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The TOMCAT Offline Transport Model

Part II. Dynamics and Advection

Martyn Chipperfield and Pascal Simon

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Martyn Chipperfield[1] and Pascal Simon[2]

1. Centre For Atmospheric Science, University of Cambridge, U.K.
2. Météo-France, Toulouse, France.

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1 Introduction

TOMCAT is an off-line three-dimensional (3D) chemical transport model (CTM). The model was initially written in 1991 by Pascal Simon and Martyn Chipperfield at the Centre National de Recherches Météorologiques at Météo France in Toulouse. Since that time some further development has occurred.

TOMCAT can use winds and temperatures from a variety of sources such as meteorological analyses or GCM output. By default tracer transport is achieved using the scheme of Prather [1986]. This can be used with the conservation of second order moments, conservation of first order moments or conservation of zero order moments. TOMCAT can be used to simply advect passive tracers or can be coupled with a chemistry scheme. The TOMCAT `nupdate` library contains a stratospheric chemistry scheme which can be used with the model. Alternatively the user can supply his/her own.

A related model to TOMCAT is SLIMCAT [Chipperfield, 1996a] which is also a 3D CTM but it is formulated on isentropic levels. This model uses the same forcing files of winds and temperatures as TOMCAT and also advects tracers using the Prather [1986] scheme. The stratospheric chemistry scheme (when used) is common to both models.

A further related model is TOPCAT [Chipperfield et al., 1995]. This is a model which calculates 3D particle trajectories again using the same forcing files as TOMCAT. The TOMCAT chemistry scheme can also be used to calculate chemistry along these trajectories.

This report is Part II of a series of three reports describing the TOMCAT off-line chemical transport model (CTM). Part I [Chipperfield, 1996b] describes the TOMCAT stratospheric chemistry scheme and part III [Stockwell and Chipperfield, 1996] describes the parameterisations of convection and vertical diffusion in the troposphere.

Section 2 contains some basic definitions of quantities used in the model. Section 3 describes the formulation of the model including a detailed description of the Prather advection scheme. Section 4 lists the sources of winds and temperatures that can be used to force TOMCAT. Section 5 describes how to access standard job decks and how to run the model. Users who are just interested in running the model should skip sections 2 and 3.

2 Basic Equations

This section lists some basic equations of atmospheric motion which are used in the detailed description of the transport part of TOMCAT (section 3). The symbols used are summarised in Appendix 1.

The continuity equation is

$$\frac{\partial}{\partial\eta}(\frac{\partial p}{\partial t}) + \nabla.(\vec{\mathbf{v_h}}\frac{\partial p}{\partial\eta}) + \frac{\partial}{\partial\eta}(\eta\frac{\partial p}{\partial\eta}) = 0 \tag{1}$$

Integrating this equation from the top of the atmosphere to the ground gives the rate of change of surface pressure:

$$\frac{\partial p_s}{\partial t} = -\int_o^1 \nabla.(\vec{\mathbf{v_h}}\frac{\partial p}{\partial\eta})d\eta \tag{2}$$

Integrating the continuity equation (1) from the top of the atmosphere to level η gives the equation for the vertical velocity. In pressure coordinates this is:

$$\omega = \frac{\partial p}{\partial t} = -\int_o^\eta \nabla.(\vec{\mathbf{v_h}}\frac{\partial p}{\partial\eta})d\eta + \vec{\mathbf{v_h}}.\nabla p \tag{3}$$

In hybrid vertical coordinates the vertical velocity is:

$$\eta\frac{\partial p}{\partial\eta} = -\frac{\partial p}{\partial t} - \int_o^\eta \nabla.(\vec{\mathbf{v_h}}\frac{\partial p}{\partial\eta})d\eta \tag{4}$$

The divergence is defined as:

$$D = \frac{1}{a}\left(\frac{1}{1-\mu^2}\frac{\partial U}{\partial\lambda} + \frac{\partial V}{\partial\mu}\right) \tag{5}$$

The relative vorticity is defined as:

$$\zeta = \frac{1}{a}\left(\frac{1}{1-\mu^2}\frac{\partial V}{\partial\lambda} + \frac{\partial U}{\partial\mu}\right) \tag{6}$$

The streamfunction (ψ) and the velocity potential (χ) are given by:

$$U = \frac{1}{a}\left\{-(1-\mu^2)\frac{\partial\psi}{\partial\mu} + \frac{\partial\chi}{\partial\lambda}\right\} \tag{7}$$

$$V = \frac{1}{a}\left\{\frac{\partial\psi}{\partial\lambda} + (1-\mu^2)\frac{\partial\chi}{\partial\mu}\right\} \tag{8}$$

$$\zeta = \nabla^2\psi \tag{9}$$

$$D = \nabla^2\chi \tag{10}$$

3 Formulation of the Transport Model

This section discusses the transport part of TOMCAT and the Prather advection scheme is described in some detail.

3.1 The Prather Advection Scheme

The default advection scheme used in TOMCAT (and SLIMCAT) is a gridpoint scheme which is based on the conservation of second order moments of the tracer distribution within the gridboxes. This scheme possesses the properties of being stable, accurate, conservative and is one of the best performing of the transport schemes available. The second order moments scheme was developed by Prather [1986]. The TOMCAT model can also be used with the conservation of first order moments (equivalent to the slopes scheme of Russell and Lerner [1981]) or conservation of only zero order moments. However, the following discussion concentrates on describing the second-order moments scheme.

After describing the principle of the advection method in the simple case of 2D transport in cartesian coordinates, we will show how it is used in the more general 3D case in spherical coordinates.

3.1.1 Definitions

Consider a domain D in the cartesian grid Oxy covered by a regular grid of spacing X and Y (in the following discussion the boxes of the grid will be referenced by the indices n in the direction Ox and k in the direction Oy). Considering a portion B of the grid, of which, for simplicity, the lower left hand corner is the origin of the grid (i.e. $B = [0, X] \times [0, Y]$), we can define the local functions on this portion:

$$K_0(x,y) = 1 \tag{11}$$

$$K_x(x,y) = \frac{2}{X}\left(x - \frac{X}{2}\right)$$

$$K_y(x,y) = \frac{2}{Y}\left(y - \frac{Y}{2}\right)$$

$$K_{xx}(x,y) = \frac{6}{X^2}\left(x^2 - Xx + \frac{X^2}{6}\right)$$

$$K_{yy}(x,y) = \frac{6}{Y^2}\left(y^2 - Yy + \frac{Y^2}{6}\right)$$

$$K_{xy}(x,y) = \frac{4}{XY}\left(x - \frac{X}{2}\right)\left(y - \frac{Y}{2}\right)$$

These functions K_α form a basis for the ensemble of the polynomial functions of order less than or equal to 2 over the box B. In addition, this basis is orthogonal because:

$$\int_0^X \int_0^Y K_\alpha(x,y).K_\beta(x,y)\,dxdy = 0 \tag{12}$$

for all pairs (α, β) in $\{0, x, y, xx, xy, yy\}$ which satisfy $\alpha \neq \beta$. However, the basis is not normalised, and we have:

$$\int_0^X \int_0^Y K_0^2(x,y)\,dxdy = XY = S \tag{13}$$

$$\int_0^X \int_0^Y K_x^2(x,y)\,dxdy = S/3$$

$$\int_0^X \int_0^Y K_y^2(x,y)\,dxdy = S/3$$

$$\int_0^X \int_0^Y K_{xx}^2(x,y)\,dxdy = S/5$$
$$\int_0^X \int_0^Y K_{yy}^2(x,y)\,dxdy = S/5$$
$$\int_0^X \int_0^Y K_{xy}^2(x,y)\,dxdy = S/9$$

The moments of a function $r(x,y)$ over the box B are defined by the following equations:

$$M_0 = \int_0^X \int_0^Y \rho\, K_0(x,y)\, r(x,y)\,dxdy \tag{14}$$
$$M_x = 3\int_0^X \int_0^Y \rho\, K_x(x,y)\, r(x,y)\,dxdy$$
$$M_y = 3\int_0^X \int_0^Y \rho\, K_y(x,y)\, r(x,y)\,dxdy$$
$$M_{xx} = 5\int_0^X \int_0^Y \rho\, K_{xx}(x,y)\, r(x,y)\,dxdy$$
$$M_{yy} = 5\int_0^X \int_0^Y \rho\, K_{yy}(x,y)\, r(x,y)\,dxdy$$
$$M_{xy} = 9\int_0^X \int_0^Y \rho\, K_{xy}(x,y)\, r(x,y)\,dxdy$$

where ρ represents the mass density, taken to be uniform in the box B.

Equally, knowledge of the moment of a function $r(x,y)$ allows us to have an analytic expression of the function, or more exactly of its projection over the basis of K_α:

$$r(x,y) = \frac{1}{M}\sum_\alpha M_\alpha K_\alpha(x,y) \tag{15}$$

where $M = \rho S$ is the total mass of the box B.

Interpretation of the moments

As the functions K_α are dimensionless, if the function $r(x,y)$ is the mass mixing ratio of a constituent, the moments of r as defined above have the dimension of mass. In particular, the zero order moment, M_0, represents the total mass of tracer contained in the box B. The moment of order 1 in a given direction represents the "average" gradient over the box in this direction; the first order moments also give the position, relative to the centre of the box B, of the centre of mass of the tracer whose distribution is represented by $r(x,y)$. The second order moments are proportional to the curve of the tracer distribution, and give the matrix of the moments of inertia of the tracer distribution $r(x,y)$ for the box considered. The variance of the distribution inside the box can equally be determined from the different moments:

$$\int_0^X \int_0^Y \rho\, r(x,y)\,dxdy = M_0 \tag{16}$$
$$\int_0^X \int_0^Y \rho\, r(x,y)^2 dxdy = M_0 + \frac{1}{3}(M_x + M_y) + \frac{1}{5}(M_{xx} + M_{yy}) + \frac{1}{9}M_{xy}$$

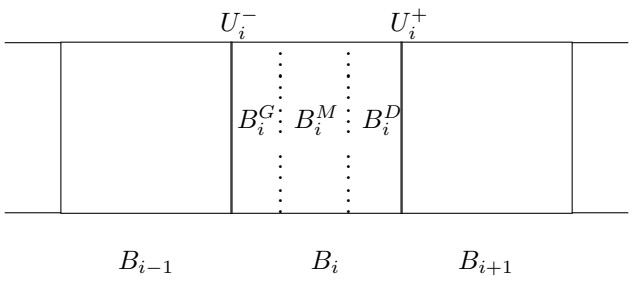


Figure 1: Example one-dimensional grid.

An important property, which arises from the above definitions, is that the moments of a function $r(x, y)$ contain the intrinsic properties of the grid in the sense that they remain invariant under all transformation on the coordinate system; in other words, all solid translations and/or stretches (compressions) of the box B do not change the moments.

3.1.2 Principle of scheme

Using the above definitions, the advection of a tracer over the period t to $t + dt$, is performed in several steps:

1. Split each box of the domain into several sub-boxes, as a function of the mass flux at the interfaces between the boxes at the instant t.

   Considering a box B_i (figure 1) and motion along the direction Ox, 3 cases are possible depending on the values of U_i^- and U_i^+, the mass fluxes across the interfaces (B_{i-1}, B_i) and (B_i, B_{i+1}).

   a) U_i^- and U_i^+ are of the same sign

   b) U_i^- positive and U_i^+ negative (convergence)

   c) U_i^- negative and U_i^+ positive (divergence).

   The box B_i is this split into a maximum of 3 sub-boxes:

   - B_i^G contains the air which is going to leave the box B_i by the left face (if U_i^- is negative).
   - B_i^D contains the air which is going to leave the box B_i by the right face (if U_i^+ is positive).
   - B_i^M contains the air which is going to stay in the box B_i during the timestep.

2. Calculate the sub-moments of each sub-box.

   The following equations allow the calculation of the sub-moments of two sub-boxes B^D and B^G of the box B split into two along Ox. For the right sub-box $B^D = [X', X] \times [0, Y]$:

$$M_0^D = \alpha \left[M_0 + (1-\alpha) M_x + (1-\alpha)(1-2\alpha) M_{xx} \right] \tag{17}$$

$$M_x^D = \alpha^2 \left[M_x + 3(1-\alpha) M_{xx} \right]$$

$$M_{xx}^D = \alpha^3 M_{xx}$$

$$M_{xy}^D = \alpha^2 M_{xy}$$
$$M_y^D = \alpha \left[M_y + (1-\alpha) M_{xy} \right]$$
$$M_{yy}^D = \alpha M_{yy}$$

and for the left sub box $B^G = [0, X'] \times [0, Y]$:

$$M_0^G = (1-\alpha) \left[M_0 - \alpha M_x - \alpha (1-2\alpha) M_{xx} \right] \tag{18}$$
$$M_x^G = (1-\alpha)^2 \left[M_x - 3\alpha M_{xx} \right]$$
$$M_{xx}^G = (1-\alpha)^3 M_{xx}$$
$$M_{xy}^G = (1-\alpha)^2 M_{xy}$$
$$M_y^G = (1-\alpha) \left[M_y - \alpha M_{xy} \right]$$
$$M_{yy}^G = (1-\alpha) M_{yy}$$

where $\alpha = (X - X')/X$ represents the fraction of mass of the box B contained in the box B^D

3. Regroup the different sub-boxes to reconstruct the new boxes at the instant $t + dt$.

   We use the following equations (the reverse of the above) to calculate the moments of a box B from those of the two sub-boxes B^D and B^G which comprise it:

$$M_0 = M_0^G + M_0^D \tag{19}$$
$$M_x = \alpha M_x^D + (1-\alpha) M_x^G + 3 \left[(1-\alpha) M_0^D - \alpha M_0^G \right]$$
$$M_{xx} = \alpha^2 M_{xx}^D + (1-\alpha)^2 M_{xx}^G + 5\alpha (1-\alpha) \left[M_x^D - M_x^G \right]$$
$$M_{xx} = +5 (1-2\alpha) \left[(1-\alpha) M_0^D - \alpha M_0^G \right]$$
$$M_y = M_j^G + M_y^D$$
$$M_{yy} = M_{yy}^G + M_{yy}^D$$
$$M_{xy} = \alpha M_{xy}^D + (1-\alpha) M_{xy}^G + 3 \left[(1-\alpha) M_y^D - \alpha M_y^G \right]$$

   where $\alpha = M_0^D / (M_0^D + M_0^G)$

Reconstruction of a box

When it is necessary to reconstruct a box from three sub-boxes B_1, B_2 and B_3, we proceed by first regrouping B_1 and B_2 (using 19), then adding B_3 to this result. We can verify that the final result is identical to that obtained if we begin by first regrouping B_2 and B_3, and then add B_1. The same result is valid for the splitting of a box into 3 sub-boxes.

Alternate Directions ("Time-splitting")

In a multi-dimensional motion, the method of evaluating the total advection by successively calculating the advection along each direction is known as "time-splitting". This method is not the only one possible, because, in principle, it is possible to proceed in one step by splitting each box into 3N sub-boxes according to the destination of the tracer mass. However, it is is much easier, and less costly, to proceed by separating the directions. In addition, this method gives the possibility of using a different timestep according to the direction, in relation to the different Courant numbers in each direction. Thus, for their experiments with a 3D off- line CTM, Prather et al. [1987] used the following sequence for the advection steps:

- Advection along X (Δt_x)
- Advection along Y (Δt_y)
- Advection along X (Δt_x)
- Advection along Z (Δt_z)
- Advection along X (Δt_x)
- Advection along Y (Δt_y)
- Advection along X (Δt_x)

with $\Delta t_z = 4\Delta t_x$ and $\Delta t_y = 2\Delta t_x$.

The validity of this approach depends on the shear of the wind, rather than on its magnitude. In the case of a uniform wind field, the successive treatment of different directions does not introduce an error with respect to a simultaneous treatment; however, in regions of strong wind shear, to treat directions successively can cause errors in the transport, but it is difficult to estimate the effect quantitatively.

3.2 Generalisation of the Scheme

Case of a variable density

In the above we assumed that the density was constant and uniform over all of the domain; in fact, the equations obtained remain valid even if this is not the case, due to the property described above. Suppose that we had calculated the moments of a box B from those of the two sub-boxes with different density which compose it. Considering box B_1 of density ρ_1, and dimension X_1, box B_2 of density ρ_2, and dimension X_2 and box B of density ρ with:

$$\rho = \frac{X_1\rho_1 + X_2\rho_2}{X_1 + X_2}$$

We proceed as if the boxes B_1 and B_2 had a density of ρ: therefore B_1 becomes B_1' of length X_1' by compression and B_2 becomes B_2' of length X_2' by stretching (if $\rho_2 \geq \rho_1$), this does not change their moments. Thus it is the case of regrouping two boxes of identical density and this is achieved by using (19).

Extension to three dimensions

The extension of the definitions and of the equations (17), (18) and (19) to three dimensions is straightforward; for example, the equations (17) must be completed by:

$$M_z^D = \alpha\left[M_z + (1-\alpha)\, M_{xz}\right]$$

$$M_{xz}^D = \alpha^2 M_{xz}$$

$$M_{yz}^D = \alpha M_{yz}$$

$$M_{zz}^D = \alpha M_{zz}$$

Properties of the scheme

The Prather scheme possesses the following properties:

- Stability: the scheme (forward Eulerian) is stable in the limit $\alpha \leq 1$, which is rigourously equivalent to the CFL condition: $u\,dt/dx \leq 1$.
- Conservation: the formulation of the scheme in flux form assures the exact conservation of the total mass of each tracer.
- Accuracy: compared to finite difference schemes, for which the mixing ratio is only known at the centre of the gridbox, additional information is provided by the storage of the first and second order moments and the calculation of their evolution. Prather [1986] estimated that the conservation of second order moments conferred on his scheme an accuracy comparable to a fourth order finite difference scheme.
- Small diffusivity and local character: the scheme is well adapted to the representation of localised phenomena, because the advection is performed by exchange between adjacent boxes (therefore there are no "distance" effects with this scheme). It should be noted that there is no continuity condition imposed on the tracer distribution at the interfaces of the boxes.
- Upwind character: in contrast to centred finite difference schemes, advection by the Prather scheme of any feature only affects the grid boxes downstream of this feature.

CPU memory and time requirement

The major inconvenience of the Prather scheme, which explains why it is not more widely used, is the cost in CPU memory and also CPU time. For each advected tracer the scheme requires (for N dimensions):

- 1 array for the zero order moment
- N arrays for the first order moments
- $N(N+1)/2$ arrays for the second order moments

Thus, for a 3D model using the conservation of second order moments, there are 10 3D arrays required for each tracer (and 6 2D arrays for a 2D model).

If the available memory is too limited (for example in high resolution or with a large number of tracers), it should be noted that it is possible to "truncate" the scheme to the conservation of first order moments only, which limits the number of arrays per tracer to $N + 1$, i.e. 4 in three dimensions. Of course, the accuracy of the scheme and the characteristic low diffusivity are affected by this operation; according to Prather [1986], the scheme truncated in this way, equivalent to the "slope-scheme" of Russell and Lerner [1981], has an accuracy comparable to that of a 2nd order finite difference scheme.

However, it should be noted that effective doubling of the resolution obtained by the conservation of 2nd order moments can be achieved at a lower cost in CPU memory (multiplication by a factor 2.5 in 3D) and in CPU time (depending on the problem) than by increasing the number of gridboxes.

3.3 Use in Spherical Geometry

The Prather scheme first requires a grid to be defined over the model domain and second the calculation of the mass fluxes at the interfaces of all of the gridboxes thus defined. Here we show how the scheme can be implemented in a transport model using spherical geometry, and then how the mass fluxes at the box interfaces can be calculated exactly when the wind field is read in as spectral coefficients.

The results obtained here can obviously be used in an "off-line" transport model forced by analyses or from output from a spectral model (i.e. TOMCAT), or alternatively for the "on-line" transport of tracers (e.g. water vapour) in a spectral GCM.

3.3.1 Definition of the grid

A rectangular grid in spherical geometry is defined by the latitudes of the north/south interfaces and the longitudes of the east/west interfaces, i.e. by a series of latitudes $\phi_k, k = 0, 1...K$ and longitudes $\lambda_i, i = 0, 1, ...I$. The gridboxes $B_{i,k}$ defined by $B_{i,k} = [\lambda_{i-1}, \lambda_i] \times [\phi_{k-1}, \phi_k]$ cover the whole globe so that:

$\phi_0 = -\frac{\pi}{2}$ (south pole)

$\phi_K = \frac{\pi}{2}$ (north pole)

$\lambda_0 = \lambda_I$ (periodicity in longitude).

Note that at no stage do we assume that the grid is regular. Any rectangular grid which satisfies the above conditions is suitable for use with the scheme within TOMCAT.

3.3.2 Grid associated with a Gaussian grid

A spectral truncation is associated with a grid in physical space, a Gaussian grid, where the physical and non-linear terms are calculated. When the CTM is coupled with winds from a spectral CGM it is natural to use this grid for the basis of the Prather scheme. This will avoid using two grids and the problems of interpolation between the two.

The definition of such a grid is made by use of the following:

- The boxes are centred in longitude on the Gaussian grid:

$$\lambda_i = 2\pi \frac{(i - .5)}{I}$$

  The grid is therefore regular in longitude, like the Gaussian grid.

- The latitudes ϕ_k are defined successively from $\phi_0 = -\pi/2$ by using the Gaussian weights ω_k and the formula:

$$\mu_k - \mu_{k-1} = \omega_k$$

  where $\mu_k = sin\,(\phi_k)$

Remembering that

$$\sum_{k=1,K} \omega_k = 2 \tag{20}$$

this defines a grid which satisfies the above conditions, for which the surface area of the grid is:

$$S_{i,k} = \frac{2\pi a^2}{I}\,\omega_k \tag{21}$$

In TOMCAT the latitudes at the interfaces of the grid are given by `DLAT2`. Values of these are contained in the file `grid_data` in `/home/j90/kd/tomcat` for most common resolutions.

3.3.3 Calculation of the mass fluxes at the interfaces:

Suppose that the grid on the sphere has been defined with no further assumptions. Now suppose that we know the horizontal wind field that will force the model in terms of spectral coefficients of streamfunction ψ and velocity potential χ.

The relations between (χ, ψ) , (U, V) and (η, ζ) are the following:

$$\eta = \frac{1}{a^2\left(1-\mu^2\right)}\left[\frac{\partial U}{\partial \lambda} + \left(1-\mu^2\right)\frac{\partial V}{\partial \mu}\right] \tag{22}$$

$$\zeta = \frac{1}{a^2\left(1-\mu^2\right)}\left[\frac{\partial V}{\partial \lambda} - \left(1-\mu^2\right)\frac{\partial U}{\partial \mu}\right]$$

$$\eta = \nabla^2 \chi \tag{23}$$

$$\zeta = \nabla^2 \psi$$

$$U = \frac{\partial \chi}{\partial \lambda} + \left(1-\mu^2\right)\frac{\partial \psi}{\partial \mu} \tag{24}$$

$$V = \frac{\partial \psi}{\partial \lambda} - \left(1-\mu^2\right)\frac{\partial \chi}{\partial \mu}$$

In the following we will also use the zonal η^λ and meridional η^μ divergences defined by:

$$\eta = \eta^\lambda + \eta^\mu \tag{25}$$

$$\eta^\lambda = \frac{1}{a^2\left(1-\mu^2\right)}\frac{\partial U}{\partial \lambda} \tag{26}$$

$$\eta^\mu = \frac{1}{a^2}\frac{\partial V}{\partial \mu} \tag{27}$$

It is possible to calculate exactly the mass fluxes at the interfaces of a rectangular grid, on the condition that this grid is regular in longitude, but not necessarily in latitude (of which a Gaussian grid is a particular example).

1. Zonal mass flux:

   Let $F^\lambda_{i,k}$ be the mass flux across the interface between the boxes $B_{i,k}$ and $B_{i+1,k}$.

   By definition:

   $$F^\lambda_{i,k} = \int_{\phi_{k-1}}^{\phi_k} \rho u a d\phi \tag{28}$$

   which can also be written:

   $$F^\lambda_{i,k} = \int_{\mu_{k-1}}^{\mu_k} \rho \frac{1}{(1-\mu^2)} U d\mu$$

2. Meridional mass flux:

   Let $F^\phi_{i,k}$ be the mass flux across the interface between the boxes $B_{i,k}$ and $B_{i,k+1}$.

   By definition:

   $$F^\phi_{i,k} = \int_{\lambda_{i-1}}^{\lambda_i} \rho v a cos\phi d\lambda \tag{29}$$

   which can be written:

   $$F^\phi_{i,k} = \int_{\lambda_{i-1}}^{\lambda_i} \rho V d\lambda$$

If we consider the box $B_{i,k}$, our problem is therefore to calculate: $F^{\lambda}_{i-1,k}$, $F^{\lambda}_{i,k}$, $F^{\mu}_{i,k-1}$ and $F^{\mu}_{i,k-1}$.

a) calculation of the meridional flux:

The first step consists of calculating the Fourier coefficients of V at the north-south interfaces of the grid by using the values of P_{nm} tabulated at the latitudes of the interfaces.

For example:

$$V_m\left(\mu^-\right) = \sum_n V_n^m Y_n^m \tag{30}$$

Performing a direct Fourier transform on these coefficients will give us the values of V at the points regularly spaced in longitude. Instead of this, note that we can use the Fourier decomposition of V:

$$V(\lambda,\mu) = \sum_m V_m(\mu)\, e^{im\lambda}$$

to write:

$$\int_{\lambda_{i-1}}^{\lambda_i} V d\lambda = \sum_m V_m(\mu) \int_{\lambda^{i-1}}^{\lambda_i} e^{im\lambda} d\lambda \tag{31}$$

If we note $\lambda_i^G = \frac{1}{2}(\lambda_{i-1} + \lambda_i)$ the longitudes of the Gaussian grid, and $\Delta\lambda$ the longitude increment of this grid, we can easily transform the integrals to:

$$\int_{\lambda_{i-1}}^{\lambda_i} e^{im\lambda} d\lambda = \frac{1}{im} e^{im\lambda}\left(e^{\frac{im\Delta\lambda}{2}} - e^{\frac{-im\Delta\lambda}{2}}\right) \tag{32}$$

$$\int_{\lambda_{i-1}}^{\lambda_i} e^{im\lambda} d\lambda = \frac{2}{m} sin\left(\frac{m\Delta\lambda}{2}\right) e^{im\lambda}$$

and finally we obtain, for the meridional mass flux F, a formula analogous to that giving V, with a multiplication of the Fourier coefficients V_m by precalculated factors:

$$F_m = V_m \frac{2}{m} sin\left(\frac{m\Delta\lambda}{2}\right)$$

After calculating V_m as indicated above, we therefore multiply them by a factor precalculated before performing the FFT which leads exactly to the integrated value of the meridional mass flux at the interfaces.

$$F^{\phi} = \sum_m F_m e^{im\lambda}$$

This method requires the prior tabulation of the Legendre functions $P_{nm}(\mu)$ and their derivatives $(1-\mu^2)dP_{nm}/d\mu$ at the latitudes of the specified box interfaces (in the file `LEGIyy` - see section 5.4).

b) calculation of the zonal flux:

We proceed differently for the calculation of the zonal mass flux. If we consider the same grid as before, we will first calculate the divergence of the zonal mass flux, obtained from the total divergence of the mass flux minus the meridional divergence.

The total divergence of the mass flux is calculated by using a similar approach to that for the calculation of the meridional mass flux. The meridional divergence is obtained immediately by the difference between the meridional fluxes at the north and south interfaces of the box.

Finally, we obtain the divergence of the zonal mass flux, which allows us to calculate in turn the zonal flux itself at the east/west interfaces of the gridboxes, in terms of a constant from the condition of periodicity in longitude. This constant is determined from the zonal mean of the zonal mass flux.

This method requires the prior tabulation of the values of the Legendre functions averaged over the boxes in the employed grid (also in the file `LEGIyy`).

Note that it would be possible to calculate directly the zonal flux without using the divergence, by using the formula:

$$\frac{U}{(1-\mu^2)} = \frac{1}{(1-\mu^2)}\frac{\partial \chi}{\partial \lambda} + \frac{\partial \psi}{\partial \mu} \tag{33}$$

but this requires the additional tabulation of the derivatives of P_{nm}

This allows the calculation in terms of a constant (from the periodic condition over the longitudes). This constant is determined from:

$$\sum_i F^{\lambda}_{i,k} = \sum_i F^{\lambda}_{i,k} \tag{34}$$

i.e. the calculation of the zonal mean of the zonal wind from the values at the centres of the boxes or from the values at the interfaces leads to the same result.

Thus, the total mass flux $F_{i,k}$ entering a box $B_{i,k}$ is given by:

$$F_{i,k} = F^{\lambda}_{i-1,k} - F^{\lambda}_{i,k} + F^{\phi}_{i,k-1} - F^{\phi}_{i,k}$$

and we can verify that

$$F_{i,k} = -S_{i,k}\,\eta^{-}_{i,k} \tag{35}$$

High latitudes

The stability of the Prather scheme is conditional on the constraint: $\alpha \leq 1$, rigourously equivalent to the CFL condition: $u\Delta/\Delta x \leq 1$ (for advection along Ox). While this constraint does not pose any particular problems and allows the use of reasonable timesteps for the advection along latitudes or in the vertical, it is not the same for the advection along longitude, because of the convergence of the meridians towards the poles and the reduction of Δx which follows ($\Delta x = acos(\phi)\Delta\lambda$). To avoid very small timesteps, the model uses "extended polar zones", as named by Prather et al. [1987] at high latitudes. This correction consists of grouping several adjacent boxes situated on the same latitude circle and advecting this block along the longitude in the same way as a single box of larger size. The number of boxes grouped together depends on the latitude, on the size of the boxes $\Delta\lambda$, on the timestep Δt, as well as on the maximum wind that will be encountered. The number of boxes grouped together at each latitude is `NUM` which is set up in the routine `CALNUM`. Before the advection step in the x direction the boxes are regrouped by using (17), then, when the zonal advection is complete, the original boxes are reconstructed using the reciprocal formulae (19).

Problem of the flux across the pole

As shown above the meridional mass flux F_ϕ across an element of surface situated at latitude ϕ is given by:

$$F^{\phi}_{i,k} = \int_{\lambda_{i-1}}^{\lambda_i} \rho v a.cos(\phi).d\lambda \tag{36}$$

In particular, the mass flux across the pole is zero even if the cross-polar wind is not zero. The quantity of mass passing directly from one polar gridbox to the gridbox diametrically opposite the pole is therefore

not always zero. The mass flux from one box to the other occurs by crossing one by one the neighbouring boxes, therefore it is a case of a zonal mass flux and not a meridional one.

Unfortunately, the zonal flow to a neighbouring box is poorly represented near the pole in the Prather scheme as discussed above. In effect, one of the characteristics of the scheme is that the mass flux calculated at the interfaces of the boxes are spread over these interfaces as of they were due to a uniform velocity (this does not mean that the calculation of the mass flux does not take account of the wind shear on the interface). Thus, in planar geometry, the volumes transported from one box to another are rectangular slabs, the velocity being assumed uniform over the sides of the boxes; in our case of interest (spherical geometry) the volumes transported along longitude are in reality angular sectors, which is equivalent to considering the angular velocity $\alpha = d\lambda\ dt = u/cos(\phi)$ constant over the interface. In particular, for the boxes neighbouring the pole, the motion is that of a rotation about the pole, which returns to taking a zero velocity at that point. In summary, the scheme implicitly considers in part that the mass flux across the pole is zero, which is true, but equally that the velocity at the pole is zero, which is not true in general.

In fact, the operation of uniformly spreading the mass flux over the whole length of the interface is equivalent to substituting the real wind field with a discretised one which has the following properties:

- The mass flux across the interfaces of the grid are the same with the discretised wind field as with the real wind field. In particular, if the real wind field is non divergent, the same is true of the discretised wind field.
- The meridional velocity v is uniform over the north/south interfaces.
- The zonal velocity $u/cos(\phi)$ is uniform over the east/west interfaces.

In addition, it follows that the discretised wind field has discontinuities at the interfaces of the gridboxes: there is a discontinuity in the meridional component at the east/west interfaces and a discontinuity in the zonal component at the north/south interfaces.

The problem of the treatment of the pole (a singularity) in a gridpoint model is a classical problem. A test to verify the performance of a numerical advection scheme in the case of cross polar flow is to consider a solid rotation about and axis inclined at 90 degrees to the polar axis. This test has been used, for example, by Williamson and Rasch [1989] for a semi-lagrangian scheme, taking an initial tracer distribution of a localised structure at the equator of the solid rotation.

The equation of the motion is the following:

$$u = Usin\lambda cos\phi$$

$$v = -Usin\lambda$$

As the motion is a solid rotation, the initial structure moves on the sphere without being deformed and returns to its initial position after travelling around the globe and crossing the two poles.

A method sometimes employed to solve this deficiency is to cover the pole by a "polar box", a circular zone centred on the pole inside which the mixing ratio of tracers is taken to be uniform. Therefore the treatment of the singular point is avoided. This method has been used by Rood et al. [1991] with the Van Leer scheme and seems capable of giving good results. Therefore it was tested with the Prather scheme by taking the polar box to be the ensemble of boxes which touch the pole. However, this approach gave transport across the pole which was too rapid. Therefore, in TOMCAT the mass flux across the pole is obtained by calculating the wind vector at the pole and determining the mass of each triangular box which would be transported to the diametrically opposite box in each timestep. This then gives the mass flux across the pole.

3.4 Correction of Negative Values

As advection schemes are not perfect it is necessary to couple them with a certain number of fixes to correct their intrinsic deficiencies. A well-known problem with classical transport schemes (spectral and finite difference) is their non-positiveness. For minor constituents (e.g. water vapour, ozone) it is obvious that negative values are purely a numerical artefact and that these negative values can be a problem in chemical or physical calculations.

Contrary to what is sometimes assumed, the formulation of the Prather scheme does not ensure the positiveness of a tracer without an additional correction. This can be seen in the example in figure 3 of Prather [1986]. In a one dimensional example, if the tracer at t_0 is localised in a single box B_i of the grid (with the 1st and 2nd order moments set to zero), and the wind u_i is directed towards the right.

$$M_0^i = 1 \tag{37}$$

$$\begin{aligned} M_x^i &= 0 \\ M_{xx}^i &= 0 \\ M_0^{i+1} &= 0 \\ M_x^{i+1} &= 0 \\ M_{xx}^{i+1} &= 0 \end{aligned} \tag{38}$$

After a timestep dt, the structure is globally displaced towards the right, and only the distributions of the boxes B_i and B_{i+1} are modified; the distribution at $t_0 + dt$ in the box B_{i+1} calculated using (17),(18) and (19) is the following:

$$M_0^i = (1-\alpha) \tag{39}$$

$$\begin{aligned} M_x^i &= 3\alpha\,(1-\alpha) \\ M_{xx}^i &= 5\alpha\,(2\alpha-1)\,(1-\alpha) \end{aligned}$$

$$\begin{aligned} M_0^{i+1} &= \alpha \\ M_x^{i+1} &= -3\alpha\,(1-\alpha) \\ M_{xx}^{i+1} &= -5\alpha\,(2\alpha-1)\,(1-\alpha) \end{aligned} \tag{40}$$

At the following timestep, for certain values of the wind α, the quantity of tracer mass which will be transported into the box B_{i+2} will be negative, which, bearing in mind the absence of tracer in this box at $t_0 + dt$ will create a negative values at the instant $t_0 + 2dt$. As can be seen, the appearance of negative values is due to the fact that during the reconstruction of the boxes at $t_0 + dt$ using the formulae (19), a distribution is created which is globally positive ($M_0 \geq 0$ even in the box B_{i+1}), but not the local positiveness, allowing the advection of negative quantities of mass. Therefore, this problem can be solved by correcting the first and second order moments before this advection to give a distribution which is positive everywhere: the correction proposed by Prather [1986] consists of:

$$M_x^* = min\left[\frac{3}{2}M_0, max\left(-\frac{3}{2}M_0, M_x\right)\right] \tag{41}$$

$$M_{xx}^* = min\left[2M_0 - \frac{1}{3}|M_x^*|, max\left(|M_x^*| - M_0, M_{xx}\right)\right] \tag{42}$$

Note that this correction slightly increases the diffusivity of the initial scheme, but this effect is very small as the creation of negative values as described above is comparatively rare and the correction consists of a redistribution of tracer mass within a gridbox. This correction is termed "flux limiting" as it consists of avoiding negative mass fluxes. However, the use of such a flux limiter will destroy tracer correlations. Generally, it is best to avoid the use of the limiter if negative tracer values can be tolerated.

3.5 Convection and Vertical Diffusion

The implementation of the Tiedtke [1989] convection scheme and the Louis [1979] vertical diffusion scheme in TOMCAT is described in Part III of this series of UGAMP Internal Reports.

4 Forcing Winds and Temperatures

This section describes the various sources of winds and temperatures that can be used to force TOMCAT. These forcing files are identical to those used in the SLIMCAT 3D model and the TOPCAT 3D trajectory model.

4.1 ECMWF Analyses

The ECMWF analyses that can be used to force TOMCAT are stored on the Cray in the directories `/home/j90/mpc/FORCAGE` (T21) and `/home/j90/mpc/FORCT42` (T42). The files contain the spectral coefficients of the streamfunction, velocity potential, temperature and specific humidity on 17 of the original 31 ECMWF model levels as well as the surface pressure. The table lists the periods that are currently available:

Period	Resolution
26/11/91 to 15/3/92	T21
26/11/91 to 29/2/92	T42
22/8/92 to 2/10/92	T42
26/11/92 to 25/3/92	T21
26/11/93 to 20/2/94	T42
13/5/94 to 8/6/94	T42
22/8/94 to 29/10/94	T42
26/11/94 to 30/4/95	T42
26/11/95 to 29/4/96	T42

4.2 UK Meteorological Office UARS Analyses

TOMCAT can also be run using the gridpoint analyses of the U.K. Meteorological Office produced for the UARS mission. However, this is not recommended as the calculation of vertical motion from the divergence leads to noisy fields. It is better to use the SLIMCAT isentropic model with UKMO analyses. These analyses are produced on 22 isobaric levels from 0.3hPa down to 1000hPa. The analyses are produced on an Arakawa 'B' grid so that the wind fields (u and v) are not given at the same location as temperature and geopotential. TOMCAT reads the data on this staggered grid; the fields are interpolated to the model grid within TOMCAT. This data is stored in `/home/j90/mpc/FORUKMO` and also `/home/j90/kd/tomcat/FORUKMO`. The table lists the periods that are currently available:

Period	Resolution
21/10/91 to 23/3/92	2.5 x 3.75
13/5/94 to 8/11/94	2.5 x 3.75
26/11/94 to 30/4/95	2.5 x 3.75

All other days from October 1991 are available on tape or by ftp from the British Atmospheric Data Centre (BADC).

4.3 (E)UGCM Output

TOMCAT can equally be forced using winds from any (E)UGCM experiment. A GCM run should be performed which saves MARS files ideally every six hours. The winds can be saved in any resolution. A program to convert GCM MARS files into SLIMCAT forcing files can be found in `/home/j90/kd/tomcat/jobs/conmars_job` on the Cray. The job uses a similar format to a UMAP job to access the MARS files. This program can be used to change the spectral truncation of the GCM output.

5 Running the Model

The standard version of the model is 'tomcati' which is contained in the directory `/home/j90/kd/tomcat`. The processed nupdate decks are in `TOMCATI` and there is a listing (with linenumbers) in `tomcati_list`.

5.1 Jobdecks

Example jobdecks for TOMCAT can be found on the Cray in the directory `/home/j90/kd/tomcat/jobs`. At present the following standard jobdecks are there:

- `transport_job` Job to run TOMCAT as a transport model only. The user can supply his own chemistry by writing an interface subroutine called CHIMIE to update the advected tracers.
- `chem_job` Job to run TOMCAT with its own stratospheric chemistry scheme.
- `inimod_job` Job to create initial data for TOMCAT.
- `conres_job` Job to convert output PDG file to different horizontal resolution for use as a restart file.
- `pdgcut_job` Job to split PDG file into smaller files (e.g. to put on tape).

5.2 Initial Data and Restart Runs

A file containing the initial tracer fields will need to be set up before TOMCAT is run. An example initialisation job is `inimod_job` (see above). For more sophisticated initialisation procedures (e.g. with full chemistry) contact `martyn@atm.ch.cam.ac.uk`. In this job the user needs to define the horizontal grid required for the model run and the vertical levels of the forcing files and TOMCAT (using `FLT` and `GLT`). The file `grid_data` in the directory `kd/tomcat` contains `fortran` data statements which define common horizontal and vertical grids. These can be cut and pasted into the initialisation job.

A TOMCAT run creates two output files: a PDG file which contains the 3D tracer distributions at specified intervals throughout the run and a REST file which contains the tracer fields at the end of the run. This REST file can be used as 'initial data' for a restart run (see below).

5.3 Parameters

The table lists some of the main parameters in TOMCAT.

Parameter	Meaning
LAT	number of latitudes
LON	number of longitudes
MI0	spectral truncation of winds after conversion
MI1	spectral truncation of winds read in
MLAT	number of latitudes in gridpoint forcing file
MLON	number of longitudes in gridpoint forcing file
NIV	number of levels

5.4 Model Switches and Variables

The following switches can be set in the model jobdeck:

Switch	Meaning
LECMWF	TRUE for spectral forcing
LUKMET	TRUE for gridpoint forcing
LCONV	TRUE to include convection
LVDIF	TRUE to include vertical diffusion

The length of the TOMCAT model run is controlled by the variables read in on channel 94

```
cat <<'eof'> fort.94
240   NO OF FILES TO JUMP IN FORCING FILE
0     =0 INITIALLY, =1 RESTART
40    NCYCLT (NDAYS * NO FORCING FILES/DAY)
48    NFFILE (NO FORCING OUTPUTS PER FILE)
eof
```

The first line indicates the number of analysis times to jump over from the start of the first forcing file. The second line indicates whether the start data comes from an initial data file or from a restart file. The third line specifies the length of the run in numbers of analysis times. NFFILE is the number of analysis times per forcing file.

```
#
#  file at forcing resolution
cp $MARTYN/UTIL/TRONxx  fort.2
#  files at model grid resolution
cp $MARTYN/UTIL/TRONyy  fort.1
cp $MARTYN/UTIL/LEGCyy  fort.20
cp $MARTYN/UTIL/LEGIyy  fort.21
#
```

The above data files need to be correctly set according to the values of MI0 and MI1. xx=MI1 and yy=MI0.

The model outputs 2 files. On channel 9 the model output a PDG file which contains the 3D tracer arrays at intervals specified by the variable NSO1. On channel 30 the model outputs REST file which can be used to restart a continuation run.

```
#
# jour=n results
cp fort.9  $WORK/xx.PDGxx
cp fort.30 $WORK/xx.RESTxx
#
```

The following lines in the subroutine INIEXP control the length of the model timestep and frequency of output.

```
DT0 =3600.                                                    INIEXP.54
NITERT=6                                                      INIEXP.55
NDYN=1                                                        INIEXP.56
NSO1=24                                                       INIEXP.57
```

DT0 is the basic model timestep. This is split into NDYN dynamical subtimesteps. NITERT is the number of iterations in one cycle, i.e. the time between the forcing files divided by DT0. Output is written to the PDG file every NSO1 iterations.

The Prather advection scheme can use a limiter to prevent negative mixing ratios, as described by Prather [1986]. This limiter can be switched on by setting the variable LIMIT to TRUE. Note that the use of this limiter can destroy tracer correlations (as the advection is no longer independent of the tracer distribution) and so should be used with care.

```
LIMIT=.FALSE.                                                 ADVEC.13
```

The following table lists some of the main model variables and the Fortran common decks in which they are stored.

Variable	Common Deck	Meaning	Units
FLT	GRILLE	defines interlevel pressure	none
GLT	GRILLE	defines interlevel pressure	none
DPL	FOR3D	pressure difference across level	Pa
PL	FOR3D	centrelevel pressure	Pa
PLT	FOR3D	interlevel pressure	Pa
Q3D	FOR3D	specific humidity at box centre	kg/kg
SM	MOMENTS	total mass of box	kg
S0	MOMENTS	zero order moment	kg*vmr
SX	MOMENTS	fist order moment in x direction	kg*vmr
SXX	MOMENTS	second order moment in x direction	kg*vmr
SURF	GRILLE	surface area of grid cell	m^2
T3D	FOR3D	temperature at box centre	K
U3D	FOR3D	velocity in x direction at box centre	ms^{-1}
V3D	FOR3D	velocity in y direction at box centre	ms^{-1}

5.5 Fortran Channels

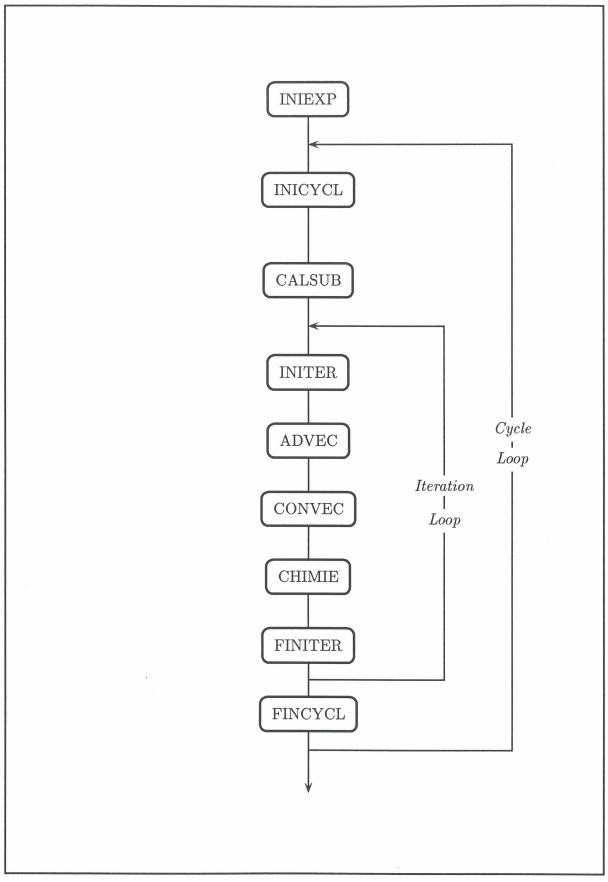
The models makes use of the following fortran channels during execution:

Channel	Variable	Common Deck	Purpose
1	ITAB		Read file TRONyy
2	ITAB1		Read file TRONxx
9	IFSO1	REDEM	Write PDG file
18	IEVAP	REDEM	Read file EVAPxx
19	ICON	REDEM	Writing/reading convection/diffusion matrix
20	IFPP0		Read file LEGCyy
21	IFPP1		Read file LEGIyy
30	IFRD	REDEM	Read/write restart file
40	IFORC	REDEM	Read forcing files
94			Read information about length of run etc.

IFORC increases from 40 during the run as the forcing files are read sequentially.

5.6 Subroutines

The following diagram shows the structure of the model. The cycle loop corresponds to the frequency of the forcing winds and temperatures (typically 6 or 24 hours). The iteration loop corresponds to the basic model timestep (set by DT0).



- ADVEC Calls the subroutines to perform advection in the three directions.
- ADVX0 Advection in x direction with conservation of 0 order moments
- ADVX1 Advection in x direction with conservation of 1st order moments
- ADVX2 Advection in x direction with conservation of 2nd order moments
- CHIMIE Interface between the chemical model and the dynamical model.
- CALSUB Sets up convection and vertical diffusion terms.
- CONVEC Applies convection and vertical diffusion.
- FINCYCL End of cycle. Writes REST file.
- FINITER End of iteration. Writes PDG file.
- INICYCL Start of cycle (period of forcing analyses).
- INIEXP Initialise experiment.
- INITER Start of iteration (DT0 timestep).

5.7 Universal Constants

The following table lists the variable names of the universal constants in TOMCAT. They are contained in the fortran common block CSTES which is in the nupdate common deck CSTUNI.

Variable	Description	
CONV	180/XPI	Value
CP	Specific heat capacity of dry air at constant p	1005.46 $JK^{-1}kg^{-1}$
CPSG	CP/GG	
CPSL	CP/XL	
CPV	Specific heat capacity of water vapour at constant p	1869.46 $JK^{-1}kg^{-1}$
CPVMCP	CPV - CP	
DEUOMG	2*OMEGA	
ECPH	CPV/(CP-1)	
ETV	RVSRA -1	
ETVQ	1 - RASRV	
GG	Acceleration due to gravity	9.80665 ms^{-2}
GSCP	GG/CP	
GSRA	GG/RA	
OMEGA	Earth's speed of rotation	7.292x10^{-5} rad s^{-1}
RA	gas constant for dry air	287.05 $JK^{-1}kg^{-1}$
RASCP	RA/CP	
RASCP2	RA/(2CP)	
RASL	RA/XL	
RASRV	RA/RV	
RTER	radius of the earth	6371229 m
RTER2	RTER*RTER	
RV	gas constant for water vapour	461.51 $JK^{-1}kg^{-1}$
RVSRA	RV/RA	
STEFAN		5.6697x10^{-8} ms^{-2}
TMERGL		271.23K
TOO	ice melting temperature	273.16K
UNSCP	1/CP	
UNSG	1/GG	
VKARMN	von Karman constant	0.4
XL	Latent heat of condensation at 0^oC	2.5008x10^6 Jkg^{-1}
XLF	XLI -XL	
XLI	latent heat of sublimation	2.83456x10^6 Jkg^{-1}
XLISCP	XLI/CP	
XLISG	XLI/GG	
XLSCP	XL/CP	
XLSG	XL/GG	
XLSRV	XL/RV	
XPI	π	3.14159..
XPOO	reference pressure	10^5 Pa

5.8 User Supplied Chemistry

TOMCAT can be used simply as a model to advect passive tracers with the user supplying code to calculate chemistry. The simplest way to to this is to name the top level subroutine of the new chemistry as CHIMIE

and not use the TOMCAT subroutine of this name. An example subroutine would be as follows:

```
      SUBROUTINE CHIMIE
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C     User supplied chemistry interface
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
*CALL PARADI
*CALL MOMENTS
C
C     Modify advected tracers
      DO 1 JV=1,NTRA
      DO 1 L=1,NIV
      DO 1 K=1,LAT
      DO 1 I=1,LON
        S0(I,K,L,JV)=0.5*S0(I,K,L,JV)
 1    CONTINUE
C
C     Store advected tracers in output array
      DO 2 L=1,NIV
      DO 2 K=1,LAT
      DO 2 I=1,LON
        ST(I,K,L,1)=S0(I,K,L,1)
        ST(I,K,L,2)=S0(I,K,L,3)
        ST(I,K,L,1)=S0(I,K,L,1) + S0(I,K,L,2)
 2    CONTINUE
C
      RETURN
      END
```

5.9 Grib Packing

The TOMCAT output (PDG) files can become very large. Ben Edgington has written code which enables the output normally stored as Cray binary in the PDG file to be packed using GRIB. The user can specify the accuracy required and so the saving in space can be dramatic (e.g a factor of 6 without significant loss of precision). Full details of the GRIB packing with TOMCAT output is given in `grib.doc` in `kd/tomcat/docs` on the RAL Cray.

5.10 Analysing TOMCAT Output

A number of programs exist for looking at TOMCAT data. These can generate UTF files for use with UPLOT. Jobs also exist so that the UMAP program can be used. It is best to contact `martyn@atm.ch.cam.ac.uk` directly if you need help with this.

If you use the GRIB facility to pack the output in the PDG files there are a range of options on the `ungrib` facility which allows the quick generation of some UTF files. See `grib.doc` for details.

6 Acknowledgements

We are grateful to M. Prather for helpful comments concerning his advection scheme.

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7 Appendix 1. Notation

Symbol	Meaning	Value
a	radius of the earth	6.371x10^6 m
D	divergence	
p	pressure	
p_s	surface pressure	
t	time	
T	temperature	
u	zonal wind	
v	meridional wind	
U	u cos(latitude)	
V	v cos(latitude)	
$\vec{\mathbf{v_h}}$	horizontal wind vector	
ϕ	latitude	
λ	longitude	
μ	$= sin\phi$	
ζ	relative vorticity	
η	vertical coordinate	
ω	pressure coordinate vertical velocity	

8 Appendix 2. Chemically Updating Tracer Moments

When using the Prather [1986] advection scheme in the basic TOMCAT (and SLIMCAT) models, any change in tracer mass due to chemistry only acts upon the zero order tracer moment (`S0`). Strictly, the first and second order moments should also be modified. This would increase the chemical resolution of the model and could reduce the rate of chemical reaction between two tracers with opposite gradients within a gridbox, for example. However, chemically updating the 1st and 2nd order moments would be prohibitively expensive in a full chemistry simulation.

Consider the integrals over a gridbox (in two dimensions) of the products of any 3 basis functions of the moments (equation (11) above). If one of the functions is the zero order moment (K_o) we get:

$$\int_0^X \int_0^Y K_0 K_0^2 (x,y)\, dxdy = XY = S \tag{43}$$

$$\int_0^X \int_0^Y K_0 K_x^2 (x,y)\, dxdy = S/3 \tag{44}$$

$$\int_0^X \int_0^Y K_0 K_y^2 (x,y)\, dxdy = S/3 \tag{45}$$

$$\int_0^X \int_0^Y K_0 K_{xx}^2 (x,y)\, dxdy = S/5 \tag{46}$$

$$\int_0^X \int_0^Y K_0 K_{yy}^2 (x,y)\, dxdy = S/5 \tag{47}$$

$$\int_0^X \int_0^Y K_0 K_{xy}^2 (x,y)\, dxdy = S/9 \tag{48}$$

Otherwise, the integrals give

$$\int_0^X K_x^3(x,y)\,dx = 0 \tag{49}$$

$$\int_0^X K_x(x,y)\,K_{xx}^2(x,y)\,dx = 0 \tag{50}$$

$$\int_0^X K_x^2(x,y)\,K_{xx}(x,y)\,dx = 2S/15 \tag{51}$$

$$\int_0^X K_{xx}^3(x,y)\,dx = 2S/35 \tag{52}$$

$$\int_0^Y \int_0^X K_x(x,y)\,K_y(x,y)\,K_{xy}(x,y)\,dxdy = S/9 \tag{53}$$

$$\int_0^Y \int_0^X K_{xy}^2(x,y)\,K_{xx}(x,y)\,dxdy = 2S/45 \tag{54}$$

Similar results are obtained for K_y and K_{yy}, or K_z and K_{zz}. All of the other products involving the 'cross terms' (mixtures of x,y, and z) are zero (see equation (12) above).

Consider two chemical tracers whose distributions in two dimensions are given by:

$$r_A(x,y) = \frac{1}{M}\sum_\alpha A_\alpha K_\alpha(x,y) \tag{55}$$

and

$$r_B(x,y) = \frac{1}{M}\sum_\alpha B_\alpha K_\alpha(x,y) \tag{56}$$

The rate of the chemical reaction between the two species depends on the product of the concentrations:

$$rate = k[A][B]$$

$$rate = k^{'}(A_0K_0+A_xK_x+A_{xx}K_{xx}+A_yK_y+A_{yy}K_{yy}+A_{xy}K_{xy})(B_0K_0+B_xK_x+B_{xx}K_{xx}+B_yK_y+B_{yy}K_{yy}+B_{xy}K_{xy})$$

The effect on the zero order moment is proportional to:

$$\int_0^X \int_0^Y ABK_0 dxdy = A_0B_0 + \frac{1}{3}(A_xB_x + A_yB_y) + \frac{1}{5}(A_{xx}B_{xx} + A_{yy}B_{yy}) + \frac{1}{9}A_{xy}B_{xy} \tag{57}$$

So, in addition to the product of the average concentration of A with the average concentration of B (first term on RHS), the zero order moments of A and B are modified by products of the higher order moments.

The effect on the first order moment in the x direction is proportional to:

$$\int_0^X \int_0^Y ABK_x dxdy = \frac{1}{3}(A_xB_0 + A_0B_x) + \frac{2}{15}(A_xB_{xx} + A_{xx}B_x) + \frac{1}{9}(A_yB_{xy} + A_{xy}B_y) \tag{58}$$

and similarly for the y direction.

The effect on the second order moment in the x direction is proportional to:

$$\int_0^X \int_0^Y ABK_{xx} dxdy = \frac{1}{5}(A_{xx}B_0 + A_0B_{xx}) + \frac{2}{15}(A_xB_x) + \frac{2}{35}(A_{xx}B_{xx}) + \frac{2}{45}(A_{xy}B_{xy}) \tag{59}$$

The effect on the second order moment in the xy direction is proportional to:

$$\int_0^X \int_0^Y ABK_{xy} dxdy = \frac{1}{9}\left(A_0 B_{xy} + A_{xy} B_0\right) + \frac{1}{9}\left(A_y B_x + A_x B_y\right) + \frac{2}{45}\left(A_{xy} B_{xx} + A_{xx} B_{xy} + A_{yy} B_{xy} + A_{xy} B_{yy}\right) \tag{60}$$

Therefore, to chemically update the 0, 1st and 2nd order moments of a chemical tracer in three-dimensions would require integrating the chemistry 10 times. As chemical integration is generally by far the most costly part of a CTM, this is prohibitively expensive. However, it may be practical to use the higher order moments to update just the zero order moments (equation (57)).

9 Appendix 3. Flowtrace

Below is a flowtrace on a Cray YMP8 from a 1 day run with `NIV=19, LON=128, LAT=64` with (6-hourly) ECWMF winds and 2 tracers. The job included convection and vertical diffusion.

```
+ flowview -Luc
                        Flowtrace Statistics Report
              Showing Routines Sorted by CPU Time (Descending)
                     (CPU Times are Shown in Seconds)

Routine Name     Tot Time  # Calls Avg Time Percentage  Accum%
---------------- -------- -------- -------- ----------  -------
ADVX2            4.03E+01       96 4.20E-01      22.88    22.88  *****
ADVY2            3.40E+01       96 3.54E-01      19.28    42.15  ****
CONSOM           2.73E+01       48 5.69E-01      15.49    57.64  ***
ADVZ2            1.59E+01       48 3.32E-01       9.02    66.67  **
CALSUB           1.31E+01        4 3.28E+00       7.43    74.10  *
CONVMA           9.88E+00    32768 3.01E-04       5.60    79.70  *
MUHERM           5.76E+00   131072 4.40E-05       3.27    87.58
CHIMIE           4.74E+00       48 9.87E-02       2.69    90.26
CALFLU           3.80E+00        5 7.59E-01       2.15    92.42
INITER           2.39E+00       48 4.98E-02       1.36    93.77
CLOUD            1.94E+00    32768 5.91E-05       1.10    94.87
FINCYCL          1.80E+00        4 4.51E-01       1.02    95.89
QSAT             1.38E+00   292132 4.71E-06       0.78    96.67
DQSATDT          8.62E-01   168175 5.13E-06       0.49    97.16
LOUIS            6.44E-01    32768 1.96E-05       0.36    97.53
PELF             5.85E-01        5 1.17E-01       0.33    98.22
SUBSCAL          5.05E-01    32768 1.54E-05       0.29    98.51
REEMDT           4.55E-01        1 4.55E-01       0.26    98.76
PEFL             4.51E-01      160 2.82E-03       0.26    99.02
PEFP             3.27E-01      320 1.02E-03       0.19    99.20
TOMCAT           2.63E-01        1 2.63E-01       0.15    99.35
INIEXP           2.58E-01        1 2.58E-01       0.15    99.50
REEZNOT          2.49E-01        1 2.49E-01       0.14    99.64
PEPF             2.46E-01      320 7.70E-04       0.14    99.78
```

```
ADVEC            1.67E-01       48 3.49E-03       0.09    99.88
INICYCL          7.08E-02        4 1.77E-02       0.04    99.92
CEP              3.25E-02      320 1.01E-04       0.02    99.93
CEF1             3.04E-02      320 9.51E-05       0.02    99.95
CONVEC           2.33E-02       48 4.85E-04       0.01    99.96
ALRET            2.27E-02        5 4.54E-03       0.01    99.98
CEF2             1.26E-02      320 3.92E-05       0.01    99.98
CORPOLE          8.40E-03        5 1.68E-03       0.00    99.99
CHTRON           7.03E-03      385 1.83E-05       0.00    99.99
FINITER          6.79E-03       48 1.41E-04       0.00   100.00
INICSF           2.64E-03        5 5.27E-04       0.00   100.00
WRCHK            2.12E-03        1 2.12E-03       0.00   100.00
FINEXP           8.28E-05        1 8.28E-05       0.00   100.00
INICSTE          3.46E-06        1 3.46E-06       0.00   100.00
INCHK            2.26E-06        1 2.26E-06       0.00   100.00
================================================================================
Totals           1.76E+02   725361
Jun 12 19:31 mpc        77.95 Mflops    191.93s a.out
```

The most expensive routines are the second order moments advection scheme and `CONSOM` which applies the convection/diffusion matrix to the tracers. However, the code is written efficiently for the Cray.