U.G.A.M.P.
INTERNAL REPORT

UK Universities Global Atmospheric Modelling Programme

UGAMP Internal Report No. 44c

The TOMCAT Offline Transport Model

Part III. Convection and Vertical Diffusion

Zoe Stockwell and Martyn Chipperfield

August 1996

The TOMCAT Offline Transport Model
Part III. Convection and Vertical Diffusion

D. Zoe Stockwell and Martyn Chipperfield

Centre For Atmospheric Science, University of Cambridge, U.K.

August 1996

Version 1.0

Contents

1 Introduction

The TOMCAT offline three-dimensional (3D) chemical transport model (CTM) has been widely used for stratospheric studies and it has recently been developed for tropospheric chemistry. A very important part of this development was the inclusion of parameterisations of tracer transport due to convection and vertical diffusion. This report describes the implementation of these parameterisations in the basic TOMCAT model.

Convective and diffusive processes vertically mix air and it is important to represent this vertical mixing in the troposphere. Not only do the lifetimes of many important gases depend on altitude with, for example, an increase in the lifetime of O_3 and NO_x with height in the troposphere, but mixing can dilute concentrations. Under high NO_x conditions this dilution can result in a greater ozone production potential. Dry convection is treated here as a diffusive process and occurs when the environment is unstable with respect to the dry adiabat. Vertical diffusion also depends on the wind shear. Moist convection can occur as shallow, deep and mid-level cumulus when the environment is unstable with respect to the moist adiabat. Neither cumulus convection nor vertical diffusion are resolved by the spatially-averaged meteorological analyses (e.g. ECMWF) even at their highest resolution. It is therefore necessary to parameterize these processes in 3D global models. In TOMCAT we have implemented the Tiedtke [1989] mass flux convection scheme and the Louis [1979] vertical diffusion scheme, based on code written and kindly supplied by Martin Heimann of the Max Planck Institute in Hamburg. These schemes are suitable for use in an offline CTM because they only require the large scale fields of winds, temperature and humidity.

This report is Part III of a series of three reports describing the TOMCAT off-line chemical transport model (CTM). Part I describes the TOMCAT stratospheric chemistry scheme and Part II describes the basic model dynamics and advection scheme.

2 Sub-grid Vertical Transport

Forcing files are read into TOMCAT at the start of every meteorological cycle (e.g. 6 hours for ECMWF analyses). At this time, the instantaneous convective and vertical diffusive fluxes are calculated for every model grid box column. These fluxes are additive and are computed to form a 2D matrix ($\mathbf{M}$) which has dimensions $\mathcal{N}$ x $\mathcal{N}$ ($\mathcal{N}$ = number of vertical levels in the model). The element $\mathbf{M}_{k,j}$ of this matrix represents the mass fraction of tracer in level j transferred to level k (s^{-1}) due to all sub-gridscale vertical processes. The tracer masses after sub-gridscale vertical transport can be related to their initial values by calculation of a second matrix $\mathbf{C}$ ($= (\mathbf{I} - \mathbf{M})^{-1}$). Vertical mass redistribution is achieved by applying this matrix to the initial tracer mass and moments[1], and is performed throughout the entire cycle before the next forcing files are input to the model, at which stage the sub-gridscale fluxes are recalculated. In effect, this means that the fluxes from moist convection and vertical diffusion do not vary in time over the meteorological cycle (e.g. 6 hours).

The remainder of this section describes the Tiedtke [1989] mass flux convection scheme and the Louis [1979] vertical diffusion scheme as implemented in TOMCAT, and describes how the 2D matrix $\mathbf{C}$ is calculated.

2.1 The Convection Scheme

The convection scheme implemented in TOMCAT is based on the work of Tiedtke [1989]. It is a mass flux scheme which explicitly represents the cloud fields and their circulation in order to determine the effect

[1] Moment redistribution is treated differently depending on the direction, (see Section 2.3).

of convection on the large-scale budgets of heat and moisture. Representing this circulation is vital for tracer transport because the convective-induced fluxes are needed. Other schemes, such as the convective adjustment scheme of Betts and Miller [1984] and the Kuo scheme [1974] do not explicitly represent this circulation. By using a simple bulk model to represent the cloud ensemble, the contribution of convection to the large-scale budget equations of heat and moisture can be calculated in the Tiedtke scheme as:

$$
\begin{aligned}
\frac{\partial \bar{s}}{\partial t} + \mathbf{v}\cdot\nabla\bar{s} + \bar{w}\frac{\partial \bar{s}}{\partial t} = & - \frac{1}{\bar{\rho}_{air}}\frac{\partial}{\partial z}[M_u s_u + M_d s_d - (M_u + M_d)\bar{s}] + \mathrm{L}(c_u - e_d - \tilde{e}_l - \tilde{e}_p) \\
& - \frac{1}{\bar{\rho}_{air}}\frac{\partial}{\partial z}(\bar{\rho}_{air}\overline{w's'})_{tu} + \bar{Q}_R \qquad (1)
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial \bar{q}}{\partial t} + \mathbf{v}\cdot\nabla\bar{q} + \bar{w}\frac{\partial \bar{q}}{\partial t} = & - \frac{1}{\bar{\rho}_{air}}\frac{\partial}{\partial z}[M_u q_u + M_d q_d - (M_u + M_d)\bar{q}] + \mathrm{L}(c_u - e_d - \tilde{e}_l - \tilde{e}_p) \\
& - \frac{1}{\bar{\rho}_{air}}\frac{\partial}{\partial z}(\bar{\rho}_{air}\overline{w'q'})_{tu} \qquad (2)
\end{aligned}
$$

where s is the dry static energy, q the specific humidity, ρ_{air} the density of air, $\mathbf{v}$ the horizontal velocity vector, w the vertical velocity, c the rate of condensation, e the rate of evaporation and Q_R the radiative heating. Overbars denote grid area means, primes denote deviations from the mean. $\tilde{e}_l$ is the evaporation of cloud air that has been detrained into the environment and $\tilde{e}_p$ is the evaporation of precipitation in the unsaturated subcloud layer. The index tu denotes boundary layer turbulence. For both expressions the first two terms on the right side represent the perturbation to the heat and moisture budgets by convection.

The convection scheme implemented in TOMCAT is identical to that described by Tiedtke [1989] apart from the following differences: in TOMCAT midlevel convection and convective downdrafts are not included, and there is no organized entrainment of environmental air above cloud base. The scheme does include cumulus updrafts in the vertical column, entrainment of environmental air into the cloud and detrainment of cloud air to the environment. The magnitudes of these are related to horizontal convergence of moisture below cloud and the difference between cloud and environmental specific humidity at cloud base. Mass balance within the vertical column is maintained by including sub-grid subsidence of environmental air, (induced by convection), within the same timestep. Subsidence is parameterized differently to Tiedtke [1989].

2.1.1 Convective Updraft

The $\mathcal{N}$ vertical levels in TOMCAT extend from level $\mathcal{N}$, closest to the Earth's surface, to level 1 (e.g. at 10 hPa in the stratosphere with ECMWF analyses). Thermodynamic and other variables are defined either at the centre of model levels or at level interfaces, (see Figure 1).

Air at the top of level $\mathcal{N}$ (i.e. at interface $\mathcal{N}-1$) is lifted through model level $(\mathcal{N}-1)$ along the dry adiabat:

$$\frac{dT_p}{dz} = -\frac{g}{c_p}$$

(The notation used in this report is summarised in Appendix 2).

The temperature of the lifted parcel at the top of level $(\mathcal{N}-1)$ (i.e. interface $\mathcal{N}-2$) is given by

$$T_p^{\mathcal{N}-2} = T_p^{\mathcal{N}-1} - (z^{\mathcal{N}-2} - z^{\mathcal{N}-1})g/c_p$$

Although the specific humidity remains constant with parcel lifting, at this higher level the temperature of the lifted parcel is lower than at interface $(\mathcal{N}-1)$ and therefore the relative humidity (RH) increases. If

Centre of Levels	Updraft and Subsidence Variables	Level Interfaces
	....	0
1	――――――――――――――――	
	....	1
2	――――――――――――――――	
	....	2
	.	
	.	
	....	$k-1$
k	$E_u^k \rightarrow$ ―――――――― $D_u^k \rightarrow$	
	.... $M_u^k \uparrow$ $M_s^k \downarrow$	k
$k+1$	$E_u^{k+1} \rightarrow$ ―――――――― $D_u^{k+1} \rightarrow$	
	...... $M_u^{k+1} \uparrow$ $M_s^{k+1} \downarrow$	$k+1$
$k+2$	――――――――――――――――	
	....	$k+2$
	.	
	.	
$\mathcal{N}-2$	――――――――――――――――	
	...... $T^{\mathcal{N}-2}, z^{\mathcal{N}-2}, q^{\mathcal{N}-2}$	$\mathcal{N}-2$
$\mathcal{N}-1$	――――――――――――――――	
	...... $T^{\mathcal{N}-1}, z^{\mathcal{N}-1}, q^{\mathcal{N}-1}$	$\mathcal{N}-1$
$\mathcal{N}$	――――――――――――――――	
	....	$\mathcal{N}$

Figure 1: TOMCAT vertical levels

the lifted parcel becomes supersaturated at interface ($\mathcal{N}$ - 2) so that $RH > 100\%$, then the first criterion for cloud occurrence in the column has been met and this interface is set as cloud base. If $RH < 100\%$, the parcel is lifted to the next level, tested for supersaturation, and so on until cloud base is found.

At cloud base, the lifted parcel now lies in a regime of moist adiabatic ascent. Excess moisture is condensed and the specific humidity q_p, and temperature T_p, are iteratively adjusted to their saturation (RH = 100%) values q_p', T_p', using

$$\begin{aligned} q_p' &= q_p - \frac{q_p - q_{sat}(T_p)}{1 + \frac{L}{c_p}\frac{dq_{sat}(T_p)}{dT}} \\ T_p' &= T_p - (q_p' - q_p)\frac{L}{c_p} \end{aligned}$$

from

$$\triangle T = - \triangle q \frac{L}{c_p}, \qquad \triangle q = q' - q$$

and

$$q' \simeq q_{sat}(T) + \frac{dq_{sat}}{dT} \triangle T$$

To achieve convergence towards saturation values, in each subsequent iteration the new values of q'_p and T'_p replace q_p and T_p. Finally, cloud liquid water content is set equal to the total condensate.

The lifted parcel is now tested for buoyancy with respect to the environmental air[2]. If the virtual static energy of the parcel, s_{vp}, is less than that of the environment, s_{ve}, then the parcel is not buoyant and the model vertical column is set as non-convecting.

$$\begin{aligned} s_{vp} &= s_p + c_p\, T_p\, (0.608\, q_p - LWC) \\ s_{ve} &= s_e + c_p\, T_e\, (0.608\, q_e) \end{aligned}$$

where

$$\begin{aligned} s_p &= \mathrm{c}_p\, T_p + \mathrm{g\ z} \\ s_e &= \mathrm{c}_p\, T_e + \mathrm{g\ z} \end{aligned}$$

If $s_{vp} > s_{ve}$ the parcel is buoyant and the second criterion for convective cloud occurrence within the column is met. The final criterion is the horizontal convergence of moisture below cloud base. This is calculated using:

$$- \int_{\text{surface}}^{\text{cloud base}} \{\mathbf{v}.\nabla \rho_w\}\, dz = \int_{\text{surface}}^{\text{cloud base}} \{\rho_w\ \nabla.\mathbf{v} - \nabla(\rho_w\ \mathbf{v})\}\, dz$$

If this integral is positive the grid column is convectively unstable and **deep convection** occurs. However, if there is a divergence of moisture, a further check is made to determine whether the column is unstable with respect to **shallow convection**. Shallow convection depends less on large-scale moisture convergence than on evaporation of moisture from the surface. If addition of this local surface evaporative flux to the integral above results in a positive water vapour flux at cloud base, then shallow convection occurs within the column. If there is still a divergence of moisture below cloud base, the model column is set as cloudless.

To maintain moisture content during convection, a moisture balance is imposed below cloud base. The updraft mass flux of air through cloud base is therefore calculated (for shallow and deep convection) as:

$$M_u^{base} = \frac{- \int_{\text{surface}}^{\text{cloud base}} \mathbf{v}.\nabla \rho_w dz \; + \; \text{surface evaporation}}{(q_p - q_e)_{\text{at cloud base}}}$$

and the updraft cloud base mass flux of tracer Tr_u^{base} as;

$$Tr_u^{base} = M_u^{base}\ \chi_p^{tr}\ .$$

The updraft mass flux at cloud base is generated by organized entrainment of air from levels below cloud base. The fraction originating from each of these levels is set proportional to the level mass.

The lifted parcel is raised through the next model level. During this process, turbulent entrainment into (E_u) and detrainment out of (D_u) the cloud are parameterized as:

$$E_u = M_u\ \epsilon_u \quad ; \qquad D_u = M_u\ \delta_u$$

[2]No test is made below cloud base for parcel buoyancy, because it is assumed that large scale moisture convergence, (which is the final boundary condition for cloud occurrence), sufficiently destabilizes the below cloud levels and ensures thermals reach the lifting condensation level, LCL. (Note that if buoyancy is not achieved at the LCL, in this parameterization scheme there is no further lifting of the parcel to test for a higher level of free convection).

where the fractional entrainment/detrainment rates (ϵ_u, δ_u) depend inversely on cloud radii. Clouds of smaller sizes are assumed to occur in the absence of large-scale convergence (i.e. shallow convection), and it is further assumed that $\epsilon_u = \delta_u$, so that a simple form is used:

$$\epsilon_u = \delta_u = \left\{ \begin{array}{ll} 1\text{x}10^{-4}\ m^{-1}, & \text{for deep convection} \\ 3\text{x}10^{-4}\ m^{-1}, & \text{for shallow convection} \end{array} \right\}$$

The updraft mass flux and tracer mass flux vary as

$$\begin{aligned} \frac{\partial M_u}{\partial z} &= E_u - D_u \\ \frac{\partial Tr_u}{\partial z} &= E_u\ \chi_e - D_u\ \chi_p = E_u\ \chi_e - D_u\ \frac{Tr_u}{M_u} \end{aligned}$$

During ascent through the level, T_p and q_p are adjusted along the wet adiabat and modified for entrainment of environmental air and detrainment of cloud air.[3] Any condensate is added to the liquid water loading. Detrainment of liquid water to the environment is included. At the level top, the lifted parcel is tested for buoyancy as before; if it is buoyant then lifting through subsequent levels continues, otherwise the lower interface of the model level in which buoyancy is lost is set as the top of the cloud column, k_{top}, (see Figure 2).

Centre of Levels		Level Interfaces
	....	k_{top-2}
k_{top-1}	$D_u^{k_{top-1}} \leftarrow$ ———————— $\rightarrow D_u^{k_{top-1}}$	
	....	k_{top-1}
k_{top}	$D_u^{k_{top}} \leftarrow$ ———————— $\rightarrow D_u^{k_{top}}$	
	cloud top $\cdots M_u^{k_{top}} \uparrow$	k_{top}

Figure 2: Showing cloud top and detrainment of cloud air

Organized detrainment occurs above cloud top[4] and allows for some small shallow cumuli overshooting the level of zero buoyancy [Tiedtke, 1989]. It is parameterized as

$$\begin{aligned} D_u^{k_{top}} &= (1-\beta)\ M_u^{k_{top}-1} \\ D_u^{k_{top}-1} &= \beta\ M_u^{k_{top}-1} \end{aligned}$$

$$\beta = \begin{cases} 0.3 & \text{for shallow convection,} \\ 0.0 & \text{for deep convection.} \end{cases}$$

Discretization

At a model level k

$$M_u^k - M_u^{k+1} = E_u^{k+1} - D_u^{k+1}\ .$$

The tracer updraft mass flux can be implicitly calculated as;

$$Tr_u^k - Tr_u^{k+1} = E_u^{k+1}\ \chi_e^{k+1} - D_u^{k+1}\ \frac{Tr_u^k}{M_u^k}.$$

[3]No modification is made to the large scale (environmental) thermodynamic properties (q_e, T_e), even though a change in these would be expected due to detrainment of cloud air.

[4]Note that there is turbulent entrainment into and detrainment out of level k_{top} in addition to organized detrainment.

$$\begin{array}{ccc}
\cdots\cdots\cdots\cdots & \uparrow M_u^k,\ \uparrow Tr_u^k & \cdots\cdots\cdots\cdots \\
E_u^{k+1} \longrightarrow & \rule{4cm}{0.4pt} & \longleftarrow D_u^{k+1} \\
\cdots\cdots\cdots\cdots & \uparrow M_u^{k+1},\ \uparrow Tr_u^{k+1} & \cdots\cdots\cdots\cdots
\end{array}$$

Substituting $M_u^k = M_u^{k+1} + E_u^{k+1} - D_u^{k+1}$, and $\chi_e^{k+1} = S0^{k+1}/SM^{k+1}$, and solving for Tr_u^k gives;

$$Tr_u^k = (Tr_u^{k+1} + E_u^{k+1}\frac{S0^{k+1}}{SM^{k+1}})(1 - \frac{D_u^{k+1}}{M_u^{k+1} + E_u^{k+1}}). \tag{3}$$

The updraft tracer flux through interface k can be represented as a linear function

$$Tr_u^k = \sum_{j=\mathcal{N}}^{1} S0^j \ \Phi_{k,j}^u$$

where $\Phi_{k,j}^u$ **is the fractional tracer mass from level j transferred through interface k in the convective updraft**. From the condition that, at the lowest model interface $\mathcal{N}$, $M_u^{\mathcal{N}} = Tr_u^{\mathcal{N}} = 0$, it can be seen that

$$\Phi_{\mathcal{N},j}^u = 0 \qquad\qquad j = 1, 2, \ldots, \mathcal{N},$$

i.e. there is no flux through the lowest model interface. From equation (3) a recursion formula can be used to determine general column values of $\Phi_{k,j}^u$:

$$\Phi_{k,j}^u = (\Phi_{k+1,j}^u + \delta_{k,j-1}\frac{E_u^{k+1}}{SM^{k+1}})(1 - \frac{D_u^{k+1}}{M_u^{k+1} + E_u^{k+1}})$$

where

$$\delta_{k,j-1} = \begin{cases} 1 & \text{if } j = k+1 \text{ (adjacent levels),} \\ 0 & \text{otherwise.} \end{cases}$$

2.1.2 Subsidence

Outside of the cloud a sub-gridscale subsidence flux is induced to maintain mass balance within the column. The mass flux through interface k, M_s^k is given by

$$M_s^k = -M_u^k$$

so that the tracer flux is $Tr_s^k = -M_u^k\ \chi_e^k$, and $\Phi_{k,j}^u = -\frac{M_u^k}{SM^k}\delta_{k,j}$.

2.2 Vertical Diffusion

The Louis [1979] vertical diffusion scheme in TOMCAT is a local K-closure scheme, which is a valid parameterization for models that resolve the planetary boundary layer (PBL) explicitly.

It is assumed that vertical diffusion can be treated similarly to molecular diffusion, with tracer fluxes set proportional to their gradients [Louis, 1979]:

$$Tr = -K_z\ \left(\frac{\partial \rho_{tr}}{\partial z}\right).$$

Calculation of K_z is identical to that used by both the ECMWF forecast model [ECMWF, 1986], and the TM2 model [Heimann, 1995]:

$$\begin{aligned} K_z &= l^2 \left| \frac{\partial \mathbf{v}}{\partial z} \right| f_h(Ri), & (4) \\ \text{the mixing length, } l &= \frac{kas\ z}{1 + (kas\ z/\lambda)}\ , & (5) \\ \text{and the Richardson number, } Ri &= \frac{g}{\theta} \frac{\frac{\partial \theta}{\partial z}}{\left| \frac{\partial \mathbf{v}}{\partial z} \right|^2}\ . & (6) \end{aligned}$$

Ignoring adiabatic processes and substituting θ using $c_p\ T\ \partial\ ln\theta \simeq \partial s$ [Holton, 1992], gives

$$Ri = \frac{g\ \partial z\ \partial s}{c_p\ T\ |\partial \mathbf{v}|^2}\ .$$

Ri relates the likelihood of vertical turbulence to the static stability of the atmosphere and vertical wind shear stress [Houghton, 1991]. Persistence of turbulence is generally expected for $Ri < 1$ [Holton, 1992], so for surface heating and an unstable lapse rate ($\partial\theta/\partial z < 0$) Ri is negative and convective overturning occurs. Under statically stable conditions Ri is positive. However, increasing vertical wind shear decreases Ri and, if mechanical production ($|\partial \mathbf{v}/\partial z|^2$) exceeds buoyancy damping ($g\partial\theta_v/\theta_v\partial z$), turbulence can be sustained, (see Equation 6).

The stability function, $f_h(Ri)$, depends on the static stability of the atmosphere.
For an unstable or neutral atmosphere, $Ri \leq 0$, and $f_h(Ri)$ is parameterized as

$$\begin{aligned} f_h(Ri) &= 1 - \frac{3\ b\ Ri}{1 + G(Ri)}, \\ G(Ri) &= 3\ b\ c\ l^2 \sqrt{\frac{-Ri}{z} \left[\frac{1}{\partial z} \left(1 + \frac{\partial z}{z} \right)^{1/3} - 1 \right]^3}. \end{aligned}$$

If the atmosphere is statically stable, $Ri > 0$, and $f_h(Ri)$ is parameterized as

$$f_h(Ri) = \frac{1}{1 + 3\ b\ Ri\sqrt{1 + e\ Ri}}\ ,$$
$$\text{(where } b = c = e = 5\text{m).}$$

Under statically stable conditions, an increase in vertical wind shear acts to decrease Ri, increase $f_h(Ri)$, and increase the vertical diffusion coefficient, K_z. For unstable conditions, an increase in vertical wind shear makes Ri less negative, and $f_h(Ri)$ smaller, which is opposite to that expected. The overall effect on K_z (Equation 5) for unstable conditions is dependent on the extent of static instability and the wind shear magnitude.

Non-local vertical diffusion schemes are not solely dependent on the local potential temperature gradient (as here in the local scheme). They therefore account for large eddy transports than can occur throughout the PBL even when part of the depth of the PBL is statically stable [Deardorff, 1972; Holtslag and Boville, 1993]. These schemes thus give a more well-mixed PBL than the Louis scheme. The Louis scheme is further limited because it does not account for entrainment at the top of the PBL. It is therefore likely that, in TOMCAT, diffusive mixing is under-predicted both within the PBL and between the PBL and free troposphere. This underestimate is likely to effect considerably the model-predicted distributions of surface-emitted tracers.

Discretization

The diffusive flux through interface k is given by

$$
\begin{aligned}
Tr_d^k &= Tr_{d,up}^k + Tr_{d,down}^k \\
Tr_{d,up}^k &= +K_z^k \left(\frac{\partial \rho_{tr}}{\partial z}\right)_{k+1\to k} \\
&= +K_z^k \frac{\rho_{air}^k}{z^k - z^{k+1}} \left(\frac{S0}{SM}\right)_{k+1} \\
Tr_{d,down}^k &= -K_z^k \left(\frac{\partial \rho_{tr}}{\partial z}\right)_{k\to k+1} \\
&= -K_z^k \frac{\rho_{air}^k}{z^k - z^{k+1}} \left(\frac{S0}{SM}\right)_{k}
\end{aligned}
$$

ρ_{tr} is the local density of tracer, z^k is defined at full model level k, K_z^k and ρ_{air}^k are defined at interface k. In general terms

$$
\begin{aligned}
Tr_d^k &= \sum_{j=1}^{\mathcal{N}} \Phi_d^{k,j}\ S0^j, \\
\Phi_d^{k,j} &= -K_z^k \frac{\rho_{air}^k}{z^k - z^{k+1}} \left[\left(\frac{\delta_{k,j}}{SM^k}\right) - \left(\frac{\delta_{k,j-1}}{SM^{k+1}}\right)\right].
\end{aligned}
$$

2.3 Matrix Calculation

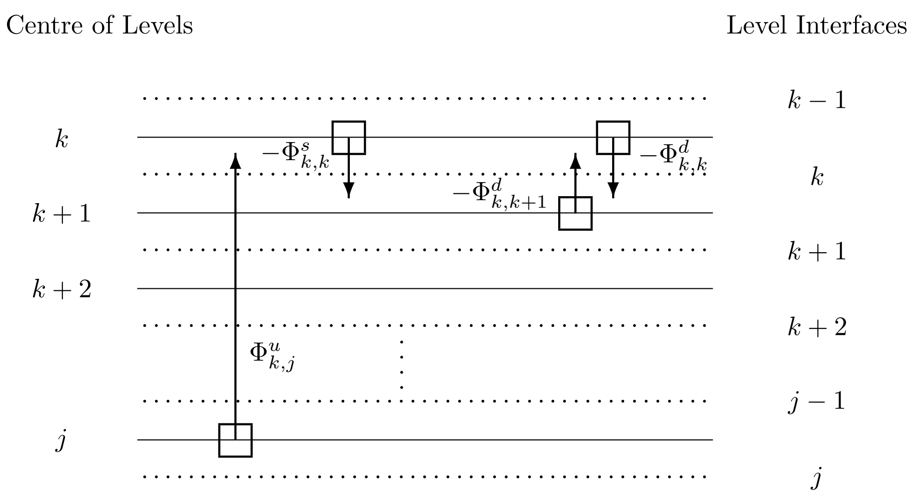


Figure 3: Fluxes associated with convective updraft, subsidence and vertical diffusion.

The matrix $\mathbf{C}$ can now be calculated. Linear addition of the individual fluxes (s^{-1}) from convection, subsidence and vertical diffusion (Figure 3) gives the fractional mass of tracer in level j transported to level k as

$$\mathbf{M}_{k,j} = \Phi^u_{k,j} + \Phi^s_{k,j} + \Phi^d_{k,j}$$

so that the change in tracer mass in level j due to sub-grid vertical transport ($\mathrm{kg_{tracer}\ s^{-1}}$) is given by

$$\frac{\partial S0^j}{\partial t} = \sum_{k=1}^{\mathcal{N}} \mathbf{M}_{k,j}\ S0^j$$

and the entire column can be represented in vector form,

$$\frac{\partial \mathbf{S0}}{\partial t} = \mathbf{M} \cdot \mathbf{S0}.$$

Finally, implicit integration gives

$$\begin{aligned} \mathbf{S0}(t + \triangle t) &= \mathbf{S0}(t) + \triangle t\ \mathbf{M} \cdot \mathbf{S0}(t + \triangle t) \\ &= (\mathbf{I} - \triangle t\ \mathbf{M})^{-1} \cdot \mathbf{S0} \\ &= \mathbf{C} \cdot \mathbf{S0}. \end{aligned}$$

Sub-grid processes therefore modify the tracer continuity equation from

$$\begin{aligned} \frac{\partial \chi_{tr}}{\partial t} &= \nabla(\mathbf{u} \cdot \chi_{tr}) + P - L\chi_{tr}, \text{ to} \\ \frac{\partial \chi_{tr}}{\partial t} &= \nabla(\mathbf{u} \cdot \chi_{tr}) + P - L\chi_{tr} + \mathbf{M} \cdot \chi_{tr}\ . \end{aligned}$$

2.4 Application to Tracer Moments

The default advection scheme in TOMCAT is the Prather [1986] second order moments scheme which stores not only the average tracer mass within each gridbox, but also the gradient and curvature of the tracer mass. These first and second order moments also need to be updated during convection and vertical diffusion.

In the horizontal, modification of the first and second order tracer moments follows that for **S0**, i.e.

$$\begin{aligned} \mathbf{SX}(t + \triangle t) &= \mathbf{C} \cdot \mathbf{SX}(t) \\ \mathbf{SXX}(t + \triangle t) &= \mathbf{C} \cdot \mathbf{SXX}(t), \end{aligned}$$

and similarly for **SY**, **SYY** and **SXY**.

It is assumed that vertical mixing reduces the vertical tracer gradient and therefore the vertical moments. These are therefore modified as

$$\begin{aligned} \mathrm{SZ}^j(t + \triangle t) &= \mathbf{C}_{j,j}\ \mathrm{SZ}^j(t) \\ \mathrm{SXZ}^j(t + \triangle t) &= \mathbf{C}_{j,j}\ \mathrm{SXZ}^j(t), \end{aligned}$$

and similarly for SYZ and SZZ.

3 Using the Convection and Diffusion Schemes in TOMCAT

The standard version of TOMCAT is `TOMCATI` in the nupdate library `/home/j90/kd/tomcat`. A listing of the model (with line numbers) is in `/home/j90/kd/tomcat/tomcati_list`.

3.1 Switches and Variables

To use the convection and/or vertical diffusion schemes set the switches LCONV and/or LVDIF to TRUE.

```
      PARAMETER(LCONV=.TRUE.,LVDIF=.TRUE.)                SWITCH.11
```

You must also access the relevant subroutines in the nupdate library e.g.

```
*C,CONVEC,CONSOM,DIFCON
```

3.2 First Order Moments Advection

The default convection scheme is set up to deal with the second order moment Prather [1986] advection scheme. If you are using only first order moments advection (e.g. to save CPU time and memory) you must change the following line in CONVEC

```
      CALL CONSOM                                         CONVEC.9
```

to call the routine CONFOM.

3.3 Fortran Channels

The convection/diffusion schemes make use of the following fortran channels during execution:

Channel	Variable	Common Deck	Purpose
18	IEVAP	REDEM	Read file EVAPxx
19	ICON	REDEM	Writing/reading convection/diffusion matrix

The file EVAPxx contains the evaporation fluxes of H_2O on the horizontal model grid. There are standard files for the common model grids in /home/j90/kd/tomcat/UTIL.

3.4 Subroutines

The subroutines in the convection and vertical diffusion schemes are listed here, along with some other principal subroutines of the model.

- CALSUB Main routine for setting up convection/diffusion matrix.
- CLOUD Calculates convection using Tiedtke [1989] scheme.
- CONVEC Calls CONSOM, CONFOM or CONZOM
- CONMA Calculates convection/diffusion matrix.
- CONSOM Applies convection/diffusion matrix to 0, 1st and 2nd order moments.
- CONFOM Applies convection/diffusion matrix to 0 and 1st order moments.
- CONZOM Applies convection/diffusion matrix to 0 order moments.
- DQSATDT Calculates d(QSAT)/dT.
- FINCYCL End of cycle.

- `FINITER` End of iteration.
- `INICYCL` Start of cycle (period of forcing analyses).
- `INIEXP` Initialise experiment.
- `INITER` Start of iteration (basic model timestep).
- `LOUIS` Calculates vertical diffusion coefficients using Louis [1979] scheme.
- `MUHERM` Performs cubic interpolation.
- `QH2O` Calculates specific humidity.
- `QSAT` Calculates saturation specific humidity.
- `SUBSCAL` Calls `LOUIS` and `CLOUD` for a model column.

4 Tests

The convections and vertical diffusion schemes have been tested in the following experiments.

4.1 Compiler Tests

- The model compiles with no ERRORS or WARNINGS.
- The model runs with variables initialised indefinite (`-f indef`).
- The model was checked for arrays going out of bounds (`-Rbc` in cft77).

4.2 Mass Conservation

The convection and vertical diffusion schemes redistribute tracer mass between levels within a model column. Therefore the total tracer mass within a column should be conserved whenever these processes are occurring. A model experiment was performed in which the total column tracer mass was diagnosed at every timestep. The total tracer masses were indeed conserved following convection and vertical diffusion.

4.3 TOMCAT 3D Experiments

4.3.1 Vertical Fluxes

TOMCAT was run using a T42 Gaussian grid and 19 vertical levels. The vertical mass fluxes from convection and vertical diffusion calculated by TOMCAT are shown in Figure 4. The results are an average over 15 days using meteorological data for December 27, 1990 - January 11, 1991. Model output was saved every 6 hours (giving an average of 60 model outputs). The vertical mass fluxes calculated by the schemes are reasonable.

4.3.2 Convective Rainfall

Although TOMCAT is an offline model where the humidity fields are specified from meteorological analyses, the Tiedtke convection scheme diagnoses the convective rainfall. In TOMCAT this rainfall is parameterized as described in Tiedtke [1989] and evaporation of rain below cloud base is ignored. Figure 5 shows the July mean convective rainfall calculated in TOMCAT in an experiment using a T42 Gaussian grid, 19 vertical levels and meteorological data for 1990. The distribution of convective rainfall is sensible.

4.3.3 Surface-Emitted Tracer Distribution

The model was run using a T42 Gaussian grid, 31 vertical levels and meteorological data for 1994. The effect of convection and vertical diffusion on the zonal mean distribution of a radioactive, short-lived ($\tau_{1/2} \sim 3.825$ days), surface-emitted tracer, radon, was investigated. Radon is emitted from all non-iced land surfaces; emissions from iced land surfaces are less as are oceanic emissions. Figure 6 illustrates the effects of convection and vertical diffusion on the resultant radon distribution predicted by TOMCAT. The convection and diffusion schemes clearly transport radon from the surface into the free troposphere. The vertical diffusion is most effective near the surface; at higher altitudes convection is more important.

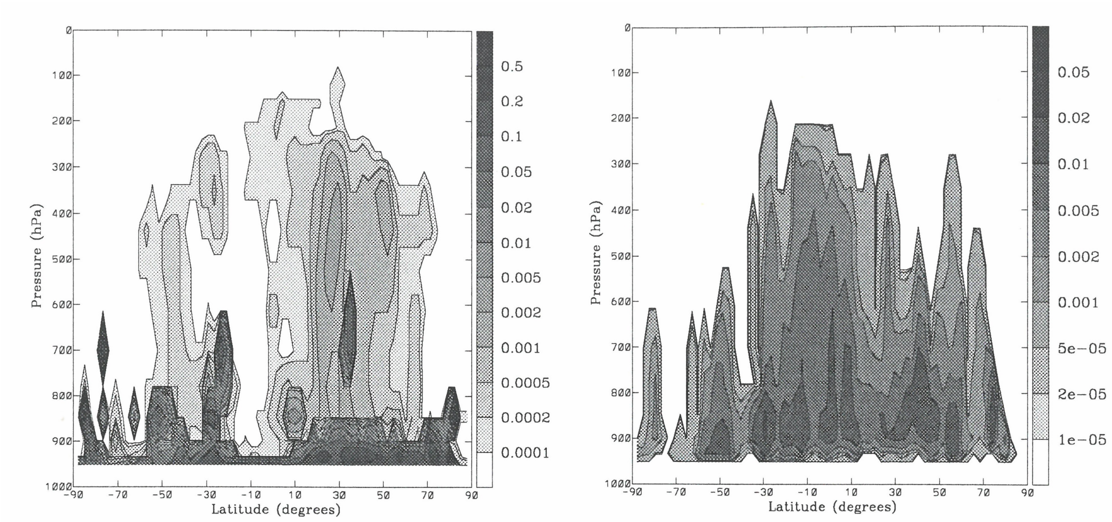


Figure 4: TOMCAT zonal mean upward vertical mass flux from a) vertical diffusion and b) convection. Averaged over December 27, 1990 - January 11, 1991. (kg_{air} m^{-2} s^{-1}).

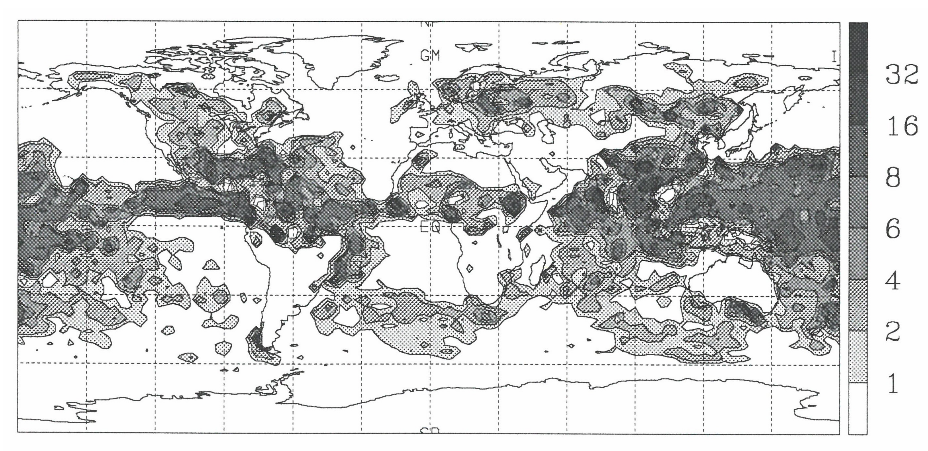
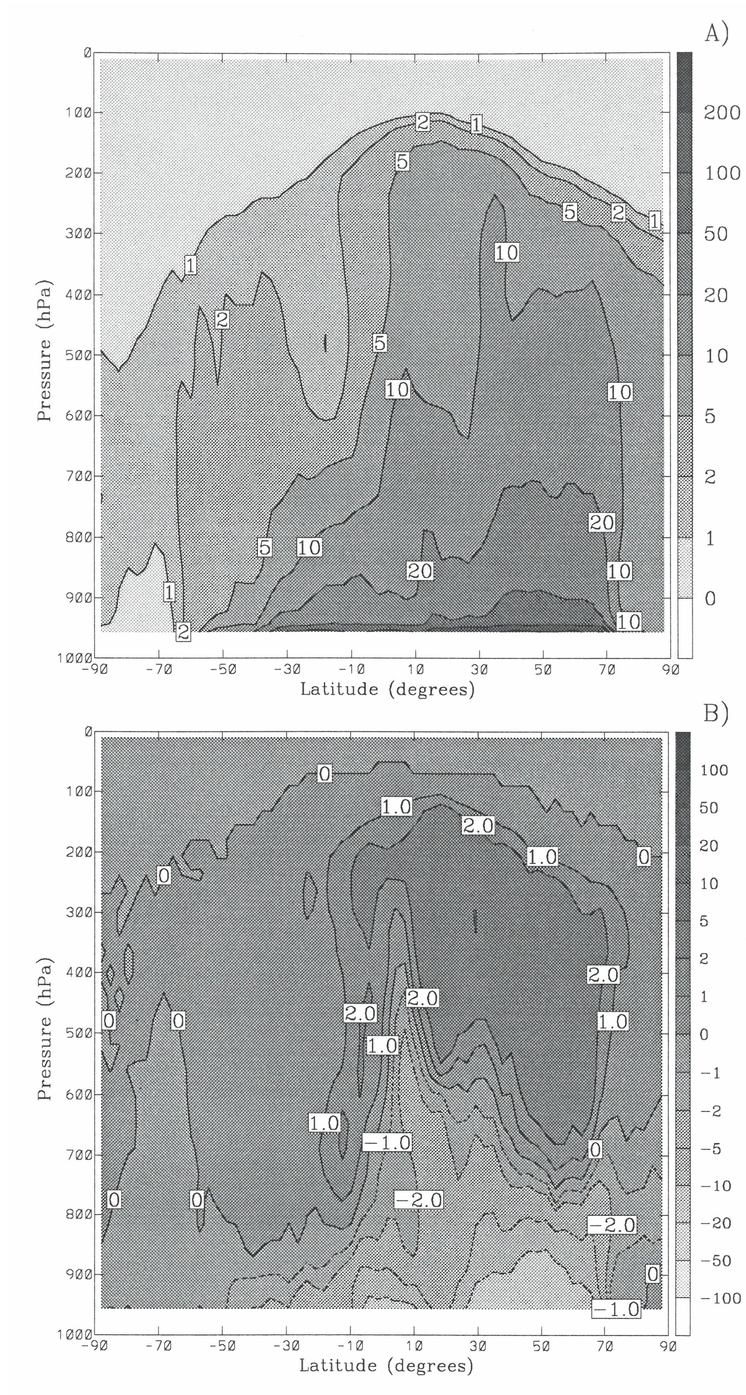


Figure 5: July rainfall (mm day^{-1}) diagnosed by TOMCAT at T42 horizontal resolution.



A)
Pressure (hPa)
Latitude (degrees)
0
100
200
300
400
500
600
700
800
900
1000
-90
-70
-50
-30
-10
10
30
50
70
90
200
100
50
20
10
5
2
1
0
B)
Pressure (hPa)
Latitude (degrees)
100
50
20
10
5
2
1
0
−1
−2
−5
−10
−20
−50
−100

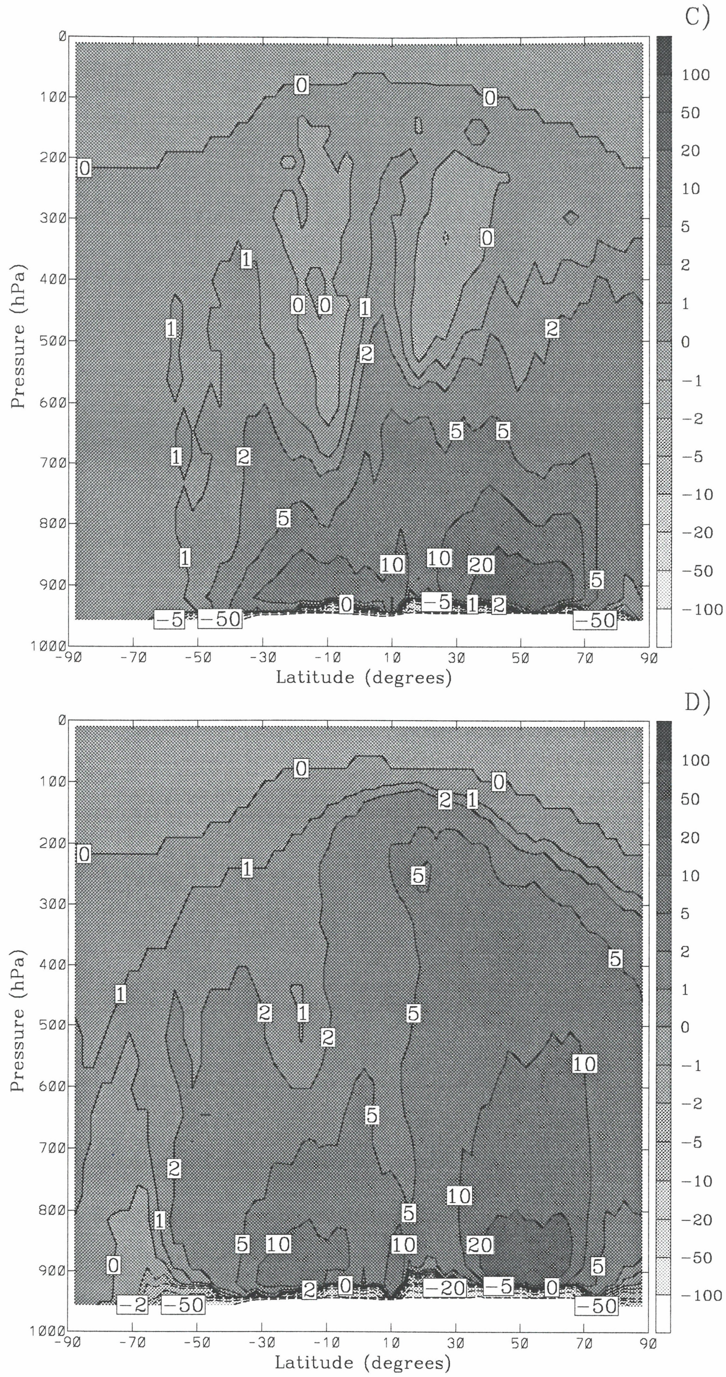


Figure 6: a) Zonal mean distribution of Radon (in pico curie m^{-3} at STP) in May 1994 from the TOMCAT run including convection and vertical diffusion. b) Difference between Figure 6a) and a model run with no convection (i.e. effect of convection). c) Difference between Figure 6a) and a model run with no vertical diffusion (i.e. effect of vertical diffusion). d) Difference between Figure 6a) and a model run with no vertical diffusion or convection.

5 Acknowledgements

We are very grateful to Martin Heimann for supplying us with his original code, and to Mike Blackburn for many helpful discussions.

References

[1] Betts, A.K., and M.J. Miller, A new convective adjustment scheme, *ECMWF Technical Report No. 43*, 1984.

[2] Chipperfield, M.P., The TOMCAT offline chemical transport model. Part I. Stratospheric chemistry code, UGAMP Internal Report No. 44a. 1996.

[3] Chipperfield, M.P., and P. Simon, The TOMCAT offline chemical transport model. Part II. Dynamics and advection, UGAMP Internal Report No. 44b. 1996.

[4] Deardorff, J.W., Theoretical expression for the countergradient vertical heat flux, *J. Geophys. Res.*, *77*, 5900-5904, 1972.

[5] ECMWF, Research Manual 3, 1986.

[6] Heimann, M., The global atmospheric tracer model TM2, Technical Report no. 10, *Deutsches Klimarechenzentrum, Hamburg*, 1995.

[7] Holton, J.R., An introduction to dynamic meteorology (3rd edition), *Academic Press*, 1992.

[8] Holtslag, A.A.M, and B.A. Boville, Local versus nonlocal boundary-layer diffusion in a global climate model, *Jour. of Climate*, *6*, 1825-1842, 1993.

[9] Houghton, J.T., The physics of atmospheres (2nd edition), *Cambridge University Press*, 1991.

[10] Kuo, H.L., Further studies of the parameterization of the influence of cumulus convection of large scale flow, *J. Atmos. Sci.*, *31*, 1232-1240, 1974.

[11] Louis, J.-F., A parametric model of vertical eddy fluxes in the atmosphere, *Boundary Layer Meteorol.*, *17*, 187-202, 1979.

[12] Prather, M. J., Numerical advection by conservation of second-order moments, *J. Geophys. Res.*, *91*, 6671-6681, 1986.

[13] Tiedtke, M., A comprehensive mass flux scheme for cumulus parameterization in large-scale models, *Mon. Wea. Review*, *117*, 1779-1800, 1989.

6 Appendix 1. Flowtrace

Below is a flowtrace on a Cray YMP8 from a 1 day TOMCAT run with `NIV=19, LON=128, LAT=64` with (6-hourly) ECWMF winds and 2 passive 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 convection/vertical diffusion scheme is efficient and suitable for use in a 3D model. The most expensive routine in the scheme is `CONSOM` which applies the convection/diffusion matrix to the tracers and takes 15% of the total time. `CALSUB`, `CONVMA` and `MUHERM` also contribute to the total cost. However, advection by the Prather [1986] scheme (which is efficiently coded) dominates the total cost. If chemistry was included, this would then be the most costly part of the model.

7 Appendix 2. Notation

The following two tables summarise the notation and variables used in this report.

Symbol	**Meaning**
	Superscripts and Subscripts
u	updraft
s	subsidence
d	vertical diffusion
p	lifted parcel
e	environmental

Symbol	Meaning	Value/Units
T	Temperature	K
z	Geopotential height	m
g	Gravitational acceleration	m s^{-2}
c_p	Average heat capacity of atmospheric gases at constant pressure	= 1005.46 J K^{-1} kg^{-1}
L	Latent heat of condensation at 0^oC	J kg^{-1}
q	Specific humidity	kg(water)/kg(air)
RH	Relative humidity; ratio of water vapour pressure to saturation water vapour pressure at air temperature	
LWC	Liquid water content	kg(water)/kg(air)
s	Dry static energy	J kg^{-1}
s_v	Virtual static energy	J kg^{-1}
ρ_w	Water density	kg(water) m^{-3}
ρ_{tr}	Tracer density	kg(tracer) m^{-3}
ρ_{air}	Air density	kg(air) m^{-3}
$\mathbf{v}$	Horizontal wind vector	m s^{-1}
χ^{tr}	Tracer mass mixing ratio	kg/kg(air)
$S0^j$	Tracer mass in level j	kg(tracer)
SM^j	Air mass in level j	kg(air)
M^k	Mass flux of air through interface k from updraft, subsidence or vertical diffusion	kg(air) m^{-2} s^{-1}
Tr^k	Mass flux of tracer through interface k from updraft, subsidence or vertical diffusion	kg(tracer) m^{-2} s^{-1}
$\Phi_{k,j}$	Fraction of tracer mass from level j transferred through interface k from updraft, subsidence or vertical diffusion	
K_z	Vertical diffusion coefficient	m^2 s^{-1}
l	Mixing length	m
kas	Asymptotic mixing length	= 438.18 m
λ	Von Karman's constant	= 0.4 m
θ	Potential temperature	K
Ri	Richardson's number	adimensional
$f_h(Ri)$	Stability function	adimensional
K	Constant for precipitation parameterization	= 2.0 x 10^{-3}
$M_{k,j}$	Fraction of tracer mass from level j transferred through model interface k due to all sub-gridscale processes	