(t) \right] . \qquad (5.5a)$$

The second step, the corrector, gives

$$c_i(t+\Delta t) = c_i(t) + \frac{1}{2} \Delta t \left[\sum_j L[\underline{\phi}(t)]_{ij} \, c_j(t) + R_i(t) + \right.$$

$$\left. \sum_j L[\underline{\phi}(t+\Delta t)]_{ij} \, c_j^*(t+\Delta t) + R_i(t+\Delta t) \right] . \qquad (5.5b)$$

Efficient use of storage in the computer is achieved by using a routine that takes a given vector $\underline{x}$ and adds to it

$$\sum_j L(\underline{\phi}) \, c_j .$$

The integration scheme can then be schematically written at time t as

$$x_i \leftarrow 0$$

$$x_i \leftarrow x_i + \sum_j L(\underline{\phi}(t))_{ij} \, c_j(t) + R_i \qquad\qquad *$$

$$c_i \leftarrow c_i + \Delta t \, x_i$$

$$x_i \leftarrow -x_i$$

$$t \leftarrow t + \Delta t$$

$$x_i \leftarrow x_i + \sum_j L(\underline{\phi}(t)) \, c_j(t) + R_i \qquad *$$

$$c_i \leftarrow c_i + \tfrac{1}{2}\Delta t \, x_i \, .$$

The routine to add the rate of change to the vector $\underline{x}$ is used in the two steps denoted *. Note that in the second step t and c refer to updated variables.

Integration of an initial value problem from t_o to $t_o + n\Delta t$ can now be carried out by applying the predictor-corrector method n times. The linear transport term is described by the right-hand side of eq.(5.2) divided by $m(I,J)$.

This expression is always well defined provided that the boundary conditions described in Section 4 are applied. If there are M levels in the vertical and N zones in the horizontal then these boundary conditions become

$$\psi^*(0,J) = Q_s(0,J) = Q_{pp}(0,J) = 0, \qquad (5.6a)$$

$$\psi^*(M,J) = Q_s(M,J) = 0, \; C(M+1,J) = C(M,J), \qquad (5.6b)$$

$$\psi^*(I,0) = Q_s(I,0) = Q_{yy}(I,0) = 0 \, , \qquad (5.6c)$$

$$\psi^*(I,N) = Q_s(I,N) = Q_{yy}(I,N) = 0 \, , \qquad (5.6d)$$

In fact, because the above conditions involve setting terms in eq.(5.2) equal to zero, the computer code can be written so that it is not necessary to refer to indices of I and J outside the ranges 1 to M and 1 to N respectively. However, an alternative version of the transport routine using vector instructions explicitly requires certain boundary values to be zero.

The above description of the numerical method does not indicate what values of Δt should be used. An upper limit on Δt is provided by the stability criteria.

A stability analysis is carried out after rewriting eq.(5.1) as

$$\frac{\partial c}{\partial t} = K_{\alpha\alpha} \frac{\partial^2 c}{\partial \alpha^2} + K_{\beta\beta} \frac{\partial^2 c}{\partial \beta^2}$$

$$+ \frac{1}{m_{\alpha\beta}} \left[\frac{\partial}{\partial \alpha} (m_{\alpha\beta} K_{\alpha\alpha}) + \frac{\partial \psi^*}{\partial \beta} \right] \frac{\partial c}{\partial \alpha} + \frac{1}{m_{\alpha\beta}} \left[\frac{\partial}{\partial \beta} (m_{\alpha\beta} K_{\beta\beta}) - \frac{\partial \psi^*}{\partial \alpha} \right] \frac{\partial c}{\partial \beta} \, .$$

$$(5.7)$$

The source and sink terms have been neglected and for tractability it is also assumed that $K_s = 0$, i.e. there is no off-diagonal diffusion.

We then define the diffusion numbers

$$S_\alpha = \frac{K_{\alpha\alpha}\Delta t}{(\Delta\alpha)^2} \quad , \quad S_\beta = \frac{K_{\beta\beta}\Delta t}{(\Delta\beta)^2} \quad , \tag{5.8}$$

and the effective Courant numbers

$$C_\alpha = \frac{1}{m_{\alpha\beta}} \left[\frac{\partial}{\partial\alpha} (m_{\alpha\beta} K_{\alpha\alpha}) + \frac{\partial\psi^*}{\partial\beta} \right] \Delta t/\Delta\alpha,$$

$$C_\beta = \frac{1}{m_{\alpha\beta}} \left[\frac{\partial}{\partial\beta} (m_{\alpha\beta} K_{\beta\beta}) - \frac{\partial\psi^*}{\partial\alpha} \right] \Delta t/\Delta\beta \ . \tag{5.9}$$

(If $\frac{\partial}{\partial\alpha} (m_{\alpha\beta} K_{\alpha\alpha}) = \frac{\partial}{\partial\beta} (m_{\alpha\beta} K_{\beta\beta}) = 0$ then these become the more usual

Courant numbers).

We have applied a Von Neumann linear stability analysis (as described in Noye, 1982, p.31) to study eq.(5.7) for centred space differencing and predictor-corrector time integration. The scheme will be stable provided that S_α, S_β, C_α and C_β all satisfy certain restrictions. For the diffusion coefficient there are necessary and sufficient conditions, viz.,

$$S_\alpha \geqslant 0, \ S_\beta \geqslant 0 \ \text{and} \ S_\alpha + S_\beta \leqslant \tfrac{1}{2} \quad . \tag{5.9}$$

Two sets of sufficient conditions have been found for the Courant numbers. These are

$$|C_\alpha| \leq \surd 2 \ S_\alpha, \ |C_\beta| \leq \surd 2 \ S_\beta \ , \tag{5.10}$$

and

$$C_\alpha^2 \leq S_\alpha \ [1-2(S_\alpha+S_\beta)]/2, \ C_\beta^2 \leq S_\beta \ [1-2(S_\alpha+S_\beta)]/2. \tag{5.11}$$

If S_α, $S_\beta > 1/8$ then conditions (5.10) are less restrictive, but if S_α, $S_\beta < 1/8$ then conditions (5.11) should be applied.

The first two conditions of eq.(5.9) are necessary for diffusion to be down-gradient. We have discussed this in some detail in section 4.

The third of conditions (5.9) shows (after using eq.5.8) that

$$\Delta t \leq \left[\frac{2\ K_{\alpha\alpha}}{(\Delta\alpha)^2} + \frac{2\ K_{\beta\beta}}{(\Delta\beta)^2} \right]^{-1} \tag{5.12}$$

for stability. In practice, eq.(5.12) sets the upper limit on the time step for the transport coefficients used by us. This is quite restrictive because if the spatial resolution is doubled then the time step must be quartered.

The sufficient conditions (5.10) and (5.11) indicate that in regions where S_α or S_β are small then the integration might become unstable. In practice however this difficulty never arises. As mentioned in Section 4 we usually impose physically realistic lower bounds on the $K_{\alpha\alpha}$ and $K_{\beta\beta}$. This serves not only to satisfy the restrictions on the Courant numbers but also to smooth out the $O(\Delta\alpha^2, \Delta\beta^2)$ errors due to the spatial differencing.

Equation (5.11) indicates a further advantage of the predictor corrector method over the forward time differencing. The latter method has a necessary and sufficient stability criteria of $C_\alpha \leq 2S_\alpha$, $C_\beta \leq 2S_\beta$. For small S_α, S_β this is much more restrictive than eq.(5.11).

6. Source specificiation and deduction

The time integration scheme described in Section 5 uses a combined source and sink term, denoted by $R(I,J)$ in eq.(5.2). The specification of this term requires some care.

In the general formalism c represents a scaled mixing ratio of the particular constituent. The total amount of the constituent is proportional to $\int mc\,d\alpha\,d\beta$, where m is the "density" in terms of α,β coordinates. In the finite difference form the mean, scaled atmospheric mixing ratio is

$$c = \sum_i m_i\ c_i\ \Delta\alpha\ \Delta\beta \ / \ \sum_i m_i\ \Delta\alpha\ \Delta\beta \ . \tag{6.1}$$

Note that if coordinates other than p-y are used then the denominator of eq.(6.1) will differ slightly from 1 because of discretization errors.

Multiplying c by M_A, the number of moles of air, gives the total number of moles of the tracer.

It is this quantity that the model conserves to within rounding errors.

From these specifications it follows that a source of S_i moles per unit time will give

$$m_i \frac{\partial c_i}{\partial t} = S_i / (M_A \, \Delta\alpha \, \Delta\beta) \quad . \tag{6.2}$$

Thus, in the notation of eq.(5.2),

$$m(I,J) \, R(I,J) = S(I,J) / (M_A \, \Delta\alpha \, \Delta\beta), \tag{6.3}$$

where $S(I,J)$ is the number of moles of tracer being put into cell I,J per unit time.

In section 5 it was explained how, given $R(I,J)$, the time evolution of $c(I,J)$ can be deduced. However, the simple relationship between $\partial c(I,J)/\partial t$ and $R(I,J)$ in eq.(5.2) makes it clear that for any cell it is just as easy to deduce the $R(I,J)$ if $\partial c(I,J)/\partial t$ is known.

This property has been used in a second version of the model. In this case $R(I,J)$ is deduced for the cells near the lower boundary and $C(I,J)$ is found as a function of time for the other cells. The procedure is practicable because the most complete observations of tracers are usually made near the ground whereas the sources and sinks of tracers are generally most complicated there. Enting (1984) and Enting and Mansbridge (1986) have described the use of the present model in the deduction of surface sources.

7. Relation to the older model

As indicated in the introduction, the development of this model arose from earlier two-dimensional modelling work within the CSIRO Division of Atmospheric Physics. There are two main differences between the 'old' and the 'new' models. Firstly the transport fields are different and secondly the technical details of the implementation of the model have been refined.

The refinement of the transport fields has come about through the use of transport fields obtained from a general circulation model (Plumb and Mahlman, 1985). The present report describes the general computer implementation of the model in a form that accepts as an input any set of transport coefficients (subject to the stability requirements in Section 5). The discussion of the refinement of the transport coefficients is outside the scope of this report, but has been given by Enting and Mansbridge (1986).

The main differences in technical details between the old and new models are:

(i) The new model gives a choice of coordinates and a choice of spatial resolution.

(ii) The new model uses diffusion coefficients that match the coordinate system that is in use, unlike the old model which uses K_{zz} on what is predominantly an equal pressure grid and $K_{\phi\phi}$ on an equal y grid. The new model takes the spectral expansion defined on the p-y grid and evaluates the fields at equal intervals of p or z and y or ϕ as appropriate and then performs any necessary conversion of the diffusion coefficients.

(iii) The new model uses mass stream functions rather than velocities to specify the advection. This reduces the storage requirements and automatically ensures the conservation of atmospheric mass.

(iv) The new model uses a spatial differencing scheme that is correct to second order in the grid spacing. In contrast, the old model uses upwind differencing for the advective terms and is correct only to first order. The consequences of this are that the results of the old model depend more strongly on the resolution than would be the case with a higher order scheme. As part of this effect the upwind differencing scheme produces a 'numerical diffusion' (Noye, 1982) that is so large in certain critical regions that the effective diffusion coefficients may be more than 100% larger than the diffusion coefficients tabulated by Hyson et al. (1980). Hyson et al. do not give any analysis of the accuracy of their 'mismatched' diffusion scheme (see (ii) above) but any errors that arise from this aspect are likely to be less serious than those arising from the use of upwind differencing of the advective transport. The higher order accuracy in the new model means that accurate results can be obtained with low resolution.

(v) The new model uses a spectral representation of the time variation and so the transport coefficients can be made to vary more smoothly than in the old model. Theoretical and numerical studies indicate that it is appropriate to update the transport fields at intervals of $\Delta t = 0.01$ years. This gives a much smoother behaviour than the monthly and seasonal updating used in the old model and yet still gives substantial savings in time compared to updating at each time step. As long as the coefficients are set to values for the midpoint of the interval Δt, the errors will be of order $(\Delta t)^2$.

(vi) The new model is implemented in a more modular fashion than the old model. This makes it possible to use it in a more flexible manner. The most striking example of this is the use of the new

model in the 'source-deduction' mode described in Section 6 above. Enting (1984) gives an example of how using a well-structured Pascal/Algol-like language, only 6 statements need to be added to convert a conventional numerical integration procedure into a procedure for carrying out the source deduction calculations.

The new model has been implemented in Fortran-77 on two different computers in the HP1000 series running under two different operating systems. An alternative version of the transport routine has been written in order to take advantage of the vector instructions available on the machines.

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