32640

COO-2249-2

Department of Meteorology, 54-1517

Massachusetts Institute of Technology

Cambridge, Massachusetts 02139

Transport Processes and Trace Constitutents in the Stratosphere

Progress Report

for the period

November 20, 1972 - June 30, 1973

Research conducted under Contract no. AT (11-1) - 2249

Principal Investigator: Dr. Derek M. Cunnold

April 2, 1973

Table of Contents (April 1973)

Section

Appendices

Introduction

During the current contract period progress has been made in all areas of our program. The progress in each of the task areas is outlined below with the details of the development of the numerical model being discussed in the main body of the report.

(I) The numerical model

The major portion of our research funds are being devoted to this task and substantial progress has been made in writing the necessary computer codes. The vorticity and thermodynamic equations have been programmed with the friction and heating omitted and the model has been run barotropically (i.e. no coupling between levels) at several levels for 12 days of prediction (300 time steps) using a Lorenz n-cycle scheme. Energy was found to be conserved at all levels. The model will be run baroclinically (i.e., including vertical coupling between levels) very shortly using an arbitrary specified vertical velocity field. It is anticipated that by the end of April the coding of the vertical velocity program will be complete and the model may be run baroclinically with an internally consistent vertical velocity field.

The most time consuming portions of the chemistry and heating rate codes have been programmed. A program for evaluating the vertical column concentration of ozone above any level is complete as is a code which derives the daily average values of the photodissociation coefficients, J_{O_2}, J_{O_3}, and J_{NO_2}, at every grid point from the predicted ozone mixing ratios. This code also calculates the atmospheric heating rate at each grid point resulting from the absorption of solar ultraviolet and visible energy. The code will shortly be extended to include the small additional contribution that molecular oxygen makes to the heating rate. By the end of April it should be possible to predict the photoequilibrium ozone concentrations at every grid point for any specified solar declination angle and similarly to evaluate the contribution of chemical processes to the loss of ozone (i.e., to evaluate the term $(d\chi_{O_3}/dt)_C$ in equation (1.31)). The programming necessary to complete the specification of atmospheric heating (which includes the infra-red contributions) will also be finished shortly.

As initial conditions for the model we shall specify the Z and T fields. We have obtained tapes of climatological monthly mean values of these parameters on a 5° grid below 100 mb and from pole to pole. A code has been completed for converting this information to spectral form. Between 100 and 10 mb we are using other data sources such as those obtained for task II which unfortunately apply only to the Northern Hemisphere. Above 10 mb there is little data available and an arbitrary initialisation will be imposed.

The lower boundary condition on the dynamics - that is the orographical distribution - is already coded but the lower boundary condition on the ozone concentration remains to be programmed.

The major coding task remaining is to couple the dynamics with the chemistry. This requires a program for transforming back and forth rapidly between grid and spectral space. We anticipate that the coding of the numerical model will be complete by the end of the current contract period. Estimates of computation time needed to run the model continue to be approximately 3 seconds per model day or 8 hours per model year (see table 0.1). The remote terminal to the IBM 360/95 at Goddard Institute for Space Studies was installed at M.I.T. at the beginning of January and has performed probably as well as may be expected for these first few months of operation.

(II) The stratospheric climatological data analysis

The conversion of the 5 years of daily values of Z and T on the NMC to a 5° latitude-longitude grid will be completed shortly. A generalised computer program for obtaining the daily and monthly statistics from the Northern Hemisphere grid data is complete. The output will be fed onto data tapes from which conventional printout and plotting routines can be accessed. For the 1964 statistics the data has been satisfactorily compared with prior computations. The data will probably be displayed on hemispherical grids via contour routines presently being constructed. It is anticipated that the data and the displays for the years 1964-1968 will be completed at the end of this contract period. This information will be analysed during the succeeding contract period.

With regard to the portion of this task relating to the computation of vertical velocities it has become clear that Dopplick's computer code should undergo considerable revision (e.g., the cloud statistics should be updated). We feel that the vertical velocities derived from the present code may not be used as a climatological data base against which the predictions of the numerical model may be compared. The technique for evaluating ω in the numerical model is potentially more accurate than is Dopplick's computer code while to modify the latter is a considerable undertaking. No progress in deriving vertical velocities from climatological data has therefore been made largely because Dr. G. Boer has not been replaced. This fact is reflected in the financial statements.

(III) Heating by trace constituents

The activities involved during this period have typically represented becoming familiar with and obtaining source information. Specifically we have updated a visible radiation code by converting radiation energy density to gas temperature changes. This visible heating code will be incorporated as one portion of the total aerosol heating code.

A second area of activity has been in the preparation of the infra-red radiative transfer codes. This code will be utilized in computing the direct infra-red solar heating and the stratospheric warming by ground emissions. Combining these two infra-red heating codes with the visible heating code will give the total aerosol heating from all sources..

The inputs to the radiative transfer codes which have required recent updating are the physical and optical properties of the aerosol. In the case of physical characteristics both size and projected number density have been the focus of attention. Recent static tests of the SST engine will be utilized to obtain size information concerning the non-gaseous emissions; however, preliminary indications are that coagulation will inevitably take place and will have to be estimated. Data which is missing and important to the basic understanding of the processes involved in the coagulation is aerosol size data vs. distance from the SST engine. Projected number density of aerosols from engine emission data indicate that concentrations of 3 particles/liter may be expected under global conditions. Optical properties of the aerosol such as index of refraction and the absorption characteristics are being measured in a combined CSDL/AFCRL experiment on an SST engine emission sample obtained from T. Broderick DOT-TSC. Preliminary results indicate that the samples are optically different than auto and chimney partiuclates. It has been found that 25% → 85% by weight of the samples contained (assumed to be) unburned fuel or a by-product. Further analysis of the properties and optical characteristics is underway.

The principal investigator has been employed full-time on this contract during the current contract period. In early December he attended a C.I.A.P. workshop in Ft. Lauderdale where he contributed to a chapter of the monograph on the neutral stratosphere concerning the simulation of stratospheric dynamics. During February Dr.'s Cunnold and Prinn attended the C.I.A.P. workshop in Boulder, Colorado at which the first draft of the monograph on the perturbed stratosphere was written and Dr. Alyea attended the workshop of the following week when monograph 4 on perturbations of the troposphere was prepared. Dr.'s Cunnold, Alyea and Phillips have submitted a paper regarding the modeling work to the AIAA/AMS meeting to be held in Denver in June and plan to be represented there.

TABLE 0.1 Estimate of calculation times

	Calculation	Time (in seconds per time step) on GISS 360/95
1.	Nonlinear terms; i.e., Jacobians in S. T, and O_3 prediction equations. Total $\sim$ 2-2/3 Jacobians at 24 active levels with 2566 nonlinear interactions at each level.	$\lesssim$ 1.00
2.	Photochemical reaction rates (values for terms containing transcendental functions are taken from tables using machine language routines.	.05
3.	Photodissociation rates (transcendental functions from tables as in 2.	.83
4.	Heating due to O_3 (transcendental functions as in 2).	.20
5.	Spectral-grid-spectral transformations for 2, 3, and 4.	$\lesssim$ .80
6.	Inversion of W-equation (see Chapter 8)	$\lesssim$ .30
7.	Totals	
	a. For one time step	$\lesssim$ 3.18 sec
	b. For one year of 1-hour steps (8760 steps)	$\lesssim$ 7-3/4 hrs.

1. Basic dynamical equations and coordinate system.

The horizontal coordinate system will be longitude (positive eastward) and latitude, denoted by λ and φ. This dependence will be represented in spherical surface harmonics, except that certain terms, such as part of the heating and photochemistry will be evaluated point-wise at selected values of λ and φ. In the vertical direction pressure (p) will be used as a coordinate with finite-differences being employed. These pressure levels will be distributed at equal intervals of log P in order to give roughly equal intervals in height. We define

$$P = p \div (100\,\text{cbar}) \qquad Z = -\ln P, \quad P = e^{-Z} \tag{1.1}$$

From the hydrostatic relation $dp = -\rho g\, dz$ and $\rho = p/RT$, we have

$$dZ = -\frac{dp}{p} = \frac{g}{RT}\, dz \tag{1.2}$$

The vertical levels will be separated by a uniform value of ΔZ. To the extent that the temperature T is approximately uniform a change of one in Z corresponds to a height change of the order of 7 km. The bottom of the atmosphere will for simplicity be taken at $Z = 0$, i.e. at p = 100 cb instead of at the conventional sea-level pressure of 101.325 cb. The top of the "atmosphere" will be artificially set at $Z = Z_{TOP}$ corresponding to a geometric height of about 70 km.

The dynamical system not only assumes hydrostatic balance, but also a "quasi-geostrophic balance" in the horizontal equations of motion. Because we must consider global processes over the entire sphere, this balance must allow for complete variability of the coriolis parameter f:

$$f = 2\Omega \sin\varphi \qquad (1.3)$$
$$\Omega = 7.292 \times 10^{-5} \text{ rad sec}^{-1}$$

The quasi-geostrophic balance in question is obtained as follows (Lorenz, Tellus, 1960, P. 364). First, we divide the horizontal velocity $\vec{v}$ into a non-divergent part $\hat{k} \times \nabla\psi$ given by a stream function ψ and a divergent part $-\nabla\chi$, given by a velocity potential χ :

$$\vec{v} = \hat{k} \times \nabla\psi - \nabla\chi \qquad (1.4)$$

If the eastward and northward components of $\vec{v}$ are represented by u and v and a is the radius of the earth, this is equivalent to

$$u = a\cos\varphi\frac{d\lambda}{dt} = -\frac{1}{a}\frac{\partial\psi}{\partial\varphi} - \frac{1}{a\cos\varphi}\frac{\partial\chi}{\partial\lambda} \qquad (1.5)$$
$$v = a\frac{d\varphi}{dt} = \frac{1}{a\cos\varphi}\frac{\partial\psi}{\partial\lambda} - \frac{1}{a}\frac{\partial\chi}{\partial\varphi}$$

The vertical component of relative vorticity, ζ, and the horizontal divergence of $\vec{v}$ are related to ψ and χ by

$$\zeta = \hat{k}\cdot \text{curl}\,\vec{v} = \nabla^2\psi \,; \quad \text{div}\,\vec{v} = -\nabla^2\chi \qquad (1.6)$$

where ∇^2 is the horizontal Laplacian operator on the sphere.

The condition of quasi-geostrophic balance is

$$\nabla\cdot f\nabla\psi = g\nabla^2 z \qquad (1.7)$$

where g is gravity and z is the height of a constant pressure surface. [Unless noted otherwise, all partial derivatives with respect to λ, φ, and t (time) are carried out at constant pressure (or Z)]. The hydrostatic relation,

$$g\frac{\partial z}{\partial p} = -\frac{1}{\rho} = -\frac{RT}{p} \tag{1.8a}$$

or

$$g\frac{\partial z}{\partial Z} = RT \tag{1.8b}$$

enables (1.7) to be rewritten as

$$\nabla\cdot f\nabla\frac{\partial\psi}{\partial Z} = \nabla^2 RT \tag{1.9}$$

Associated with this relation (which is a simplified form of the equation obtained by taking the horizontal divergence of the equations of motion(is the "vorticity equation":

$$\nabla^2\frac{\partial\psi}{\partial t} = -\hat{k}\times\nabla\psi\cdot\nabla(f+\nabla^2\psi) + \nabla\cdot f\nabla\chi + \nabla\cdot(\vec{F}_r\times\hat{k}) \tag{1.10}$$

where $\vec{F}_r$ is the horizontal frictional force per unit mass.

The continuity equation (conservation of mass) is

$$\frac{\partial}{\partial p}\left(\frac{dp}{dt}\right) = \frac{\partial}{\partial P}\left(\frac{dP}{dt}\right) = -\nabla\cdot\vec{v} = \nabla^2\chi \tag{1.11}$$

The upper boundary condition at $Z = Z_{TOP}$ will be that dp/dt vanishes there. Let us define

$$X = -\int_{P_{TOP}}^{P}\chi\, dP \quad , \quad \chi = -\frac{\partial X}{\partial P} \tag{1.12}$$

Equation (1.10) can then be rewritten as

$$\nabla^2\frac{\partial\psi}{\partial t} = -\hat{k}\times\nabla\psi\cdot\nabla(f+\nabla^2\psi) - \nabla\cdot f\nabla\left(\frac{\partial X}{\partial P}\right) + \nabla\cdot(\vec{F}_r\times\hat{k}) \tag{1.13}$$

If we use $Z = -\ln P$ as the vertical coordinate, the appropriate vertical advection velocity is

$$W = \frac{dZ}{dt} = -\frac{1}{P}\frac{dP}{dt} \tag{1.14}$$

The continuity equation (1.11) in terms of W is:

$$\nabla \cdot P\vec{v} + \partial(PW)/\partial Z = 0 \qquad (1.15)$$

From (1.11), (1.12) and (1.14) we get $\partial\,[\,PW - \nabla^2 X\,]/\partial P = 0$, or

$$PW = \nabla^2 X \qquad (1.16)$$

Boundary conditions on W are that W vanishes at Z_{TOP} and that it is given by orographic upslope motion at the bottom:

$$Z = Z_{TOP}: \quad W = 0 \qquad (1.17)$$

$$Z = 0: \quad W \approx \frac{\rho g \omega}{\vec{p}} = \frac{1}{H_0}\, \vec{v}_\psi \cdot \nabla h$$

where h is the orography and $\vec{v}_\psi$ is $k \times \nabla\psi$ at the first interior level for ψ. Here

$$H_0 = \frac{RT_0}{g} = 7\,km \qquad (1.18)$$

is a constant.

Friction will be represented by a vertical Austausch, $\vec{F}_r = \frac{1}{\rho}\partial\vec{\tau}/\partial z = -g\,\partial\vec{\tau}/\partial p$. Thus $\nabla \cdot \vec{F}_r \times \hat{k} = \frac{\partial}{\partial P}[\nabla \cdot (-\frac{g}{P_0}\,\vec{\tau} \times \hat{k}\,]$

In the interior regions of the model (but not at the ground) we set $\vec{\tau} = \rho K_m\, \partial(\hat{k} \times \nabla\psi)/\partial z$, giving

$$\nabla \cdot \left(-\frac{g}{P_0}\,\vec{\tau} \times \hat{k}\right) = \nabla \cdot \left[\frac{g^2 \rho^2}{P_0^2} K_m \frac{\partial \nabla\psi}{\partial P}\right]$$

Replacing ρ by p/RT and replacing g/RT by $1/H_0$ we get

$$\nabla \cdot \left[-\frac{g}{P_0}\,\vec{\tau} \times \hat{k}\right] = -\frac{K_m}{H_0^2}\, P \frac{\partial \nabla^2\psi}{\partial Z}.$$

At the ground, we can set $\vec{\tau}$ equal to 0.003 $P_0\, |\vec{v}|\, \vec{v}$, with $\overline{|\vec{v}|}$ a suitable mean anemometer speed (5 m/sec^{-1}) and the anemometer vector wind $\vec{v}$ equal to a rotated ($\alpha = 22.5$ degrees) fraction (0.5) of $\hat{k} \times \nabla\psi$ at the lowest interior level at which ψ is defined

$$\vec{\tau}_{grnd} = \left[0.003\,\bar{\rho}\,\overline{|\vec{v}|}\,(0.5)\right]\left[\cos\alpha\; \hat{k} \times \nabla\psi - \sin\alpha\; \nabla\psi\right]_{interior} \qquad (1.19)$$

$$\nabla \cdot \left[-\frac{g}{p_0}\,\vec{\tau} \times \hat{k}\right]_{grnd} = -\left\{\frac{1}{H_0}\left[.003\,\overline{|\vec{v}|}\,(0.5)\cos\alpha\right]\right\}\nabla^2\psi_{int}$$

For $H_0 = 7$ km, $|\vec{v}| = 5\ m\ sec^{-1}$ and $\cos\alpha = 0.925$, the coefficient here has the value $10^{-6}\ sec^{-1}$.

The conventional quasi-geostrophic Taylor-Ekman theory (Charney and Eliassen, Tellus, 1949, Vol. 1, No. 2, P. 38) gives a corresponding term ("Ekman pumping") of

$$-\left\{\frac{1}{H_0}\sqrt{\frac{K_m f}{2}}\ \sin 2\alpha\right\}\nabla^2\psi \tag{1.20}$$

For $K_m = 5\times10^4\ cm^2\ sec^{-1}$ and $\bar{f} = 10^{-4}\ sec^{-1}$, the coefficient in this derivation is $1.6 \times 10^{-6}\ sec^{-1}$. To summarize the friction term we can write

$$\nabla\cdot\vec{F}_r\times\hat{k} = \frac{\partial}{\partial P}(PF)$$

$$Z>0: \quad F = -\frac{K_m}{H_0^2}P\frac{\partial\nabla^2\psi}{\partial Z} \tag{1.21}$$

$$Z=0: \quad F = -k_D\nabla^2\psi_{int}$$

where k_D refers to the "surface drag-coefficient" in (1.19) or (1.20). At $Z = Z_{TOP}$, F will vanish (no stress).

The next physical statement is the thermodynamic law d (entropy) $/dt$ = rate of heating ÷ temperature. For our perfect gas system this would be

$$c_p\frac{d}{dt}\left[\ln(Tp^{-\kappa})\right] = \frac{q}{T}\ ; \quad \kappa = \frac{R}{c_p} = \frac{2}{7} \tag{1.22}$$

where q is the rate of heating per unit mass and T the temperature. In terms of T, this becomes

$$\frac{\partial T}{\partial t} = -(\hat{k}\times\nabla\psi - \nabla\chi)\cdot\nabla T - W\frac{\partial T}{\partial Z} - \kappa WT + \frac{q}{c_p} \tag{1.23}$$

We will however use a simplified form of this, obtained by ignoring $\nabla\chi\cdot\nabla T$ and by replacing T in $W\partial T/\partial Z$ and κWT by $\bar{T}$, where $\bar{T}$ is the horizontal average:

$$T = \bar{T}(p,t) + T'(\lambda,\phi,p,t)$$

$$\bar{T} = \frac{1}{4\pi a^2}\int_{-\pi/2}^{\pi/2}\cos\phi\, d\phi \int_{0}^{2\pi} T\, d\lambda \; ; \qquad \overline{T'} = 0 \tag{1.24}$$

[This definition of $\overline{(\ )}$ and $(\ )'$ will be applicable to any variable.]

This greatly simplifies the computations, and is reasonably accurate because $\nabla\psi \gg \nabla\chi$ and $\partial T'/\partial Z + \kappa T'$ is generally small compared to $\partial\bar{T}/\partial Z + \kappa\bar{T}$. The result is

$$\frac{\partial T}{\partial t} = -\hat{k}\times\nabla\psi\cdot\nabla T - W\left(\frac{d\bar{T}}{dZ} + \kappa\bar{T}\right) + q/c_p \tag{1.25}$$

However this simplification has the result that we can no longer interpret (1.25) as forecasting $\bar{T}$, the horizontally averaged T; this is because the horizontal average of (1.25) gives simply

$$\frac{\partial\bar{T}}{\partial t} = \bar{q}/c_p$$

whereas the horizontal average of the exact equation (1.23) gives

$$\frac{\partial\bar{T}}{\partial t} = \frac{\bar{q}}{c_p} - \kappa\,\overline{W'T'} - \frac{1}{p}\frac{\partial}{\partial Z}\left(p\,\overline{W'T'}\right), \tag{1.26}$$

showing the effect of vertical transports of entropy by the motion. We expect little change in $\bar{T}$ from the observed annual average $\bar{T}(Z)$, however, either with season or with changes in the ozone chemistry. [The effect of the latter will be investigated separately, as discussed later.]

In passing, we note that

$$\begin{aligned}\frac{\partial T}{\partial Z} + \kappa T &= \frac{RT}{g}\left(\frac{\partial T}{\partial z} + \frac{g}{c_p}\right)\\ &= T\frac{\partial}{\partial Z}\left[\ln\left(T p^{-\kappa}\right)\right]\\ &= \frac{N^2}{R}\left(\frac{RT}{g}\right)^2\end{aligned} \tag{1.27}$$

where N is the buoyancy frequency.

Finally, we describe the basic form of the equation for the (number density) mixing ratio of a trace substance such as O_3. Define

$$\chi_i = n_i \div n_m \tag{1.28}$$

where n_i is the number density of the i-th trace substance, n_m is the total number density, assumed to be equivalent to the "normal" constituents N_2, O_2 and CO_2 since n_i is very small.

$$n_m \cong p/kT$$

$$k = \text{Boltzman constant} = 1.380 \times 10^{-26} \text{ kilojoules deg}^{-1} \tag{1.29}$$

The equation for $d\chi_i/dt$ (the rate of change following the motion) is

$$\frac{d\chi_i}{dt} = \frac{\partial \chi_i}{\partial t} + (\hat{k} \times \nabla\psi - \nabla\chi)\cdot\nabla\chi_i + W\frac{\partial \chi_i}{\partial Z}$$

$$= \frac{1}{n_m}\left(\frac{dn_i}{dt}\right)_c + \frac{1}{\rho}\frac{\partial}{\partial z}\left(\rho K_d \frac{\partial \chi_i}{\partial z}\right)$$

where $(dn_i/dt)_c$ is the net rate of local photo-chemical generation of the substance (number per unit volume per unit time) and K_d is the vertical eddy-diffusion coefficient [with dimensions $(\text{length})^2 \div$ time]. K_d will vary only with P.

The vertical diffusion term can be rewritten by using the hydrostatic equation as

$$\frac{\partial}{\partial P}\left[K_d\left(\frac{gP}{RT}\right)^2\frac{\partial \chi_i}{\partial P}\right] \approx \frac{\partial}{\partial P}\left[-\frac{K_d}{H_0^2}P\frac{\partial \chi_i}{\partial Z}\right] \tag{1.30}$$

where we have again absorbed the variation of density with T into H_0 on the recognition that K_d itself is not a precisely known quantity. K_d (and the momentum Austausch K_m) will be prescribed functions of P. The equation for χ_i is now

$$\frac{\partial \chi_i}{\partial t} = -(\hat{k}\times\nabla\psi - \nabla\chi)\cdot\nabla\chi_i - W\frac{\partial \chi_i}{\partial Z} + \frac{1}{n_m}\left(\frac{dn_i}{dt}\right)_c + \frac{\partial}{\partial P}\left[-\frac{K_d}{H_0^2}P\frac{\partial \chi_i}{\partial Z}\right] \tag{1.31}$$

or

or $$\frac{\partial \chi_i}{\partial t} = -\frac{1}{P}\left[\nabla\cdot(P\vec{v}\chi_i) + \frac{\partial(PW\chi_i)}{\partial Z}\right] + \frac{1}{m_m}\left(\frac{dm_i}{dt}\right)_c + \frac{\partial}{\partial P}\left[-\frac{K_d}{H_0^2}P\frac{\partial \chi_i}{\partial Z}\right] \tag{1.32}$$

[having made use of (1.4) and (1.15) to obtain the last form].

The rate of change of $\overline{\chi_i}$ (the horizontal average) is obtained from the horizontal average of (1.32):

$$\frac{\partial \overline{\chi_i}}{\partial t} = \frac{\partial}{\partial P}\left[P\,\overline{W'\chi_i'}\right] + \left[\overline{\frac{1}{m_m}\left(\frac{dm_i}{dt}\right)_c}\right] + \frac{\partial}{\partial P}\left[-\frac{K_d}{H_0^2}P\frac{\partial \overline{\chi_i}}{\partial Z}\right] \tag{1.33}$$

The rate of change of χ_i' will however be obtained from a simplified form of (1.31), much as was done in the thermodynamic equation (1.25):

$$\frac{\partial \chi_i'}{\partial t} = -\hat{k}\times\nabla\psi\cdot\nabla\chi_i' - W\frac{\partial\overline{\chi_i}}{\partial Z} + \left[\frac{1}{m_m}\frac{dm_i}{dt}\right]_c' + \frac{\partial}{\partial P}\left[-\frac{K_d}{H_0^2}P\frac{\partial \chi_i'}{\partial Z}\right] \tag{1.34}$$

In contrast to $\overline{T}$, where we are for the most part content to take $\overline{T}$ as given, we must predict $\overline{\chi_i}$ as well as χ_i'. Equation (1.33) will therefore be used as well as (1.34).

Presumably (1.33) need not be applied every time step in the numerical integration, $\overline{\chi_i}$ being a slowly changing function of time. However, the term $\overline{W'\chi_i'}$ must be put equal to zero at $P = 1$ to ensure no net creation of χ_i by the large-scale motion.

The form of $(d\chi_i/dt)_c$ is discussed later. However, a special treatment must be used for the lower boundary condition on the vertical eddy flux of ozone. Galbally (Quart. J. Roy. Meteor. Soc., 1971, P. 18) shows that in the very lowest layer the vertical flux (over land) of ozone is proportional to the ground concentration

$$K_d \frac{\partial \chi}{\partial z} \simeq \frac{K_d}{H_0}\frac{\partial \chi}{\partial Z} = d\,\chi_{grnd} \tag{1.35}$$

(the surface destruction of ozone being proportional to O_3). The coefficient d has a value of about 1 cm sec^{-1}. We will apply this formulation to the lowest layer in our model ($0 \leq Z \leq \Delta Z$). Values of χ are defined at the top of the layer ($Z = \Delta Z,\ j = J-1$) and at the ground ($Z = 0,\ j = J$). Thus (dropping the i-subscript on χ),

$$\left(\frac{K_d}{H_0}\frac{\partial \chi}{\partial Z}\right)_{J-1/2} = \left(\frac{K_d}{H_0 \Delta Z}\right)_{J-1/2}(\chi_{J-1}-\chi_J) = d\,\chi_J \tag{1.36}$$

whence

$$\chi_J = \chi_{J-1} \div \left[1 + \frac{d H_0 \Delta Z}{K_d}\right]_{J-1/2} \tag{1.37}$$

and

$$\left(\frac{K_D}{H_0 \Delta Z}\right)_{J-1/2}(\chi_{J-1}-\chi_J) = \frac{d\,\chi_{J-1}}{1+(d H_0 \Delta Z/K_d)} \tag{1.38}$$

Galbally cites values of the vertical number flux of ozone molecules over land in the range 1 to 6 x 10^{11} mol cm^{-2} sec^{-1}. Aldaz (J. Geo. Res., 1969, P. 6943) estimates a global average of 1 to 1.7 x 10^{11} mol cm^{-2} sec^{-1}. Pichinga representative value of 2 x 10^{11} mol cm^{-2} sec^{-1} and equating this to $n_m K\, \partial\chi/\partial z$, we find, for $n_m = 4{,}55 \times 10^{19}\ cm^{-3}$ and $K = 10^5\ cm^2\ sec^{-1}$, that a vertical gradient of ozone number mixing ratio of

$$\frac{\partial \chi}{\partial z} \sim 0{,}5 \times 10^{-13}\ cm^{-1} = \frac{5 \times 10^{-8}}{10\ km} \tag{1.39}$$

is required. Galbally's data show a typical ground value for χ of

$5 \times 10^{11} \div 4.5 \times 10^{19} \sim 10^{-8^{1-10}}$. The typical inferred downward flux of ozone observed near the ground is compatible then with a tropospheric K of 10^5 cm^2 sec^{-1} and a tropopause (10km) value for χ of 6×10^{-8} or a 10-km value for n_3 of $(6 \times 10^{-8}) \times (8 \times 10^{18}) \sim 50 \times 10^{10}$ cm^{-3}. This value is not greatly inconsistent with values of 10^{12} cm^{-3} which seem characteristic of the tropopause level in the meridional cross section prepared by D. Wu from the data of Hering and Borden (1967).

A special treatment of the ozone equation will be necessary at high levels. At these heights, Lindzen and Goody (J. Atmos. Sci., 1965, P. 341) show that the photo-dissociation of ozone is extremely rapid, with a time constant becoming less than 1 hour at heights above 45 km. (They presumably use typical values of incident solar radiation.) The conventional methods of "time-stepping" equations such as (1.34) require a computational time step no longer than the characteristic physical times associated with terms on the right side of (1.34). Since the advective time scale is of the order of an hour or so, we must consider replacing (1.33) and (1.34) at upper levels by the equilibrium condition.

$$\chi_i = (\chi_i)_{equil} \Leftrightarrow \frac{dn_i}{dt} = 0 \tag{1.40}$$

For use in radiation computations, we need N_i, the number of molecules of χ_i in the vertical column of unit cross-section above a given pressure surface:

$$N_i = \int_z^\infty n_i \, dz = \int_z^\infty \chi_i \, n_m \, dz = \int_z^\infty \chi_i \frac{R}{k} \rho \, dz$$

$$= \frac{R p_0}{g k} \int_0^P \chi_i \, dP$$

where $R = 287$ kj ton^{-1} deg^{-1} is the gas constant for air.

This gives numerically

$$N_i = 2.12 \times 10^{29} \int_0^P \nu_i \, dP \quad \text{in (meter)}^{-2} \tag{1.35}$$

$$= 2.12 \times 10^{25} \int_0^P \nu_i \, dP \quad \text{in (cm)}^{-2}$$

In the case of molecular oxygen, ν_i is taken as uniform and equal to 0.2096, giving

$$N_{O_2} = 0.4444 \times 10^{25} P \text{ cm}^{-2} \tag{1.36}$$

The lower boundary condition for ozone

The surface destruction process for ozone must give rise to a boundary layer effect in which the ozone changes rapidly from the free air value a lower value at the ground. Our use of (approximately) 3-km height increments will not represent this adequately. Secondly, land and water surfaces differ markedly in their effect on surface ozone. Fortunately it is possible to correct for both of these complications by using the detailed analysis by P. Fabian and C. Junge (Global rate of ozone destruction at the earth's surface: Arch. Meteor., Geo., Bioklimat., (a)-Meteor. u. Geo. 19, 161-72, 1970). The important point is to obtain the correct global ratio between the lower tropospheric value of ozone and the surface destruction rate, since the former may affect the ozone amount higher up and thereby the photochemical destruction rates.

Fabian and Junge model the presumed boundary-layer ozone profile by standard methods and make allowance for different properties of land, vegetation and water (and their global distribution) and for different wind speeds. They arrive at a global surface destruction rate ranging from 3.1 to 5.6 × 10^{10} mol/cm^{2}sec, the variation being due to uncertainty in choice of surface wind speed. Using an average lower tropospheric value of

5×10^{11} mol/cm^3 for O_3, we have a global ratio of

$$d_1 \equiv \frac{3.1 \text{ to } 5.6 \times 10^{10}}{5 \times 10^{11}} \sim 0.08 \text{ cm sec}^{-1}$$

[Note that "measured" values of d at the ground range from .04 cm sec^{-1} over water to land values of 0.6 (Aldaz and 1.0 (Galbally) cm sec^{-1}.]

Referring to our model equations (1.37) and (1.38)

$$\left(\frac{K_D}{H_0 \Delta Z}\right)_{J-\frac{1}{2}} \left(\chi_{j-1} - \chi_j\right) = \frac{d\,\chi_{j-1}}{1 + \left(\frac{d H_0 \Delta Z}{K_D}\right)} = d\,\chi_j$$

we recognize the left side as the downward diffusive flux at the botton of our model, (which must equal the surface destruction rate) and χ_{J-1} as the number density (mixing ratio) in the model corresponding most closely to the 5×10^{11} number density for the free air referred to above. Our model will not include different types of surface with their differing abilities to destroy ozone. This is alright since, because of the strong horizontal advection in the atmosphere, these differing surface properties affect primarily the local boundary layer profile and surface value rather than the local free troposphere values. We must use a correct global effect, however, and we get this by simply choosing a single model value for d such that the ratio of the destruction rate to the free air value in the model matches the global observed ratio, $\bar{d}$.

$$\frac{d}{1 + \frac{d H_0 \Delta Z}{K_D}} = d_1 = 0.08 \text{ cm/sec}$$

For $H_o \Delta Z = 3$ Km, and $K_d = 10\ m^2\ sec^{-1}$, this gives $d = 0.105\ m\ sec^{-1}$. Fabian and Junge also discuss the ratio (their ε) of the surface value of O_3 to the free air value, and obtain typical values of 0.35 over land and 0.85 over water. Our model now implies a single value for this ratio of

$$\frac{\chi_j}{\chi_{j-1}} = \frac{d_1}{d} = 0.8$$

very comfortably located in the range inferred by Fabian and Junge.

Vertical diffusivity for ozone.

An upper estimate for K_d in the troposphere and lower stratosphere can be obtained from measured ozone profiles by equating

$$\left(\frac{48}{29}\right) \rho K_d \frac{\partial \chi}{\partial z} = \text{constant} = 3.5 \times 10^{-12} \text{ gm/cm}^2\text{/sec}$$

where χ is the number density mixing ratio, and 3.5×10^{-12} is the product of the mass of an ozone molecule (7.9×10^{-23} gm) with the average global surface distruction rate of 4.4×10^{10} mol $\text{cm}^{-2}\text{sec}^{-1}$ found by Fabian and Junge (reference cited earlier). Values of $\partial \chi / \partial z$ can be obtained from the middle latitude synthesis by Krueger and Minzner (A proposed mid-latitude ozone model for the U.S. Standard atmosphere. Preprint, Jan. 1973 Goddard Space Flight Center.) (Similar values are obtained from using the 3-year average ozone profiles for Bedford and Green Bay that has been analysed by D. Wu.)

z(km)	$(\frac{48}{29}\chi)$	$\frac{48}{29}\frac{\partial \chi}{\partial z}(\text{cm}^{-1})$	$\rho \frac{\text{gm}}{\text{cm}^3}$	$K_d \frac{\text{cm}^2}{\text{sec}}$
2	5×10^{-8}			
3		0.5×10^{-13}	0.9×10^{-3}	7.8×10^{4}
4	6			
5		0.5	0.74	9.4×10^{4}
6	7			
7		1.5	0.59	4×10^{4}
8	10			
9		6	0.47	1.2×10^{4}
10	22			
11		15	0.36	0.65×10^{4}
12	52			
13		15	0.26	0.90×10^{4}
14	82			
15		30	0.19	0.61×10^{4}
16	142			
17		63	0.15	0.37×10^{4}
18	267			
19		82	0.11×10^{-3}	0.39×10^{4}
20	431×10^{-8}			

At higher elevations ozone begins to no longer act as an inert tracer Here we refer to recent computations by S. Wofsy and M. McElroy (On vertical mixing in the upper stratosphere and lower mesosphere. Submitted, November 1972, to J. Geo. Res.) These authors combine (a) the suggestion by Lindzen that K might vary as $\rho^{-1/2}$ because the velocities in gravity waves - a like'y mixing process - tend to increase in this manner with height and (b) measurements by Ehhalt of methane concentration. Using a chemical model, they find that Ehhalt's measurements at 50 km fit but with a K_d distribution having small values of 2×10^3 cm^2 sec^{-1} at 16-20 km increasing to 2×10^6 at 80 km as $(n_m)^{-1/2}$. We can model this simply by noting that n_m is proportional to p for constant T, and that p in turn is proportional to exp(-Z).

The following distribution of K seems reasonable.

(a) $Z \leq Z_0 = 0.6$: $K \equiv K_0 = 10^5 \text{ cm}^2/\text{sec}$

(b) $Z_0 \leq Z \leq Z_1 = 2.4$: $K_1 = 2 \times 10^3 \text{ cm}^2/\text{sec}$

$$K = K_0 + \frac{(K_0 - K_1)(Z - Z_0)}{(Z_1 - Z_0)^2}\left[Z + Z_0 - 2Z_1\right]$$

(c) $Z \geq Z_1$: $K_2 = 9.4 \times 10^5, \quad Z_2 = 10$

$$K = K_1 + (K_2 - K_1)\,\frac{\exp\left[\frac{Z - Z_1}{2}\right] - 1}{\exp\left[\frac{Z_2 - Z_1}{2}\right] - 1}$$

These formulae and numbers give the following match for K_d with the inferred values cited above from ozone and methane.

z(km)	Z	Formula	Inferred (O_3)	Inferred (CH_4)
3	.357	100×10^3	78×10^3	300
5	.616	98	94	
7	.892	71	40	
9	1.171	48	12	
11	1.492	27	6.5	
13	1.802	13	9.0	
15	2.120	4	6.1	
17	2.433	2.4	3.7	2×10^3
19	2.719	5.7	3.9×10^3	
20	2.861	7.6		6.8
30	4.289	35.7		45
40	5.717	93.3		110
50	7.145	210.8		260
60	8.573	450.7		490
70	10.000	940.0×10^3		940×10^3

The CH_4 inferred values are from the model B profile of Wofsy and McElroy. We have given preference in the troposphere to the values deduced from ozone, shifting over at $Z > 2.4$ to the deductions based on methane.

The formulas for K given above involve 6 selectable parameters: Z_0, Z_1, Z_2, K_0, K_1, K_2. These can be changed at will to allow study of our uncertainty about K; most notably they should be interpreted as probable upper limits for K since some vertical transport of ozone will be produced by the large-scale explicitly-forecast motions of our model, whereas the method of "inferring" the K-values has ignored this.

2. Choice of vertical levels.

We want the vertical domain to extend well above the actual ozone layer. We also want it high enough that there is some opportunity for the damping effects of ozone and radiation to absorb mechanical energy generated in the baroclinic processes of the lower atmosphere. On the other hand, we cannot for practical reasons get involved in the more complicated processes of the upper atmosphere and lower thermosphere. An upper limit of about 70 km seems reasonable.

We obtain equal intervals in $Z = -\ln P$ ($P =$ pressure ÷ 100 cb) by defining

$$\left.\begin{aligned} Z_j &= \Delta Z\,(J-j) \\ P_j &= e^{-\Delta Z\,(J-j)} \end{aligned}\right\} j = 1, 2, \cdots, J. \tag{2.1}$$

$j = 1$ is at the "top" of our atmosphere, and $j = J$ at the bottom, whence

$$\Delta Z = \frac{Z_1}{J-1} = \frac{Z_{TOP}}{J-1}$$

A convenient choice is obtained by choosing

$$\begin{aligned} e^{\Delta Z} &= r\,, \qquad r = 3/2 \\ \Delta Z &= \ln r = 0.40547 \\ J &= 26 \end{aligned} \tag{2.2}$$

so that

$$\begin{aligned} Z_1 = Z_{TOP} &= (J-1)\ln r = 10.13675 \\ P_1 &= r^{-(J-1)} = 3.9605 \times 10^{-5} \end{aligned} \tag{2.3}$$

P_1 corresponds to a pressure of 39.605 dynes/cm^2, typical of the height $z \sim 71.5$ km. Successive pressure levels are separated by (roughly) 72/25 ~ 2.9 km. The relations

$$P_j = r^{-(J-j)} \quad ; \quad P_{j+1} = r\,P_j \tag{2.4}$$

are useful.

At these levels, the following basic variables will be represented

$$j = 1, 2, \ldots, J: \qquad T_j, \; W_j, \; (N_i)_j$$

together with the heating rate, the photo-chemical term , and the vertical turbulent fluxes of momentum. At the intermediate levels the streamfunction ψ_j will be represented

$$j = \frac{3}{2}, \frac{5}{2}, \ldots, J - \frac{1}{2} \quad : \quad \psi_j$$

For convenience in notation, however, ψ will be labeled with an integer subscript according to the convention

$$\psi(P = P_{j+1/2}) \equiv \psi_j$$

This results in the following scheme.

j							
1	P_1	Z_1	$W_1(=0)$,	$(N_i)_1$,	(T_1)	F_1	
			ψ_1,	ζ_1			G_1
2	P_2	Z_2	W_2	$(N_i)_2$,	T_2	F_2	
			ψ_2,	ζ_2			G_2
3	P_3	Z_3	W_3	$(N_i)_3$,	T_3	F_3	
$j-1$	P_{j-1}	Z_{j-1}	W_{j-1}	$(N_i)_{j-1}$	T_{j-1}	F_{j-1}	
			ψ_{j-1}	ζ_{j-1}			G_{j-1}
j	P_j	Z_j	W_j	$(N_i)_j$	T_j	F_j	
			ψ_j	ζ_j			G_j
$j+1$	P_{j+1}	Z_{j+1}	W_{j+1}	$(N_i)_{j+1}$	T_{j+1}	F_{j+1}	
$J-1$	P_{J-1}	Z_{J-1}	W_{J-1}	$(N_i)_{J-1}$	T_{J-1}	F_{J-1}	
			ψ_{J-1},	ζ_{J-1}			G_{J-1}
J	P_J	Z_J	W_J,	$(N_i)_J$	T_J	F_J	

(F and G are defined on pages 17 and 18.)

The following table lists the values of the more basic variables for the choice $r = 3/2$, $J = 26$. Values of $\overline{T}$ above 30 km were taken from the 1965 CIRAS annual mean, values at lower elevation coming from data based on statistics gathered by the Planetary Circulation Project at M.I.T. (To be precise, they were obtained from the latter as shown in a figure based on them in the thesis by A. Hollingsworth.) The static stability parameter S is defined later in equation (3.20).

j	p_j	Z_j	z (km) (approx)	$\overline{T}_j$	n_m $(cm)^{-3}$	$S_j/\Delta Z$
1	.0000396	10.137	71.6	211	136×10^{13}	137×10^{-4}
2	.0000594	9.731	69.0	219	196	144
3	.0000891	9.326	66.3	226.5	285	154
4	.000134	8.920	63.5	234	415	161
5	.000200	8.515	60.6	241.5	600	166
6	.000301	8.109	57.6	249.5	877×10^{13}	167
7	.000451	7.704	54.5	258.5	126×10^{14}	174
8	.000677	7.298	51.4	267	184	217
9	.00101	6.893	48.[illegible]	267.5	274	277
10	.00152	6.488	[illegible]	261.5	421	302
11	.00228	6.082	42.0	254.5	649×10^{14}	295
12	.00343	5.677	38.8	248.5	100×10^{15}	285
13	.00514	5.271	35.9	242.5	154	277
14	.00771	4.866	33.0	237	236	272
15	.0116	4.460	30.2	231	364	269
16	.0173	4.055	27.5	225	557	261
17	.0260	3.649	24.8	219.5	855×10^{15}	251
18	.0390	3.244	22.2	214.5	132×10^{16}	237
19	.0585	2.838	19.6	211.5	201	217
20	.0878	2.433	17.1	210.5	302	194
21	.132	2.027	14.8	213	449	155
22	.198	1.622	12.0	222	646	125
23	.296	1.216	9.3	234	913×10^{16}	116
24	.444	0.811	6.4	248	130×10^{17}	104
25	.667	0.405	3.4	266	182	105
26	1.000	0.0	0.1	284	455×10^{17}	122×10^{-4}

3. Non-dimensional finite-difference equations.

In this section we write the basic equation in a non-dimensional form (primarily to simplify the dynamical computations) and simultaneously introduce the vertical finite-difference representation defined in section 2. We define

$$\begin{aligned}
\mu &= \sin\phi \\
\nabla\,(\text{dim}) &= \frac{1}{a}\,\nabla\,(\text{non-dim}) \\
\nabla^2\,(\text{dim}) &= \frac{1}{a^2}\,\nabla^2\,(\text{non-dim}) \\
\psi\,(\text{dim}) &= 2\Omega a^2\,\psi\,(\text{non-dim}) \\
X\,(\text{dim}) &= 2\Omega a^2\,X\,(\text{non-dim}) \\
t\,(\text{dim}) &= \frac{1}{2\Omega}\,t\,(\text{non-dim}) \\
W\,(\text{dim}) &= 2\Omega\,W\,(\text{non-dim}) \\
T\,(\text{dim}) &= \bar{T}(Z) + \left(4\Omega^2 a^2/R\right) T\,(\text{non-dim})
\end{aligned} \tag{3.1}$$

In the last expression T (*dim*) in the "total" temperature in absolute degrees, $\bar{T}(Z)$ is the "standard atmosphere" temperature (also in degrees) given in the table at the end of section 2, while the quantity ($4\Omega^2a^2/R$) T (non- *dim*) is the variable T appearing in (1.25), having a zero horizontal average. [The total T (*dim*) is of course used in all chemical computations.]

$$\begin{aligned}
\Omega &= 7.292\times10^{-5}\ \text{rad sec}^{-1} \\
a &= 6.371\times10^{6}\ \text{meters} \\
R &= 287\ \text{kj ton}^{-1}\,\text{deg}^{-1} \\
C_p &= (7/2)\,R
\end{aligned} \tag{3.2}$$

One day, ($2\pi/\Omega$) *secs* , corresponds to

$$\Delta t\,(\text{non-dim}) = 2\Omega\left(\frac{2\pi}{\Omega}\right) = 4\pi \tag{3.3}$$

The non-dimensional ∇^2 operator is

$$\nabla^2(\ ) = \frac{1}{\cos^2\phi}\frac{\partial^2(\ )}{\partial\lambda^2} + \frac{1}{\cos\phi}\frac{\partial}{\partial\phi}\left[\cos\phi\,\frac{\partial(\ )}{\partial\phi}\right] \tag{3.4}$$

The relation

$$PW = \nabla^2 X \tag{1.16}$$

between W and X can be used to eliminate X in favor of W [in equation (1.13)] by defining the inverse Laplacian operator

$$\mathcal{L} \equiv \nabla^{-2}$$

$$X = P \mathcal{L} W \tag{3.5}$$

We also have

$$\zeta = \nabla^2 \psi \,, \quad \psi = \mathcal{L} \zeta \tag{3.6}$$

A further convenient arrangement is useful for evaluating terms of the form $\partial(PF)\partial P$, which appears in the vertical diffusion terms for vorticity and trace substances and in the term

$$\frac{\partial X}{\partial P} = \frac{\partial}{\partial P}\left[P(\mathcal{L} W)\right]$$

in the vorticity equation (1.13). We have

$$\left[\frac{\partial}{\partial P}(PF)\right]_j = \frac{P_{j+1/2} F_{j+1/2} - P_{j-1/2} F_{j-1/2}}{P_{j+1/2} - P_{j-1/2}} = \left(\frac{r}{r-1}\right) F_{j+1/2} - \left(\frac{1}{r-1}\right) F_{j-1/2} \tag{3.7}$$

where we have made use of (2.4).

The horizontal advection of a quantity F can be written as the Jacobian

$$-\vec{v}_\psi \cdot \nabla F = -\hat{k} \times \nabla\psi \cdot \nabla F = \frac{\partial F}{\partial \lambda}\frac{\partial \psi}{\partial \mu} - \frac{\partial \psi}{\partial \lambda}\frac{\partial F}{\partial \mu}$$

$$\equiv J(F, \psi) \tag{3.8}$$

The non-dimensional form of the vorticity equation (1.13), with regard to the subscript labelling defined in section 2, together with equation (1.21) and (3.5) - (3.8) is as follows.

For $j = 1, 2, \cdots, J-1$:

$$\frac{\partial \zeta_j}{\partial t} = J(\mu + \zeta_j, \psi_j) - \nabla \cdot \left\{ \mu \nabla \mathcal{L} \left[\left(\frac{r}{r-1}\right) W_{j+1} - \left(\frac{1}{r-1}\right) W_j \right] \right. \tag{3.9}$$

$$+ \left(\frac{r}{r-1}\right) F_{j+1} - \left(\frac{1}{r-1}\right) F_j$$

$$\psi_j = \mathcal{L}\,\zeta_j \tag{3.10}$$

$$F_1 = 0 \tag{3.11}$$

$$F_J = -D\,\zeta_{J-1} \tag{3.12}$$

$$F_j = E_j(\zeta_j - \zeta_{j-1}) \qquad (j = 2, 3, --, J-1) \tag{3.13}$$

$$E_j = (K_m)_j \div \left[H_o^2\, 2\Omega\, \Delta Z\right] \tag{3.14}$$

$$D = k_D \div 2\Omega \tag{3.15}$$

$$W_1 = 0 \tag{3.16}$$

$$W_J = -\mathcal{J}\left(\frac{h}{H_o}, \psi_{J-1}\right) \tag{3.17}$$

The non-dimensional form of the "thermal wind equation" (1.9) becomes

for $j = 2, 3, --, J-1$:

$$\nabla \cdot \mu \nabla(\psi_j - \psi_{j-1}) = -\nabla^2 T_j \Delta Z \tag{3.18}$$

The non-dimensional form of the thermal equation (1.25) becomes

for $j = 2, 3, --, J-1$:

$$\frac{\partial T_j}{\partial t} = \frac{1}{2}\mathcal{J}(T_j, \psi_j + \psi_{j-1}) - S_j W_j + \left[\frac{R}{c_p\, 8\Omega^3 a^2}\right] q_j \tag{3.19}$$

where

$$S_j = \left(\frac{R}{4\Omega^2 a^2}\right)\left[\frac{d\bar{T}}{dZ} + \frac{R}{c_p}\bar{T}\right]_j \tag{3.20}$$

is tabulated at the end of section 2. q_j, the rate of heating per unit mass, is still in dimensional form in (3.19). It is considered later in section 5.

The trace substance equation is

For $j = j_0, j_0+1, --, J-1$:

$$\frac{\partial \chi_j}{\partial t} = \frac{1}{2} J(\chi_j, \psi_j + \psi_{j-1}) - W_j \left(\frac{d\bar{\chi}}{dZ}\right)_j + \left(\frac{r}{r-1}\right) G_j - \left(\frac{1}{r-1}\right) G_{j-1} + \frac{1}{2\Omega}\left[\frac{1}{n_m}\left(\frac{dn}{dt}\right)_c\right]_j \qquad (3.21)$$

$$G_j = D_j (\chi_{j+1} - \chi_j) \quad ; \text{for } j = j_0, \cdots, J-2.$$

$$D_j = (K_d)_{j+1/2} \div (2\Omega H_o^2 \Delta Z) \qquad (3.22)$$

[The vertical diffusion coefficient K_d is defined at the Z_j-levels corresponding to j = integer plus 1/2, whereas the vertical exchange coefficient K_m for vorticity appearing in (3.14) is defined at integer values of j.]. At the bottom, the relation (1.38) gives

$$G_{J-1} = - \frac{\chi_{J-1}}{\left[\frac{2\Omega H_o}{d} + \frac{2\Omega H_o^2 \Delta Z}{(K_d)_{J-1/2}}\right]} \qquad (3.23)$$

The integer j_o sets the level above which (3.21) may be replaced by a photochemical equilibrium statement, as discussed near the end of section one.

4. Photochemistry.

To begin with, the photochemistry will involve only oxygen and odd nitrogen compounds, with the latter being specified as given functions of pressure (or possibly pressure and latitude). (Equations to predict the nitrogen compounds may be added later.) The reactions involved are the four main Chapman reactions and reactions of NO and NO_2 with oxygen. (The following write-up is based on analysis by R. Prinn.)

Reference:

(a)

$$O_2 + h\nu \rightarrow 2O$$

$$J_{O_2} = \int_0^{2459} \alpha_{O_2} I e^{-\chi_{O_2}-\chi_{O_3}} d\lambda \ \ \mathrm{sec}^{-1} \qquad (4.1)$$

(b)

$$O + O_2 + M \rightarrow O_3 + M \qquad (4.2)$$

$$l_1 = 1.6 \times 10^{-35} e^{\frac{1050}{T}} \ \mathrm{cm}^6 \ \mathrm{sec}^{-1}$$

(c)

$$O_3 + h\nu \rightarrow O_2 + O$$

$$J_{O_3} = \int_0^{11400} \alpha_{O_3} I e^{-\chi_{O_3}} d\lambda \ \ \mathrm{sec}^{-1} \qquad (4.3)$$

(d)

$$O + O_3 \rightarrow 2O_2$$

$$k_1 = 2 \times 10^{-11} e^{-\frac{2395}{T}} \ \mathrm{cm}^3 \ \mathrm{sec}^{-1} \qquad (4.4)$$

(e)

$$NO + O_3 \rightarrow NO_2 + O_2$$

$$k_2 = 1.7 \times 10^{-12} e^{-\frac{1310}{T}} \ \mathrm{cm}^3 \ \mathrm{sec}^{-1} \qquad (4.5)$$

(e)

$$NO_2 + O \rightarrow NO + O_2$$

$$k_3 = 3.2 \times 10^{-11} e^{-\frac{530}{T}} \ \mathrm{cm}^3 \ \mathrm{sec}^{-1} \qquad (4.6)$$

(f) $$NO_2 + h\nu \rightarrow NO + O$$

$$J_{NO_2} = \int_0^{3975} \alpha_{NO_2} I e^{-X_{NO_2} - X_{O_3}} d\lambda \quad sec^{-1} \qquad (4.7)$$

In the three radiation integrals the exponent X is

$$X_i = \frac{\alpha_i(\lambda) N_i}{\cos\psi} \qquad (4.8)$$

where $\alpha_i(\lambda)$ is the absorption cross-section, N_i is the number of i-molecules in the cm^2 vertical column above the point [See equation (1.35)] and ψ is the solar zenith angle. (The diurnal variation of ψ will be averaged as described below.) I is the incident solar radiation, a function of the wavelength λ. Note that because the ozone absorption bands overlap the absorption bands of O_2 and NO_2 we must include the depletion of solar energy by ozone in (4.1) and 4.7).

References:

(a) Kockarts, 1970: Proc. 4th Joint ESRO-ESRIN Symposium (ed. G. Fiocco). D. Reidel, Dordrecht, 1971.

Ackerman, 1970: As for Kockarts.

(b) Johnston, 1971: Science, 173, P. 517.

Schiff, 1969: Can. J. Chem., 47, P.1903.
(ℓ_1 is an average of their values)

(c) Ackerman, 1970: As for Kockarts.

(d) Schiff, 1969: As above.

(e) Schofield, 1967: Planet. Space Sci., 15, P. 643.

(f) Hall and Blacet, 1952: J. Chem. Phys. 20, P. 1745.

TABLE 4.1 Typical values of rate coefficients

Coefficient	Height (km)						Comments
	60	50	40	30	20	10	
χ_{O_3}	1.1×10^{-7}	3.0×10^{-6}	7.0×10^{-6}	7.0×10^{-6}	2.3×10^{-6}	1.1×10^{-7}	
$\bar{J}_{O_3}$	4.5×10^{-2}	2.7×10^{-3}	6.5×10^{-4}	2.7×10^{-4}	2.0×10^{-4}	1.9×10^{-4}	From Crutzen (1970)
$\bar{J}_{O_2}$	1.0×10^{-9}	6.0×10^{-10}	2.2×10^{-10}	2.6×10^{-11}	2.5×10^{-13}	4.0×10^{-18}	
χ_{NO_2}	-	-	3.0×10^{-9}	9.0×10^{-9}	2.2×10^{-9}	2.0×10^{-9}	Brasseur & Nicolet (1973)
$\bar{J}_{NO_2}$	-	-	7.0×10^{-3}	6.7×10^{-3}	6.4×10^{-3}	6.2×10^{-3}	From Crutzen (1970)
$\bar{T}$	243	268	251	230	212	232	
k_1	1.1×10^{-15}	2.5×10^{-15}	1.4×10^{-15}	0.6×10^{-15}	0.2×10^{-15}	0.6×10^{-15}	
k_3	3.6×10^{-11}	4.4×10^{-11}	3.8×10^{-11}	3.2×10^{-11}	2.6×10^{-11}	3.2×10^{-11}	
n_m	6.5×10^{15}	2.2×10^{16}	8.5×10^{16}	3.8×10^{17}	1.9×10^{18}	8.5×10^{18}	
$.20961_1 n_m$	1.6×10^{-18}	3.5×10^{-18}	1.9×10^{-17}	9.9×10^{-17}	8.4×10^{-16}	2.2×10^{-15}	
[O]	9.5×10^{9}	9.0×10^{9}	7.0×10^{8}	4.0×10^{7}	1.3×10^{6}	8.0×10^{3}	(cm^{-3}) from Crutzen (1970)
K	7.5×10^{-5}	2.1×10^{-3}	1.1×10^{-3}	3.3×10^{-4}	7.3×10^{-6}	3.0×10^{-6}	(zero at night)
$\bar{J}_{O_2}[O_2]/\bar{J}_{O_3}[O_3]$	0.4	.015	0.01	.003	1×10^{-4}	4×10^{-8}	
Q_{O_3}	4.0×10^{-20}	2.5×10^{-21}	4.7×10^{-22}	1.7×10^{-22}	-	-	joules/sec/O_3 molecule
q/C_p	2.2×10^{-4}	3.5×10^{-4}	1.7×10^{-4}	6.0×10^{-5}	-	-	dimensionless

The equation for $d[O]/dt$ (we denote temporarily number densities n_i by a square bracket) is

$$\frac{d[O]}{dt} = 2[O_2]J_{O_2} + [O_3]J_{O_3} + [NO_2]J_{NO_2} - [O]\left\{ l_1[O_2][M] + k_1[O_3] + k_3[NO_2] \right\} \tag{4.9}$$

($[M]$ is the neutral number density, equal to n_m in the table at the end of section 2.) The term $l_1[O_2][M]$ increases with decreasing elevation from a minimum of 10^{-3} sec^{-1} at 70 km, and reaches a value as large as 40 sec^{-1} at 30 km. We can therefore assume equilibrium for $[O]$:

$$[O] = \frac{2[O_2]J_{O_2} + [O_3]J_{O_3} + [NO_2]J_{NO_2}}{L(1+K)} \tag{4.10}$$

where

$$L = l_1[O_2][M]$$
$$K = \frac{k_1[O_3] + k_3[NO_2]}{l_1[O_2][M]} \tag{4.11}$$

A similar thing happens in the equation for $[NO]$,

$$\frac{d[NO]}{dt} = k_3[NO_2][O] + J_{NO_2}[NO_2] - [NO]\left\{ k_2[O_3] \right\} \tag{4.12}$$

where the product $k_2[O_3]$ is again large enough (10^{-3} sec^{-1} at 50 km, .04 sec^{-1} at 20 km) to allow us to assume $d[NO]/dt = 0$. Thus

$$[NO] = \left\{ \frac{k_3[O] + J_{NO_2}}{k_2[O_3]} \right\} [NO_2] \tag{4.13}$$

TABLE 4.2

Flux of solar photons, q, at one AU, absorption cross section of O_2 and of O_3, $\sigma(O_2)$ and $\sigma(O_3)$, for wavelength intervals $\Delta\lambda$ and wavenumber intervals $\Delta\nu$ from Ly-α to 7300 Å

No.	$\Delta\lambda$(Å)	$\Delta\nu$(cm^{-1})	q(cm^{-2} s^{-1})	$\sigma(O_2)$ (cm^2)	$\sigma(O_3)$ (cm^2)	$\sigma(NO_2)$ (cm^2)
1	Ly α 1.215,67	82.259	3.00×10^{11}	1.00×10^{-20}	2.32×10^{-17}	
2	1.170–1.163	85.500–86.000	1.03×10^{8}	2.00×10^{-20}	7.80×10^{-18}	
3	1.176–1.170	85.000–85.500	2.66	1.25×10^{-18}	7.97	
4	1.183–1.176	84.500–85.000	1.12	2.55×10^{-19}	8.66	
5	1.190–1.183	84.000–84.500	1.24	3.00×10^{-20}	9.51	
6	1.198–1.190	83.500–84.000	1.82	3.75×10^{-19}	1.25×10^{-17}	
7	1.205–1.198	83.000–83.500	1.90	4.45×10^{-18}	1.84	
8	1.212–1.205	82.500–83.000	7.40	8.35	2.19	
9	1.220–1.212	82.000–82.500	2.28×10^{9}	6.00×10^{-19}	2.30	
10	1.227–1.220	81.500–82.000	3.67	2.35	2.26	
11	1.235–1.227	81.000–81.500	1.36	4.50	2.06	
12	1.242–1.235	80.500–81.000	1.61	3.35	1.30	
13	1.250–1.242	80.000–80.500	1.32	1.75×10^{-17}	8.91×10^{-18}	
14	1.258–1.250	79.500–80.000	1.41	8.95×10^{-18}	7.24	
15	1.266–1.258	79.000–79.500	3.11	4.30	6.09	
16	1.274–1.266	78.500–79.000	1.06	1.10	5.66	
17	1.282–1.274	78.000–78.500	1.37	2.05	5.87	
18	1.290–1.282	77.500–78.000	1.02	4.43	6.47	
19	1.299–1.290	77.000–77.500	1.14	5.55	8.14	
20	1.307–1.299	76.500–77.000	7.29	4.20	1.24×10^{-17}	
21	1.316–1.307	76.000–76.500	2.20	6.85	1.52	
22	1.324–1.316	75.500–76.000	1.59	1.45×10^{-18}	1.47	
23	1.333–1.324	75.000–75.500	2.21	2.25	1.51	
24	1.342–1.333	74.500–75.000	1.24×10^{10}	2.30×10^{-18}	1.51×10^{-17}	
25	1.351–1.342	74.000–74.500	1.99×10^{9}	4.55	1.65	
26	1.360–1.351	73.500–74.000	3.09	7.23	1.54	
27	1.370–1.360	73.000–73.500	2.57	9.50	1.35	
28	1.379–1.370	72.500–73.000	2.74	1.23×10^{-17}	1.05	
29	1.389–1.379	72.000–72.500	3.10	1.32	7.97×10^{-18}	
30	1.408–1.389	71.000–72.000	7.60	1.36	7.17	
31	1.428–1.408	70.000–71.000	1.01×10^{10}	1.40	6.28	
32	1.449–1.428	69.000–70.000	1.30	1.48	5.66	
33	1.470–1.449	68.000–69.000	1.82	1.41	5.23	
34	1.492–1.470	67.000–68.000	2.33	1.29	4.47	
35	1.515–1.492	66.000–67.000	2.66	1.15	3.69	
36	1.538–1.515	65.000–66.000	2.90	9.91×10^{-18}	2.93	
37	1.562–1.538	64.000–65.000	3.60	8.24	2.19	
38	1.587–1.562	63.000–64.000	4.75	6.58	1.63	
39	1.613–1.587	62.000–63.000	6.40	4.97	1.20	
40	1.639–1.613	61.000–62.000	5.49	3.45	9.77×10^{-18}	
41	1.667–1.639	60.000–61.000	1.19×10^{11}	2.08	8.66	
42	1.695–1.667	59.000–60.000	1.76	1.23	8.14	
43	1.724–1.695	58.000–59.000	2.32	7.22×10^{-19}	8.17	
44	1.739–1.724	57.500–58.000	1.44	4.58	8.57	
45	1.754–1.739	57.000–57.500	1.83	2.74	8.40	
46	1.770–1.754	56.500–57.000	2.34	3.10×10^{-20}	8.11	
47	1.786–1.770	56.000–56.500	2.62	1.90	7.99	
48	1.802–1.786	55.500–56.000	2.88×10^{11}	1.10	7.86×10^{-19}	
49	1.818–1.802	55.000–55.500	3.14	6.00×10^{-21}	7.63	

See Ackerman (1970), Proc. 4th Joint ESRO-ESRIN Symposium (ed. G. Fiocco) D. Reidel, Dordrecht, 1971.

TABLE 4.2 (Continued)

No.	$\Delta\lambda$(Å)	$\Delta\nu$(cm^{-1})	q(cm^{-2} s^{-1})	$\sigma(O_2)$ (cm^2)	$\sigma(O_3)$ (cm^2)	$\sigma(NO_2)$ (cm^2)
50	1.835-1.818	54.500-55.000	3.81×10^{11}	3.50×10^{21}	7.29×10^{-19}	
51	1.852-1.835	54.000-54.500	4.43	1.80	6.88	
52	1.869-1.852	53.500-54.000	4.95	9.50×10^{22}	6.40	
53	1.887-1.869	53.000-53.500	5.94	4.70	5.88	
54	1.905-1.887	52.500-53.000	6.59	2.30	5.31	
55	1.923-1.905	52.000-52.500	7.26	1.30	4.80	
56	1.942-1.923	51.500-52.000	9.85	6.50×10^{23}	4.38	
57	1.961-1.942	51.000-51.500	1.27×10^{12}	3.70	4.11	
58	1.980-1.961	50.500-51.000	1.39	2.40	3.69	
59	2.000-1.980	50.000-50.500	1.53	1.70	3.30	
60	2.020-2.000	49.500-50.000	1.60	1.25	3.26	
61	2.041-2.020	49.000-49.500	1.74	1.14×10^{-23}	3.26	
62	2.062-2.041	48.500-49.000	2.31	1.05	3.51	
63	2.083-2.062	48.000-48.500	4.20	1.00	4.11	
64	2.105-2.083	47.500-48.000	7.30	9.55×10^{-24}	4.84	
65	2.128-2.105	47.000-47.500	9.42	8.93	6.26	
66	2.150-2.128	46.500-47.000	1.06×10^{13}	8.28	8.57	
67	2.174-2.150	46.000-46.500	1.34	7.60	1.17×10^{-18}	
68	2.198-2.174	45.500-46.000	1.32	6.92	1.52	
69	2.222-2.198	45.000-45.500	1.73	6.28	1.97	
70	2.247-2.222	44.500-45.000	1.80	5.65	2.55	
71	2.273-2.247	44.000-44.500	1.82	5.03	3.24	
72	2.299-2.273	43.500-44.000	2.26	4.40	4.00	
73	2.326-2.299	43.000-43.500	2.40	3.76	4.83	
74	2.353-2.326	42.500-43.000	2.25	3.09	5.79	
75	2.381-2.353	42.000-42.500	2.21	2.44	6.86	
76	2.410-2.381	41.500-42.000	2.32	1.75	7.97	4.82 10^{-20}
77	2.439-2.410	41.000-41.500	2.50	6.74×10^{-25}	9.00	4.82
78	2.469-2.439	40.500-41.000	2.73		1.00×10^{-17}	2.26
79	2.500-2.469	40.000-40.500	2.88		1.07	2.20
80	2.532-2.500	39.500-40.000	3.02		1.11	2.32
81	2.564-2.532	39.000-39.500	3.97		1.12	2.42
82	2.597-2.564	38.500-39.000	7.13		1.11	2.47
83	2.632-2.597	38.000-38.500	4.37		1.03	2.55
84	2.667-2.632	37.500-38.000	1.12×10^{14}		9.43×10^{-18}	2.83
85	2.703-2.667	37.000-37.500	1.25		8.23	3.11
86	2.740-2.703	36.500-37.000	1.16		6.81	3.40
87	2.778-2.740	36.000-36.500	1.19		5.31	3.68
88	2.817-2.778	35.500-36.000	1.38		3.99	3.97
89	2.857-2.817	35.000-35.500	1.70		2.84	4.25
90	2.899-2.857	34.500-35.000	2.46		1.92	4.53
91	2.941-2.899	34.000-34.500	3.90		1.14	5.11
92	2.985-2.941	33.500-34.000	3.99		6.60×10^{-19}	5.70
93	3.030-2.985	33.000-33.500	3.86		3.69	6.23
94	3.077-3.030	32.500-33.000	5.08		1.97	7.40
95	3.100 (± 25)	32.520-32.000	5.92		1.05	8.78
96	3.150	32.000-31.496	6.05		5.23×10^{-20}	1.03 10^{-19}
97	3.200	31.496-31.008	6.94		2.91	1.19
98	3.250	31.008-30.534	8.12		1.50	1.35
99	3.300	30.534-30.075	9.71		7.78×10^{-21}	1.53
100	3.350	30.075-29.630	8.97		3.72	1.65

TABLE 4.2 (Continued)

No.	$\Delta\lambda$(Å)	$\Delta\nu$(cm^{-1})	q(cm^{-2} s^{-1})	$\sigma(O_2)$ (cm^2)	$\sigma(O_3)$ (cm^2)	$\sigma(NO_2)$ (cm^2)
101	3.400 (± 25)	29.630–29.197	9.44×10^{14}		1.71×10^{-21}	1.78 10^{-19}
102	3.450	29.197–28.777	1.01×10^{15}		7.46×10^{-22}	1.43
103	3.500	28.777–28.369	1.03		2.66	2.09
104	3.550	28.369–27.972	1.03		1.09	2.18
105	3.600	27.972–27.586	1.04		5.49×10^{-23}	2.26
106	3.650	27.586–27.211	1.18		–	2.32
107	3.700	27.211–26.846	1.23		–	2.38
108	3.750	26.846–26.490	1.24		–	2.46
109	3.800	26.490–26.144	1.17		–	2.53
110	3.850	26.144–25.806	1.11		–	2.57
111	3.900	25.806–25.478	1.09		–	2.60
112	3.950	25.478–25.157	1.19		–	2.63
113	4.000	25.157–24.845	1.54		–	*
114	4.050	24.845–24.540	1.90		–	
115	4.100	24.540–24.242	1.99		2.91	
116	4.150	24.242–23.952	1.99		3.14	
117	4.200	23.952–23.669	2.02		3.99	
118	4.250	23.669–23.392	2.01		6.54	
119	4.300	23.392–23.121	1.94		6.83	
120	4.350	23.121–22.851	1.98		8.66	
121	4.400	22.851–22.599	2.25		1.25×10^{-22}	
122	4.450	22.599–22.346	2.39		1.49	
123	4.500	22.346–22.099	2.48		1.71	
124	4.550	22.099–21.858	2.49		2.12	
125	4.600	21.858–21.622	2.48		3.57	
126	4.650	21.622–21.390	2.50		3.68	
127	4.700	21.390–21.164	2.55		4.06	
128	4.750	21.164–20.942	2.61		4.89	
129	4.800	20.942–20.725	2.59		7.11	
130	4.850	20.725–20.513	2.46		8.43	
131	4.900	20.513–20.504	2.44		8.28	
132	4.950	20.504–20.100	2.53		9.09	
133	5.000	20.100–19.900	2.48		1.22×10^{-21}	
134	5.050	19.900–19.704	2.49		1.62	
135	5.100	19.704–19.512	2.50		1.58	
136	5.150	19.512–19.324	2.43		1.60	
137	5.200	19.324–19.139	2.43		1.78	
138	5.250	19.139–18.957	2.52		2.07	
139	5.300	18.957–18.779	2.58		2.55	
140	5.350	18.779–18.605	2.64		2.74	
141	5.400	18.605–18.433	2.67		2.88	
142	5.450	18.433–18.265	2.70		3.07	
143	5.500	18.265–18.100	2.68		3.17	
144	5.550	18.100–17.937	2.66		3.36	
145	5.600	17.937–17.778	2.66		3.88	
146	5.650	17.778–17.621	2.67		4.31	
147	5.700	17.621–17.467	2.67		4.67	
148	5.750	17.467–17.316	2.69		4.75	
149	5.800	17.316–17.667	2.71		4.55	
150	5.850	17.667–17.021	2.71		4.35	
151	5.900	17.021–16.878	2.71		4.42	
152	5.950	16.878–16.736	2.72		4.61	

---

* At wavelengths beyond 3975Å dissociation of NO_2 is not possible and the values of $\sigma(NO_2)$ are therefore not tabulated.

TABLE 4.2 (Continued)

No.	$\Delta\lambda$(Å)	$\Delta\nu$(cm^{-1})	q(cm^{-2} s^{-1})	$\sigma(O_2)$ (cm^2)	$\sigma(O_3)$ (cm^2)	$\sigma(NO_2)$ (cm^2)
153	6.000 (± 25)	16.736-16.598	2.72×10^{15}		4.89×10^{-21}	
154	6.050	16.598-16.461	2.71		4.84	
155	6.100	16.461-16.326	2.70		4.54	
156	6.150	16.326-16.194	2.70		4.24	
157	6.200	16.194-16.064	2.70		3.90	
158	6.250	16.064-15.936	2.69		3.60	
159	6.300	15.936-15.810	2.68		3.43	
160	6.350	15.810-15.686	2.67		3.17	
161	6.400	15.686-15.564	2.66		2.74	
162	6.450	15.564-15.444	2.65		2.61	
163	6.500 (± 50)	15.384-15.265	3.95		2.40	
164	6.600	15.265-15.038	5.22		2.07	
165	6.700	15.038-14.815	5.18		1.72	
166	6.800	14.815-14.598	5.14		1.37	
167	6.900	14.598-14.388	5.09		1.11	
168	7.000	14.388-14.184	5.04		9.13×10^{-22}	
169	7.100	14.184-13.986	4.99		7.93	
170	7.200	13.986-13.793	4.94		6.40	
171	7.300	13.793-13.605	4.90		5.14	

In the nighttime [NO] vanishes according to this expression. In the daytime the factor multiplying [NO_2] in (4.13) has the typical values 70, 2, 0.3 and 0.15 at 50, 40, 30 and 20 km (see table). We may then argue that at the levels of major [O_3], the major portion of [$NO + NO_2$] averaged over a day is in the form of [NO_2]. That is to say, an assumption that [$NO + NO_2$] is a given function of pressure can be replaced by an assumption that [NO_2] is an assigned function of pressure (possibly a different function, of course).

Calculations by Johnston (1971; Science, 173, P. 517) and Crutzen (1971; J. Geophy. Res., 76, P. 7311) suggest that the total odd nitrogen mixing ratio ([NO] + [NO_2]) $\div$ [M] increases considerably with height. These results do depend however on assumptions about the vertical eddy diffusion coefficient and the set of assumed reactions and reaction rates, (see Crutzen, ibid plus 1972, AMBIO, in press). The calculations by Crutzen (1971), which include HNO_3 suggest that [NO_2] $\div$ [M] is approximately constant above about 25 km while decreasing by a factor of about 10 from 25 km down to 15 km.

For the moment then, we assume that [NO_2] or [NO_2] $\div$ [M] is a prescribed function of pressure, with [NO] determined from (4.13).

The equation for [O_3] is

$$\frac{d[O_3]}{dt} = \ell_1 [O_2][M][O] - J_{O_3}[O_3] - k_1 [O][O_3] - k_2 [NO][O_3] \qquad (4.14)$$

Substitution for [O] and [NO] from (4.10) and (4.13) gives

$$\frac{d[O_3]}{dt} = \frac{1-K}{1+K} \, 2 [O_2] J_{O_2} - \frac{2K}{1+K} \left([O_3] J_{O_3} + [NO_2] J_{NO_2} \right)$$

$$= \frac{1}{1+K} \left\{ 2 [O_2] J_{O_2} - 2K \left([O_2] J_{O_2} + [O_3] J_{O_3} + [NO_2] J_{NO_2} \right) \right\} \qquad (4.15)$$

The previous table shows that K and the ratio ($[O_2]J_{O_2}$) ÷ ($[O_3]J_{O_3}$) are both equally small, of order 10^{-2} or less. A case can then be made for simplifying the above expression to

$$\frac{d[O_3]}{dt} \approx 2[O_2]J_{O_2} - 2K\left([O_3]J_{O_3} + [NO_2]J_{NO_2}\right) \tag{4.16}$$

where we have retained only the leading terms. In terms of the number mixing ratios ν_i,

$$\begin{aligned} \nu_{O_2} &= [O_2] \div n_m = 0.2096 \\ \nu_{O_3} &= [O_3] \div n_m \\ \nu_{NO_2} &= [NO_2] \div n_m \end{aligned} \tag{4.17}$$

we have

$$\left[\frac{1}{n_m}\frac{dn_{O_3}}{dt}\right] = 2(.2096)J_{O_2} - 2K\left[\nu_{O_3}J_{O_3} + \nu_{NO_2}J_{NO_2}\right] \tag{4.18}$$

$$K = \frac{k_1\nu_{O_3} + k_3\nu_{NO_2}}{(.2096)\,\ell_1\, n_m} = K(p,T) \tag{4.19}$$

At constant pressure the logarithmic derivative of n_m with T is T^{-1}, whereas the logarithmic variation of (k_1/ℓ_1) and (k_3/ℓ_1) with T is $3445/T^2 \sim \frac{10}{T}$ and $1580/T^2 \sim \frac{5}{T}$ respectively. We therefore treat n_m as a known function of pressure ($= p/k\bar{T}$;see table at end of section 2), but will compute the exact dependence of the rate constants on T.

Using $n_m = 7.243 \times 10^{21}\ P_j/\overline{T}_j$, K is computed as follows

$$K = \frac{\overline{T}_j}{P_j}\left\{ 823\,\chi_{O_3}\,e^{-\frac{3445}{T}} + 1317\,\chi_{NO_2}\,e^{-\frac{1580}{T}} \right\} \qquad (4.20)$$

The two exponentials are computed from the non-dimensional temperatures,

$$\begin{aligned} e_1 &= \exp\left[-\frac{3445}{T(\text{non-dim})}\cdot\frac{R}{4a^2\Omega^2}\right] \\ e_2 &= \exp\left[-\frac{1580}{T(\text{non-dim})}\cdot\frac{R}{4a^2\Omega^2}\right] \end{aligned} \qquad (4.21)$$

5000 values of e_1 and e_2 are stored in a table computed for values of

$$T(\text{non-dim}) = \left(\frac{10}{256}+\frac{\delta}{2}\right), \left(\frac{10}{256}+\frac{3\delta}{2}\right), \ldots\ldots, \left(\frac{10}{256}+\frac{9999}{2}\delta\right)$$

where $\delta = 16^{-4}$. It is assumed that the stratospheric model will always yield temperatures in the range

$$\frac{10}{256} = 0.0390 < T(\text{non-dim}) \leq \frac{945}{32\times 256} = 0.1154 \qquad (4.22)$$

Suppose that a model T(non-dim) is such that

$$\left(\frac{10}{256} + i\delta\right) \leq T(\text{non-dim}) < \left(\frac{10}{256} + \overline{i+1}\,\delta\right),$$

then we set $\quad e_1(T) = e_1\left(\frac{10}{256} + \frac{2i+1}{2}\delta\right)$

and $\quad e_2(T) = e_2\left(\frac{10}{256} + \frac{2i+1}{2}\delta\right).$

The maximum error introduced by evaluating the exponentials by this method is approximately 1/2 %.

Let us now consider how J_{O_2}, J_{O_3}, and J_{NO_2} are computed. Consider first J_{O_3}.

$$J_{O_3} = \int_0^{11400} \alpha_{O_3}(\lambda)\, I(\lambda)\, e^{-X_{O_3}}\, d\lambda$$

is computed as the sum

$$J_{O_3} = \sum_{i=60}^{171} \alpha_{O_3}(\lambda_i)\, F(\lambda_i)\, e^{-X_{O_3}} \qquad (4.23)$$

where the wavelengths, λ_i, the absorption coefficient, and the solar flux, $F(\lambda_i)$, integrated each wavelength interval are taken from table 4.2 (from Ackerman, 1970). The reduction of the solar flux in this wavelength range by molecular onygen is considered to be negligible. The maximum error thus introduced is certainly less than 5%.

In order to compute J_{NO_2}, we must evaluate X_{NO_2}. Using the NO_2 profile shown in table 4.1, the optical depth, X_{NO_2}, for a solar zenith angle of zero is only .01 at ground level and at 3975Å. We shall therefore neglect the reduction in $I(\lambda)$ resulting from absorption by NO_2 in our computation of J_{NO_2}. Thus the computation scheme used is

$$J_{NO_2} = \sum_{i=} \alpha_{NO_2}(\lambda_i)\, F(\lambda_i)\, e^{-X_{O_3}} \qquad (4.24)$$

J_{O_2} is evaluated as the sum

$$J_{O_2} = \sum_{i=45}^{77} \alpha_{O_2}(\lambda_i)\, F(\lambda_i)\, e^{-(X_{O_3}+X_{O_2})} \qquad (4.25)$$

in which the overlapping of the absorption bands of molecular oxygen and ozone must be included.

Values of J_{O_3}, J_{O_2}, and J_{NO_2} are calculated at levels 1 through 22.

5. Model heating

Above 30 km atmospheric heating is assumed to be the sum of two contributions - the absorption of solar ultraviolet and visible radiation by ozone and infrared heating and cooling by carbon dioxide, ozone, and water vapor. The relative magnitudes of these contributions is depicted in figure 5.1 (from calculations by Newell et al., 1970).

(a) model of solar absorption by ozone

$$Q'_{O_3} = \int_0^{7500} \alpha_{O_3}(\lambda)\, I(\lambda)\, \varepsilon(\lambda)\, e^{-X_{O_3}}\, d\lambda \quad \text{joules/sec}/O_3 \text{ mol.} \qquad (5.1)$$

where $\alpha_{O_3}(\lambda)$ is the absorption coefficient of ozone

$I(\lambda)$ is the flux of solar photons incident on the top os the atmosphere

$\varepsilon(\lambda)$ is the energy of a photon of wavelength (= $1.9872 \times 10^{-15}/\lambda$ joules for λ in Å)

X_{O_3} is the optical depth of ozone (see section 4)

For equation 1.25 we require the heating rate in dimensionless units,

$$\frac{q}{c_p} = 9.375 \times 10^7\, \chi_{O_3}\, Q_{O_3} \qquad (5.2)$$

Q_{O_3} is evaluated as the sum

$$Q_{O_3} = \sum_{i=60}^{171} \alpha_{O_3}(\lambda_i)\, F(\lambda_i)\, \frac{e^{-X_{O_3}}}{\lambda_i} \qquad (5.3)$$

where $F(\lambda_1)$ is the solar flux of photons integrated over a small wavelength interval around λ_1 (see table 4.2).

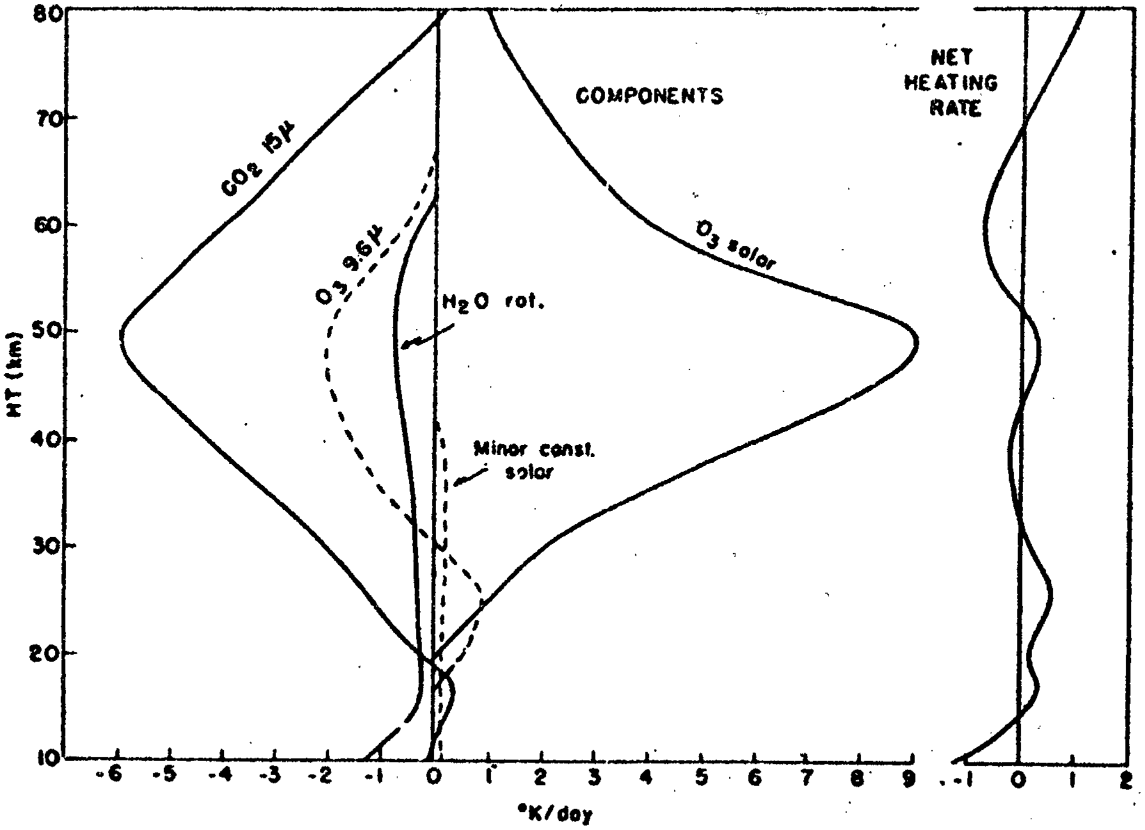

Figure 5.1. Vertical distribution of the components of the net radiative heating rate. (Newell and Gray, 1972)

(b) Tropospheric and infra-red stratospheric heating rates

In the troposphere and lower stratosphere, we follow Trenberth (Ph.D. thesis, M.I.T., 1972) in setting, at each level j,

$$\frac{\partial T}{\partial t} = \;-\;-\;-\; + h_j\left(T_j^* - T\right) \tag{5.4}$$

where h_j is a "Newtonian" cooling coefficient, T_j^* is a hypothetical equilibrium temperature field, and T is the temperature predicted by the model. (All T's in the above equation have a zero horizontal average.) For the zonally symmetric part, Trenberth divided T* into an annual average term (symmetric in latitude) and a seasonal term (an odd function of latitude):

$$T_j^*(\mu,t) = T_{j2}^* P_2^\circ(\mu) + \left[T_{j1}^* P_1^\circ(\mu) + T_{j3}^* P_3^\circ(\mu)\right] \sin \frac{2\pi}{365}(t-\phi_j) \tag{5.5}$$

Here μ is the sine of the latitude and P_n° are the legendre functions normalized so that $\int_{-1}^{1} P^2 \, d\mu = 2$.

$$\begin{aligned} P_1^\circ(\mu) &= \sqrt{3}\,\mu \\ P_2^\circ(\mu) &= \frac{\sqrt{5}}{2}\left(3\mu^2-1\right) \\ P_3^\circ(\mu) &= \frac{\sqrt{7}}{2}\,\mu\left(5\mu^2-3\right) \end{aligned} \tag{5.6}$$

t is in days and is zero at the vernal equinox. d_j is a mild time-lag introduced in the troposphere to account for delayed ocean warmth. Trenberth used the following values for his eight levels:

Z_j	P_j	z_j(km)	$h_j(\text{day}^{-}\ )$	d_j	T^*_{j2}(deg)	T^*_{j1}(deg)	T^*_{j3}(deg)
.511	.6	4	0.08	21	-15.4	6.54	0
1.204	.3	9	0.059	21	-10.3	5.97	0
2.120	.12	15	0.019	0	-2.24	8.96	1.70
3.219	.04	22	0.026	0	-4.64	11.8	3.32
4.605	.01	30.5	0.050	0	-5.39	14.0	4.57
6.214	.002	43	0.190	0	-5.37	11.7	5.45
7.601	.0005	54	0.24	0	-1.78	11.2	4.89
9.210	.0001	63	0.20	0	0	2.77	1.21

In the stratosphere, Trenberth's formula empirically represents all of the main types of radiation effects:

a. Short wave absorption by ozone and oxygen (20 km and higher)

b. 9.6 micron absorption and emission by ozone (20-30 km)

c. Infra-red absorption and emission by CO_2 (all heights)

In our model we will explicitly compute radiatinn of type a, as described elsewhere. This means that Trenberth's formulation must be changed for Z higher than 20 km ($Z \geq 2.9$). Type c can be represented by a simple Newtonian law

$$\frac{\partial T}{\partial t} = -a(p)T \tag{5.7}$$

The most recent values of a are those computed by Dickinson (A method of parameterization for infra-red cooling between altitudes of 30 and 70 km.

NCAR preprint, February 1973). He obtained these values of a(p) by careful line integration of the CO and O bands for a standard atmosphere, followed by a similar computation in which T was varied slightly. (Physically this is satisfactrry for the circumstance of cooling to space - it does not include, however, the major effect of b above, which comes from absorption of radiation emitted by the ground in the water-vapor window region.) Dickinson finds values as follows:

Z	a(day^{-1})
11.4	.016
10.0	.062
9.1	.125
8.7	.172
7.9	.200
7.4	.220
6.9	.212
6.1	.135
4.8	.080
3.9	.060

These can be fit satisfactorily by two linear segments matching the three underlined extreme values:

$$\begin{aligned} &3.9 \leq Z \leq 7.4 \qquad a = 0.22 + .045714\,(Z-7.4)\ \text{deg}^{-1} \\ &7.4 \leq Z \leq 11.4 \qquad a = 0.22 - .051\,(Z-7.4)\ \text{deg}^{-1} \end{aligned} \tag{5.8}$$

Dickinson's values are larger than the early values used by Lindzen and Goody (J. Atmos. Sci., 1965) of 0.043 and 0.06 day^{-1} for Z less than or greater than 6 (z = 40 km). Dickinson's values can also be compared with values obtained by taking the cooling rates computed by London and Kuhn

(J. Atmos. Sci., 1969) and, at each pressure level, determining a least square fit to $\delta T/\delta t = -a\ T$ from the seven latitudes at which Kuhn and London made their computations. The profile of values for a so obtained

z (km)	a(day^{-1})
77.5	0.17
72.5	0.10
67.5	0.18
61.5	0.18
56.5	0.125
50.5	0.135
44	0.125
38	0.097
32.25	0.044

,

has the same shape with height as that obtained by Dickinson, but peaks with a value of 0.18 day^{-1} at the higher level $Z \sim 9$, and in the stratosphere are typically smaller than Dickinson's values by about 0.03 day^{-1}. (The difference in the srratosphere may arise from Dickinson's having taken "hot bands" into account for CO_2

Trenberth's values of his h_j (given earlier above) exceed Dickinson's values by only 0.05, 0.02, and 0.03 day^{-1} at $Z = 6.2$, 7.6, and 9.2 and is less than Dickinson's by 0.02 at $Z = 4.6$. It therefore appears reasonable to use "Dickinson's values" given by (5.8).

Heating due to the 9.6 micron O_3 band has been computed by Dopplick (Ph.D. thesis, M.I.T., 1970) using typical observed values of O_3. It gives a heating rate more or less independent of season with a peak value of 1.1 deg day^{-1} at the poles, centered at an altitude of about 25 km ($Z = 3.5$). This may be represented most simply by

$$\frac{\partial T}{\partial t} = -\frac{0.8}{\sqrt{5}} P_2^0(\mu)\left[1 - (Z-3.5)^2\right] \qquad (5.9)$$

for $2.5 \leq Z \leq 3.5$ and zero for Z values outside this range. As such, this heating does not depend on O_3 or T. This is not too critical, however, since the physical dependence on T is primarily due to ocean surface and cloud top temperatures, and any moderate variations in O_3 from that used by Dopplick will mostly shift somewhat the height $Z = 3.5$ vertically (i.e., the existing O_3 is ample to absorb all this upwelling radiation.)

We therefore propose the following strategy for heating computations. Define

Method I.

a. Explicit computation of short wave heating

b. Infra-red cooling with the Dickinson formula (5.8) for a supplemented by $a = 0.06$ for $Z < 3.9$

c. Formula (5.9) for O_3 window radiation for $2.5 \leq Z \leq 4.5$

Method II.
Trenberth's formulas (subject to some possible re-evaluation in detail)

These methods are combined as follows for different height ranges. ($Z = 2.5$ and 4.5 corresponds roughly to heights of 17.5 and 30.3 km)

A. $Z > 4.5$: Only method I.

B. $2.5 \leqslant Z \leqslant 4.5$: Weighted average of I and II as follows

$$\left(\frac{Z - 2.5}{2}\right) \times \text{Method I} + \left(\frac{4.5 - Z}{2}\right) \times \text{Method II}$$

C. $Z \leqslant 2.5$: Only method II.

TABLE 5.1 Standard concentrations of ozone, molecular oxygen, and nitrogen dioxide.

Level	Height km	$n(O_2)$ (cm^{-3})	Column Conc. $N_{O_2}(cm^{-2})$	$n(O_3)$ cm^{-3}	Column Conc. $N^*_{O_3}(cm^{-2})$	$n(NO_2)$ cm^{-3}
1	71.6	2.86×10^{14}	1.76×10^{20}	2.8×10^{8}	8.12×10^{13}	
2	69.0	4.11	2.64	6.4	1.97×10^{14}	
3	66.3	5.99	3.96	1.5×10^{9}	4.70	
4	63.5	8.72	5.94	3.5	1.13×10^{15}	
5	60.6	1.26×10^{15}	8.91	6.5	2.52	
6	57.6	1.84	1.34×10^{21}	1.2×10^{10}	5.16	
7	54.5	2.65	2.01	2.3	1.03×10^{16}	
8	51.4	3.86	3.01	4.6	2.08	
9	48.2	5.75	4.51	9.9	4.30	
10	45.0	8.84	6.77	2.15×10^{11}	9.01	8.84×10^{6}
11	41.9	1.36×10^{16}	1.02×10^{22}	4.1	1.84×10^{17}	7.79×10^{7}
12	38.8	2.10	1.52	7.6	3.55	4.00×10^{8}
13	35.9	3.23	2.28	1.3×10^{12}	6.50	1.39×10^{9}
14	33.0	4.96	3.43	1.8	1.09×10^{18}	2.60
15	30.2	7.64	5.14	2.45	1.68	3.27
16	27.5	1.17×10^{17}	7.71	3.4	2.46	3.40
17	24.8	1.80	1.16×10^{23}	4.3	3.48	3.68
18	22.2	2.84	1.73	4.8	4.66	3.96
19	19.6	4.22	2.60	4.65	5.87	4.40
20	17.1	6.34	3.90	3.6	6.92	6.04
21	14.6	9.43	5.85	2.5	7.68	8.08
22	12.0	1.36×10^{18}	8.78	2.0	8.25	1.15×10^{10}
23	9.3	1.92	1.32×10^{24}	1.0	8.66	1.72
24	6.4	2.73	1.98	6.0×10^{11}	8.88	2.58
25	3.4	3.82	2.96	6.0	9.05	3.87
26	0.1	9.56	4.44	6.0	9.25	5.80

6. The computational procedure for evaluating the daily average values of the heating and photodissociation rates

Expressions 5.3, 4.23, 4.24, and 4.25 for Q_{O_3}, J_{O_3}, J_{O_2}, and J_{NO_2} require a knowledge of the vertical column concentrations of O_2 and O_3 (N_{O_2} and N_{O_3}) and of the solar zenith angle (ψ). N_{O_2} is given at each level by expression (1.36). N_{O_3}, on the other hand, must be evaluated at each time step using expression (1.35) and values of χ_{O_3} from the prior time step.

(a) Evaluation of N_{O_3} at each grid point and each level, P_j.

$$N_{O_3}(P_j) = 2.12 \times 10^{25} \int_0^{P_j} \chi_{O_3}\, dP \qquad (\mathrm{cm}^{-2}) \tag{6.1}$$

Clearly,

$$N_{O_3}(P_j) = N_{O_3}(P_{j-1}) + 2.12 \times 10^{25} \int_{P_j}^{P_{j-1}} \chi_{O_3}\, dP$$

Therefore N_{O_3} is evaluated first at level 1 and then sequentially at every other level. $N_{O_3}(P_1)$ need only be evaluated approximately, and we suppose that χ_{O_3} decays exponentially above level 1 with a scale height determined from the horizontal average values of χ_{O_3} at levels 1 and 2. Thus

$$N_{O_3}(P_1) = 2.12 \times 10^{25}\, \chi_{O_3}(P_1) P_1 \left[1 + \frac{1}{\Delta Z} \log_e \frac{\overline{\chi_{O_3}(P_2)}}{\overline{\chi_{O_3}(P_1)}} \right]^{-1} \tag{6.2}$$

$N_{O_3}(P_j)$ for $j \geqslant 2$ is evaluated using expression (6.1). The integral is evaluated by using a second order curve fit to χ_{O_3} with the curve forced to pass through the values of χ_{O_3} at levels j, j - 1, and j - 2. Then

$$\int_{P_j}^{P_{j-1}} \chi_{O_3}\, dP = \frac{\Delta Z}{12}\left[5P_j\,\chi_{O_3}(P_j) + 8P_{j-1}\,\chi_{O_3}(P_{j-1}) - P_{j-2}\,\chi_{O_3}(P_{j-2})\right] \qquad (6.3)$$

$\chi_{O_3}(P_0)$ is set equal to zero. For the 2.8 km level spacing typical of our model, this computational technique produces errors in $N_{O_3} \lesssim 2\%$.

(b) Evaluation of daily average values of Q_{O_3}, J_{O_3}, J_{O_2}, J_{NO_2}

We do not wish to include the diurnal variation of the solar zenith angle in our model. Thus, in principle, we wish to evaluate expressions 5.3, 4.23, 4.24, and 4.25 at daily average values of X_{O_2} and X_{O_3}, corresponding to diurnal mean solar zenith angles. This has proved not possible within acceptable error limits. However by trial and error it has been found that the mean of two values of the Q and the J's at particular solar zenith angles does yield daily average values to 5% accuracy.

We first evaluate the hour angle of sunset at each latitude using the relation

$$\cos\psi = \sin\phi\,\sin\delta + \cos\phi\,\cos\delta\,\cos h \qquad (6.4)$$

where ψ is the solar zenith angle
ϕ is the latitude
δ is the solar declination
and h is the hour angle (measured from local noon).

Sunrise and sunset are given by $h = \pm H$ with

$$\cos H = -\tan\phi \tan\delta \tag{6.5}$$

Considering only the Northern Hemisphere $(\tan\phi \geq 0)$ we have

$$\begin{array}{lll} \tan\phi\tan\delta \leq -1 & : H \equiv 0 & (\text{polar winter night}) \\ -1 < \tan\phi\tan\delta < 0 & : 0 < H < \pi/2 & \\ \tan\phi\tan\delta = 0 & : H = \pi/2 & (\text{equinox}) \\ 0 < \tan\phi\tan\delta < 1 & : \pi/2 < H < \pi & \\ 1 \leq \tan\phi\tan\delta & : H \equiv \pi & (\text{polar summer day}) \end{array} \tag{6.6}$$

The exact expression for the daily average value of q (say) is

$$\bar{q} = \frac{1}{2\pi}\int_{-H}^{H} q \, dh = \frac{1}{\pi}\int_{0}^{H} q \, dh \tag{6.7}$$

However we have found the following alogorithm to be accurate to 5%:

$$\bar{q} = \frac{H}{2.05\,\pi}\left[q\Big|_{h=\frac{H}{4}} + q\Big|_{h=\frac{3H}{4}} \right] \tag{6.8}$$

This procedure is used to evaluate $\bar{Q}_{O_3}$, $\bar{J}_{O_3}$, $\bar{J}_{NO_2}$, and $\bar{J}_{O_2}$.

(c) Tabulation of values of Q_{O_3}, J_{O_3}, J_{O_2}, and J_{NO_2}.

The evaluation of $\bar{J}_{O_2}$, for example, at a particular grid point requires the evaluation of 66 exponentials. However computation time requirements limit us to approximately 10 multiplications per grid point for the evaluation of $\bar{Q}_{O_3}$, $\bar{J}_{O_3}$, $\bar{J}_{O_2}$ and $\bar{J}_{NO_2}$. Tables of values of Q_{O_3} J_{O_3}, J_{O_2}, and J_{NO_2} are therefore stored in the machine initially as a function of N_{O_3}.

Consider for example the way in which J_{O_3} is evaluated in the determination of $\overline{J}_{O_3}$. For each level, j, a table of 2 × 240 values of J_{O_3} are stored. Thus initially J_{O_3} is evaluated for values of

$$X_{O_3}(\lambda_i) = \frac{X_k(\lambda_i)}{4}\left(1+\frac{\delta}{2}\right), \frac{X_k(\lambda_i)}{4}\left(1+\frac{3\delta}{2}\right), \ldots, \frac{X_k(\lambda_i)}{4}\left(1+\frac{479\delta}{2}\right)$$

where $\delta = 1/256$, $k = 1$ or 2, and

$$X_1(\lambda_i) = 1.1\,\alpha_{O_3}(\lambda_i)\,N^*_{O_3} \quad , \quad X_2(\lambda_i) = 2.6\,\alpha_{O_3}(\lambda_i)\,N^*_{O_3}$$

The numbers 1.1 and 2.6 are considered to be typical values of $\sec\psi$ at $h = H/4$ and $h = 3H/4$ respectively. $N^*_{O_3}$ are obtained from a standard ozone profile suggested by Krueger (1972) and are tabulated in table 5.1.

Suppose now that $h = H/4$,

$$\frac{1.1\,N^*_{O_3}(P_j)}{4}(1+\ell\delta) \leq N_{O_3}(P_j)\sec\psi \leq \frac{1.1\,N^*_{O_3}(P_j)}{4}(1+\overline{\ell+1}\,\delta) \qquad (6.9)$$

Then J_{O_3} is set equal to

$$J_{O_3}\left[\frac{1.1}{4}N^*_{O_3}\left(1+\frac{2\ell+1}{2}\delta\right)\right].$$

Except that if $N_{O_3}(P_j)\sec\psi < \frac{1.1}{4}N^*_{O_3}(P_j)$, J_{O_3} is set equal to

$$J_{O_3}\left[\frac{1.1}{4}N^*_{O_3}\left(1+\frac{\delta}{2}\right)\right] \qquad (6.10)$$

and if $N_{O_3}(P_j)\sec\psi > 4.4\,N^*_{O_3}(P_j)$, J_{O_3} is set equal to

$$J_{O_3}\left[4.4\,N^*_{O_3}\left(1-\frac{\delta}{2}\right)\right]$$

A similar procedure is used (using the second set of tabulated values) to evaluate J_{O_3} at $h = 3H/4$. $\overline{Q}_{O_3}$, $\overline{J}_{O_2}$, and $\overline{J}_{NO_2}$ are evaluated in a similar manner.

In the case of $\overline{J}_{O_2}$ there is however an additional complication, viz. that J_{O_2} depends not only on X_{O_3} but also on X_{O_2}. Again computer limitations require that we produce an approximation scheme for computing the dependence of J_{O_2} on $N_{O_2} \sec\psi$ - or, since N_{O_2} is fixed at each level, on $\sec\psi$. If $\log J_{O_2}$ is plotted against $\log \cos\psi$, a curve with but a small curvature over values of $\cos\psi$ varying by a factor of 3 or 4 is produced. Thus it was decided to make a quadratic fit to this curve. Then

$$J_{O_2}\Big|_{h=\frac{H}{4}} = J^{(1)}_{O_2} \exp\left[a_1 \log_e\left(\frac{\cos\psi}{1.1}\right) + b_1 \overline{\log_e\left(\frac{\cos\psi}{1.1}\right)}^{2}\right] \quad (6.11)$$

where $$J^{(1)}_{O_2} = \sum_{i=45}^{77} \alpha_{O_2}(\lambda_i)\, F(\lambda_i)\, e^{-(X_{O_3} + X^{(1)}_{O_2})}$$

and $$X^{(1)}_{O_2} = 1.1\, \alpha_{O_2}(\lambda_i)\, N_{O_2} .$$

J_{O_2} is evaluated by the tabulation procedure previously described. The constants, $a_1(P_j)$ and $b_1(P_j)$ are determined by

$$a_1 = \frac{(\log_e 3.0)^2 \log_e \frac{J_1}{J_s} - (\log_e 1.8)^2 \log_e \frac{J_3}{J_s}}{\log_e 1.8 \, \log_e 3.0 \, \log_e 0.6}$$

$$b_1 = \frac{\log_e 3.0 \, \log_e \frac{J_1}{J_s} - \log_e 1.8 \, \log_e \frac{J_3}{J_s}}{\log_e 1.8 \, \log_e 3.0 \, \log_e 0.6} \quad (6.12)$$

$$J_s = \sum_{i=45}^{77} \alpha_{O_2}(\lambda_i)\, F(\lambda_i)\, e^{-(X^{(1)}_{O_3} + X^{(1)}_{O_2})}$$

$$J_1 = \sum_{i=45}^{77} \alpha_{O_2}(\lambda_i) F(\lambda_i) e^{-\left(X_{O_3}^{(1)} + 1.8 X_{O_2}^{(1)}\right)}$$

$$J_3 = \sum_{i=45}^{77} \alpha_{O_2}(\lambda_i) F(\lambda_i) e^{-\left(X_{O_3}^{(1)} + 3 X_{O_2}^{(1)}\right)} \tag{6.13}$$

with $X_{O_3}^{(1)} = 1.1\, \alpha_{O_3}(\lambda_i) N_{O_3}^{*}$

A similar procedure is used to evaluate $J_{O_2}\Big|_{h=\frac{3H}{4}}$; in this case the constants are a_2 and b_2 and $X_{O_2}^{(1)}$ and $X_{O_3}^{(1)}$ are replaced by $X_{O_2}^{(2)}$ and $X_{O_3}^{(2)}$.

$$X_{O_2}^{(2)} = 2.6\, \alpha_{O_2}(\lambda_i) N_{O_2}$$

$$X_{O_3}^{(2)} = 2.6\, \alpha_{O_3}(\lambda_i) N_{O_3}^{*} \tag{6.14}$$

7. Spectral form of the equations

We define spectral solutions at arbitrary level j in the form

$$\left.\begin{aligned}
\Psi_j &= \sum_\alpha \Psi_{\alpha,j}\, Y_\alpha(\lambda,\mu) \\
\zeta_j &= \sum_\alpha \zeta_{\alpha,j}\, Y_\alpha(\lambda,\mu) \\
W_j &= \sum_\alpha W_{\alpha,j}\, Y_\alpha(\lambda,\mu) \\
F_j &= \sum_\alpha F_{\alpha,j}\, Y_\alpha(\lambda,\mu) \\
T_j &= \sum_\alpha T_{\alpha,j}\, Y_\alpha(\lambda,\mu) \\
q_j &= \sum_\alpha q_{\alpha,j}\, Y_\alpha(\lambda,\mu)
\end{aligned}\right\} \qquad (7.1)$$

and for the trace substance equation

$$\left.\begin{aligned}
x_j &= \sum_\alpha x_{\alpha,j}\, Y_\alpha(\lambda,\mu) \\
G_j &= \sum_\alpha G_{\alpha,j}\, Y_\alpha(\lambda,\mu)
\end{aligned}\right\} . \qquad (7.2)$$

In terms of longitude (λ) and latitude (μ) we have defined members of the complete set of orthogonal spherical harmonics in (7.1) and (7.2) using

$$Y_\alpha(\lambda,\mu) = e^{i l_\alpha \lambda} P_\alpha(\mu) \qquad (7.3)$$

with

$$\alpha = n_\alpha + i\, l_\alpha \qquad (7.4)$$

denoting a vector index of planetary wave number ℓ_α and degree n_α. The $P_\alpha(\mu)$ are Legendre polynomials of rank and degree given by α. Normalization of the spherical harmonics is such that integration over the unit spherical surface (s) yields the orthogonal property

$$\int_S Y_\alpha Y_\beta^* \, ds = 4\pi \, \delta_{\alpha,\beta} \quad . \tag{7.5}$$

Complex conjugate values are denoted by an asterisk. Another useful property of the set of spherical harmonics is that they satisfy the differential equation

$$\nabla^2 Y_\alpha = -c_\alpha Y_\alpha \; ; \; c_\alpha = n_\alpha(n_\alpha + 1) \, . \tag{7.6}$$

The complete set of orthonormal Legendre polynomials as used in (7.3) are defined such that

$$P_\alpha^* \equiv P_\alpha \tag{7.7}$$

and all P_α are normalized to

$$\int_{-1}^{+1} P_\alpha P_\beta \, d\mu = 2\,\delta_{\alpha,\beta} \quad . \tag{7.8}$$

We now want to substitute solutions (7.1) and (7.2) into the non-dimensional forms of our model equations, multiply through with a member of the orthogonal set (say, Y_γ^*), and integrate the resulting relationships over the unit sphere. Application of this procedure to the vorticity equation (3.9) for example yields the desired spectral form of this equation,

$$\frac{d\zeta_{r,j}}{dt} = -i\ell_r\Psi_{r,j} - A_{r,j} + \frac{D_r}{c_{r-\epsilon}}\left[\left(\frac{\Omega}{\Omega-1}\right)W_{r-\epsilon,j+1} - \right.$$
$$\left. -\left(\frac{1}{\Omega-1}\right)W_{r-\epsilon,j}\right] - \frac{E_r}{c_{r+\epsilon}}\left[\left(\frac{\Omega}{\Omega-1}\right)W_{r+\epsilon,j+1} - \right.$$
$$\left. -\left(\frac{1}{\Omega-1}\right)W_{r+\epsilon,j}\right] + \left(\frac{\Omega}{\Omega-1}\right)F_{r,j+1} - \left(\frac{1}{\Omega-1}\right)F_{r,j} \tag{7.9}$$

in which over the unit spherical surface s,

$$\left.\begin{aligned}
\frac{d\zeta_{r,j}}{dt} &= \frac{1}{4\pi}\int_s \frac{\partial\zeta_j}{\partial t}Y_r^* ds \\
i\ell_r\Psi_{r,j} &= \frac{1}{4\pi}\int_s J(\Psi_j,\mu)Y_r^* ds = \frac{1}{4\pi}\int_s \frac{\partial\Psi_j}{\partial\lambda}Y_r^* ds \\
A_{r,j} &= \frac{1}{4\pi}\int_s J(\Psi_j,\zeta_j)Y_r^* ds \quad \text{(See Appendix A)} \\
\frac{D_r}{c_{r-\epsilon}}W_{r-\epsilon,j} - \frac{E_r}{c_{r+\epsilon}}W_{r+\epsilon,j} &= -\frac{1}{4\pi}\int_s\left[\nabla\cdot\mu\nabla\mathcal{L}(W_j)\right]Y_r^* ds \\
&\qquad \text{(See Appendix B)} \\
F_{r,j} &= \frac{1}{4\pi}\int_s F_j Y_r^* ds
\end{aligned}\right\} \tag{7.10}$$

Similarly, the thernodynamic energy equation (3.19), the trace substance equation (3.21), and the thermal wind relationship (3.18) reduce to the spectral forms

$$\left.\begin{aligned}
\frac{dT_{r,j}}{dt} &= -B_{r,j} - S_j W_{r,j} + \left[\frac{R}{c_p 8\Omega^3 a^2}\right] q_{r,j} \\
\frac{d\chi_{r,j}}{dt} &= -B^{(\chi)}_{r,j} - \left(\frac{d\bar{\chi}}{dz}\right)W_{r,j} + \left(\frac{\Omega}{\Omega-1}\right)G_{r,j} - \\
&\quad - \left(\frac{1}{\Omega-1}\right)G_{r,j-1} + \frac{1}{4\pi}\int_s \frac{1}{2\Omega}\left[\frac{1}{n_m}\left(\frac{dn}{dt}\right)_c\right]_j Y_r^* ds \\
\Delta z\, c_r T_{r,j} &= -D_r\left(\Psi_{r-\epsilon,j-1} - \Psi_{r-\epsilon,j}\right) + \\
&\quad + E_r\left(\Psi_{r+\epsilon,j-1} - \Psi_{r+\epsilon,j}\right)
\end{aligned}\right\} \tag{7.11}$$

where, for example,

$$\frac{dT_{r,j}}{dt} = \frac{1}{4\pi}\int_s \frac{\partial T_j}{\partial t}Y_r^* ds \quad . \tag{7.12}$$

$$\left.\begin{aligned}
\frac{d\chi_{r,j}}{dt} &= \frac{1}{4\pi}\int_S \frac{d\chi_j}{dt} Y_r^* \, ds \\
c_r T_{r,j} &= \frac{1}{4\pi}\int_S \left(-\nabla^2 T_j\right) Y_r^* \, ds \\
B_{r,j} &= \frac{1}{8\pi}\int_S J(\psi_j+\psi_{j-1}, T_j)\, Y_r^* \, ds \quad \text{(See Appendix A)} \\
B_{r,j}^{(\chi)} &= \frac{1}{8\pi}\int_S J(\psi_j+\psi_{j-1}, \chi_j)\, Y_r^* \, ds \quad \text{(See Appendix A)} \\
D_r \psi_{r-\epsilon,j} - E_r \psi_{r+\epsilon,j} &= -\frac{1}{4\pi}\int_S \left[\nabla\cdot\nu\nabla\psi_j\right] Y_r^* \, ds \quad \text{(see Appendix B)}
\end{aligned}\right\} \qquad (7.12 \text{ cont.})$$

In addition, we want to determine the spectral form of (1.6) relating the vertical component of relative vorticity (ζ) and the streamfunction (ψ). It can be shown that

$$\zeta_{r,j} = -c_r \psi_{r,j} \qquad (7.13)$$

or

$$\psi_{r,j} = -\frac{\zeta_{r,j}}{c_r} \qquad (7.14)$$

provided that in (6.14) we stipulate $r \neq 0+i0$ (i.e., $c_r \neq 0$).

We see that the spectral relationships (7.9), (7.11), and (7.13) [or (7.14)] along with definitions (7.10) and (7.12) form a complete set of equations for solution. However, it is not convenient to attempt to integrate the model in this form as there is no explicit relationship determiming the vertical velocity field represented by W. In order to define W we must to alter the thermal wind relationship of (7.11). This development is contained in the next section. Furthermore, specification of the truncation limits to be used for series solutions (7.1) and (7.2) have not yet been established and will be discussed in a later section.

8. Determination of W in the dynamic equations

In order to obtain an explicit description of the vertical motion fields in our model atmosphere, we insert (7.14) into the thermal wind equation of (7.11) and differentiate w.r.t. time to get

$$\Delta z_j C_\gamma \frac{dT_{\gamma,j}}{dt} = \frac{D_\gamma}{C_{\gamma-\epsilon}}\left(\frac{dS_{\gamma-\epsilon,j-1}}{dt} - \frac{dS_{\gamma-\epsilon,j}}{dt}\right) - \\ - \frac{E_\gamma}{C_{\gamma+\epsilon}}\left(\frac{dS_{\gamma+\epsilon,j-1}}{dt} - \frac{dS_{\gamma+\epsilon,j}}{dt}\right) \tag{8.1}$$

for all levels j = 2, 3, ... , J - 1. We note that (8.1) does not apply for the case $\gamma = 0 + i0$. Furthermore, for notational purposes, we will stipulate that in (8.1) and all future relationships, terms which require $\gamma - \epsilon = 0 + i0$ or $n_{\gamma-\epsilon} < l_{\gamma-\epsilon}$ do not exist. This applies equally to cases in which $\gamma + \epsilon$ is not contained within the specified model truncation limits.

Let us now define

$$a_{\gamma,j} \equiv -i l_\gamma (\Psi_{\gamma,j-1} - \Psi_{\gamma,j}) - A_{\gamma,j-1} + A_{\gamma,j} + \\ - \left(\frac{1}{\Omega-1}\right) F_{\gamma,j-1} + \left(\frac{\Omega+1}{\Omega-1}\right) F_{\gamma,j} - \left(\frac{\Omega}{\Omega-1}\right) F_{\gamma,j+1}$$

$$b_{\gamma,j} \equiv -B_{\gamma,j} + \left[\frac{R}{c_p 8 \Omega^3 a^2}\right] g_{\gamma,j} \tag{8.2}$$

such that using (7.9) we can write

$$\frac{dS_{\gamma,j-1}}{dt} - \frac{dS_{\gamma,j}}{dt} = a_{\gamma,j} - \frac{1}{(\Omega-1)} \frac{D_\gamma}{C_{\gamma-\epsilon}} \left[W_{\gamma-\epsilon,j-1} - (\Omega+1) W_{\gamma-\epsilon,j} + \\ + \Omega W_{\gamma-\epsilon,j+1} \right] + \frac{1}{(\Omega-1)} \frac{E_\gamma}{C_{\gamma+\epsilon}} \left[W_{\gamma+\epsilon,j-1} - (\Omega+1) W_{\gamma+\epsilon,j} + \\ + \Omega W_{\gamma+\epsilon,j+1} \right] \tag{8.3}$$

and, the thermodynamic energy equation of (7.11) reduces to

$$\frac{dT_{\gamma,j}}{dt} = b_{\gamma,j} - S_j W_{\gamma,j} . \tag{8.4}$$

Inserting solutions (8.3) and (8.4) into (8.1) has the effect of eliminating the time dependence of (8.1) and at any given time we have

$$\Delta z_1 c_r b_{r,j} - \Delta z_1 c_r S_j W_{r,j} = \frac{D_r}{c_{r-\epsilon}} a_{r-\epsilon,j} - \frac{E_r}{c_{r+\epsilon}} a_{r+\epsilon,j} -$$
$$- \frac{1}{(\Omega-1)} \frac{D_{r-\epsilon} D_r}{c_{r-2\epsilon} c_{r-\epsilon}} \left[W_{r-2\epsilon,j-1} - (\Omega+1) W_{r-2\epsilon,j} + \Omega W_{r-2\epsilon,j+1} \right] +$$
$$+ \frac{1}{(\Omega-1)} \left(\frac{E_{r-\epsilon} D_r}{c_{r-\epsilon} c_r} + \frac{E_r D_{r+\epsilon}}{c_r c_{r+\epsilon}} \right) \left[W_{r,j-1} - (\Omega+1) W_{r,j} + \Omega W_{r,j+1} \right] -$$
$$- \frac{1}{(\Omega-1)} \frac{E_r E_{r+\epsilon}}{c_{r+\epsilon} c_{r+2\epsilon}} \left[W_{r+2\epsilon,j-1} - (\Omega+1) W_{r+2\epsilon,j} + \Omega W_{r+2\epsilon,j+1} \right]$$

or, if we define

$$\left. \begin{aligned} r_{r,j} &\equiv (\Omega-1) \left[\frac{D_r}{c_{r-\epsilon} c_r} a_{r-\epsilon,j} - \frac{E_r}{c_r c_{r+\epsilon}} a_{r+\epsilon,j} - \Delta z_1 b_{r,j} \right. \\ f_r^{(1)} &\equiv \frac{D_{r-\epsilon} D_r}{c_{r-2\epsilon} c_{r-\epsilon} c_r} \\ f_r^{(2)} &\equiv -\frac{1}{c_r^2} \left(\frac{E_{r-\epsilon} D_r}{c_{r-\epsilon}} + \frac{E_r D_{r+\epsilon}}{c_{r+\epsilon}} \right) \\ f_r^{(3)} &\equiv \frac{E_r E_{r+\epsilon}}{c_r c_{r+\epsilon} c_{r+2\epsilon}} \\ \sigma_j &\equiv (\Omega-1) \Delta z_1 S_j \end{aligned} \right\} , \quad (8.5)$$

the W-equation can be compacted to

$$\left[f_r^{(1)} W_{r-2\epsilon,j-1} + f_r^{(2)} W_{r,j-1} + f_r^{(3)} W_{r+2\epsilon,j-1} \right] -$$
$$- (\Omega+1) \left[f_r^{(1)} W_{r-2\epsilon,j} + f_r^{(2)} W_{r,j} + f_r^{(3)} W_{r+2\epsilon,j} \right] +$$
$$+ \Omega \left[f_r^{(1)} W_{r-2\epsilon,j+1} + f_r^{(2)} W_{r,j+1} + f_r^{(3)} W_{r+2\epsilon,j+1} \right] -$$
$$- \sigma_j W_{r,j} = r_{r,j} \quad (8.6)$$

in which from (1.17) we represent the boundary conditions as

$$\left.\begin{aligned} W_{\gamma,1} &= 0 \\ W_{\gamma,J} &= H_\gamma \\ H_\gamma &\equiv \frac{1}{4\pi}\int_S J(\psi_{J-1}, h/H_0)\, Y_\gamma^* \, dS \end{aligned}\right\} . \qquad (8.7)$$

In order to prepare (8.6) for inversion we want to take note of certain properties of the equations in order to reduce the calculation to a finite set of simple matrix solutions. Inspection of (8.6) shows that the equations uncouple according to planetary wave numbers, ℓ_γ . In addition, within each planetary wave the equations contain two independent sets; one of even vector elements ($n_\gamma + \ell_\gamma$ all even) and the other of odd vector elements ($n_\gamma + \ell_\gamma$ all odd). Thus, to facilitate ease of notation, let us define some new sets of indices to be applied to (8.6) by first denoting a maximum planetary wave number, L, for a given spectral truncation as

$$L = \ell_\gamma)_{max} \qquad (8.8)$$

so that we can designate K independent sets of matrix equations using index k where

$$k = 1, 2, 3, \ldots, K; \quad K = 2(L+1) . \qquad (8.9)$$

For a given matrix set we will determine k by designating

$$k = \begin{Bmatrix} 2\ell_\gamma + 1 & \text{for even vector sets} \\ 2(\ell_\gamma + 1) & \text{for odd vector sets} \end{Bmatrix} . \qquad (8.10)$$

Furthermore, within each of the K matrix equation sets it is useful to designate an element index, b_k, where

$$b_k = 1, 2, 3, \ldots, B_k \quad . \tag{8.11}$$

Thus, for a given matrix set designated by the subscript k we devise the b_k indices as follows:

1) For k odd (even vectors) let

$$N_k = n_k)_{max} \tag{8.12}$$

for which we consider only n_k from the set $n_k + \ell_k$ even. Then the value for an individual b_k is determined from

$$\left.\begin{aligned} b_k &= \frac{n_k + \ell_k + 2}{2} - \delta_{\ell_k,0} \\ B_k &= \frac{N_k + \ell_k + 2}{2} - \delta_{\ell_k,0} \end{aligned}\right\} \tag{8.13}$$

where we ingore values of b_k outside the range incicated in (7.11); i.e., when $k = 1$, $n_1 = 0$, and $\ell_1 = 0$ we do not include the value $b_1 = 0$ which designates the nonallowable equation of (7.1) in which $\gamma = 0 + i0$ [see comments following (8.1)].

Similarily,

2) For k even (odd vectors) let

$$N_k = n_k)_{max} \tag{8.14}$$

in which here we consider only n_k from the set $n_k + \ell_k$ odd. Then, we have

$$\left.\begin{aligned} b_k &= \frac{n_k - \ell_k + 1}{2} \\ B_k &= \frac{N_k - \ell_k + 1}{2} \end{aligned}\right\} \quad . \tag{8.15}$$

At this point we want to note an additional property inherent in the spectral W-equations represented by (8.6). That is, from definitions contained in (8.5) and Appendix B we can show that for any given k,

$$f_{b_k}^{(3)} = \frac{E_{\gamma_k} E_{\gamma_k+\epsilon}}{C_{\gamma_k} C_{\gamma_k+\epsilon} C_{\gamma_k+2\epsilon}}$$

$$\equiv \frac{D_{\gamma_k+\epsilon} D_{\gamma_k+2\epsilon}}{C_{\gamma_k} C_{\gamma_k+\epsilon} C_{\gamma_k+2\epsilon}} \equiv f_{b_k+1}^{(1)} . \qquad (8.16)$$

We are now prepared to convert (8.6) to matrix form. To do this we first define tridiagonal matrices $\mathcal{D}_k$ as

$$\mathcal{D}_k = \begin{pmatrix} f_1^{(2)} & f_1^{(3)} & 0 & \cdots & \cdots & \cdots & 0 \\ f_1^{(3)} & f_2^{(2)} & f_2^{(3)} & \ddots & & 0 & \vdots \\ 0 & \ddots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & & f_{b_k-1}^{(3)} & f_{b_k}^{(2)} & f_{b_k}^{(3)} & & \vdots \\ \vdots & 0 & & \ddots & \ddots & \ddots & \vdots \\ \vdots & & & & \ddots & \ddots & \vdots \\ 0 & \cdots & \cdots & \cdots & 0 & f_{B_k-1}^{(3)} & f_{B_k}^{(2)} \end{pmatrix}_k \qquad (8.17)$$

where we have made use of (8.8) - (8.16). We note from (8.17) that not only is each $\mathcal{D}_k$ <u>tridiagonal</u> but it is also symmetric. In addition, it can be shown that every principle minor determinate of $\mathcal{D}_k$ is <u>positive</u> and thus $\mathcal{D}_k$ can be said to be <u>positive definite</u>. These properties will be discussed in more detail below.

To complete the conversion of (8.6) to matrix form we define vectors

$$W_{k,j} = \begin{pmatrix} w_{1,j} \\ w_{2,j} \\ \vdots \\ w_{b_k,j} \\ \vdots \\ w_{B_k,j} \end{pmatrix}_k \quad ; \quad R_{k,j} = \begin{pmatrix} r_{1,j} \\ r_{2,j} \\ \vdots \\ r_{b_k,j} \\ \vdots \\ r_{B_k,j} \end{pmatrix}_k \tag{8.18}$$

such that (8.6) can be written in the matrix form

$$\left.\begin{aligned} &\mathcal{D}_k W_{k,j-1} - (r-1)\mathcal{D}_k W_{k,j} + \\ &+ r\mathcal{D}_k W_{k,j+1} - \sigma_j W_{k,j} = R_{k,j} \quad ; \\ &j = 2, 3, 4, \ldots, J-1 \text{ for each } k = 1, 2, 3, \ldots, K \end{aligned}\right\} . \tag{8.19}$$

We wish to modify (8.19) through diagonalization of each $\mathcal{D}_k$. However, since each tridiagonal $\mathcal{D}_k$ is real, symetric and positive definite we know that all eigenvalues of $\mathcal{D}_k$ are real and positive. Also, the sets of eigenvectors associated with these eigenvalues are orthonormal. Thus if $\mathcal{D}_k$ is of rank M, say, there exists a set of real positive eigenvalues $(\lambda_k)_p$ with p = 1, 2, 3, ... , M associated with $\mathcal{D}_k$ and M sets of orthonormal eigenvectors $q_{p,s}$ with s = 1, 2, 3, ... , M. If we let Q_k represent the matrix of eigenvectors associated with the set $(\lambda_k)p$ and matrix $\mathcal{D}_k$, we have

$$Q_k = \begin{pmatrix} q_{11} & q_{12} & \cdots & q_{1s} & \cdots & q_{1M} \\ q_{21} & q_{22} & \cdots & q_{2s} & \cdots & q_{2M} \\ \vdots & & & & & \\ q_{p1} & q_{p2} & \cdots & q_{ps} & \cdots & q_{pM} \\ \vdots & & & & & \\ q_{M1} & q_{M2} & \cdots & q_{Ms} & \cdots & q_{MM} \end{pmatrix}_k \tag{8.20}$$

such that

$$Q_k \tilde{Q}_k = \tilde{Q}_k Q_k = I \tag{8.21}$$

where I is the unit matrix and $\tilde{(\ )}$ denotes transposition. Define

$$\Lambda_k = \begin{pmatrix} (\lambda_k)_1 & 0 & \cdots & & 0 \\ 0 & (\lambda_k)_2 & & 0 & \vdots \\ \vdots & & \ddots & & \vdots \\ \vdots & & (\lambda_k)_p & & \vdots \\ & 0 & & \ddots & 0 \\ 0 & \cdots & & 0 & (\lambda_k)_M \end{pmatrix} \tag{8.22}$$

where then we know

$$\left.\begin{aligned} & \mathcal{D}_k Q_k = Q_k \Lambda_k \\ \text{and} \quad & \tilde{Q}_k \mathcal{D}_k Q_k = \tilde{Q}_k Q_k \Lambda_k = \Lambda_k \end{aligned}\right\} \tag{8.23}$$

We now want to expand the vector $W_{k,j}$ in (8.19) in the form

$$W_{k,j} = Q_k V_{k,j} \,, \quad V_{k,j} = \tilde{Q}_k W_{k,j} \tag{8.24}$$

where we note that $V_{k,j}$ is also a vector.

Inserting solutions (8.24) into (8.19) and multiplying through with $\tilde{Q}_k$ gives

$$\tilde{Q}_k \mathcal{D}_k Q_k V_{k,j-1} - (r+1) \tilde{Q}_k \mathcal{D}_k Q_k V_{k,j} + \\ + r \tilde{Q}_k \mathcal{D}_k Q_k V_{k,j+1} - \sigma_j \tilde{Q}_k Q_k V_{k,j} = \tilde{Q}_k R_{k,j}$$

or, from (8.23), we can write

$$\Lambda_k V_{k,j-1} - \left[(r+1)\Lambda_k + \sigma_j\right] V_{k,j} + r\Lambda_k V_{k,j+1} = \tilde{Q}_k R_{k,j} \quad . \tag{8.25}$$

Now, we know that there exists an inverse

$$\Lambda_k^{-1} = \begin{pmatrix} 1/(\lambda_k)_1 & 0 & \cdots & \cdots & 0 \\ 0 & 1/(\lambda_k)_2 & & 0 & \vdots \\ \vdots & & \ddots \; 1/(\lambda_k)_p & & \vdots \\ \vdots & 0 & & \ddots & 0 \\ 0 & \cdots & \cdots & 0 & 1/(\lambda_k)_m \end{pmatrix} \tag{8.26}$$

such that

$$\Lambda_k^{-1}\Lambda_k = I \quad . \tag{8.27}$$

Thus, if we multiply (8.25) through with Λ_k^{-1}, (8.25) reduces to the form

$$V_{k,j-1} - \left[(r+1)I + \sigma_j\Lambda_k^{-1}\right] V_{k,j} + rV_{k,j+1} = \Lambda_k^{-1}\tilde{Q}_k R_{k,j} \tag{8.28}$$

where for each k = 1, 2, 3, ... , K we have j = 2, 3, 4, ... , J - 1.

We now let

$$\left.\begin{aligned} &\mathcal{S}_{k,j} \equiv -\left[(r+1)I + \sigma_j\Lambda_k^{-1}\right] \\ &\text{and} \\ &\mathcal{R}_{k,j} \equiv \begin{cases} \Lambda_k^{-1}\tilde{Q}_k R_{k,2} - V_{k,1} & (\text{for } j=2) \\ \Lambda_k^{-1}\tilde{Q}_k R_{k,j} & (\text{for } 3 \le j \le J-2) \\ \Lambda_k^{-1}\tilde{Q}_k R_{k,J-1} - rV_{k,J} & (\text{for } j=J-1) \end{cases} \end{aligned}\right\} . \tag{8.29}$$

Using (8.29), (8.28) transforms to the set

$$\left.\begin{aligned} \mathcal{S}_{k,2}V_{k,2} + \Omega V_{k,3} &= R_{k,2} \ (\text{for } j=2) \\ V_{k,j-1} + \mathcal{S}_{k,j}V_{k,j} + \Omega V_{k,j+1} &= R_{k,j} \ (3 \le j \le J-2) \\ V_{k,J-2} + \mathcal{S}_{k,J-1}V_{k,J-1} &= R_{k,J-1} \ (\text{for } j=J-1) \end{aligned}\right\} \quad (8.30)$$

in which from (8.24) and the boundary conditions of (8.7) we see that in (8.29)

$$\left.\begin{aligned} V_{k,1} &= 0 \\ V_{k,J} &= \tilde{Q}_k W_{k,J} \equiv \tilde{Q}_k H_k \end{aligned}\right\} . \quad (8.31)$$

We see that for each k the system (8.30) is tridiagonal in j and thus submits readily to solution provided certain provisions are met (see Appendix C for details). Briefly, to invert (8.30) we first define

$$\left.\begin{aligned} u_{k,2} &\equiv \mathcal{S}_{k,2}^{-1} \quad (\text{for } j=2) \\ u_{k,j} &\equiv \left(\mathcal{S}_{k,j} - \Omega u_{k,j-1}\right)^{-1} \ (\text{for } 3 \le j \le J-1) \\ v_{k,j} &\equiv -\Omega u_{k,j} \quad (2 \le j \le J-1) \end{aligned}\right\} \quad (8.32)$$

and then let

$$\left.\begin{aligned} y_{k,2} &= u_{k,2} R_{k,2} \quad (\text{for } j=2) \\ y_{k,j} &= u_{k,j}\left(R_{k,j} - y_{k,j-1}\right) \ (\text{for } 3 \le j \le J-1) \end{aligned}\right\} . \quad (8.33)$$

Solutions to (8.30) thus appear as

$$\left.\begin{array}{l} V_{k,J-1} = y_{k,J-1} \quad (\text{for } j = J-1) \\ V_{k,j} = v_{k,j} V_{k,j+1} + y_{k,j} \\ \qquad (\text{for } j = J-2, J-3, \cdots, 2) \end{array}\right\} \tag{8.34}$$

provided all $u_{k,j}$ in (8.23) exist and are finite. Vectors $W_{k,j}$ are then obtained from (8.24).

9. Energetics

The kinetic energy per unit mass, K_j, at any given atmospheric level j is given in terms of nondimensional quantities in (3.1), as

$$K_j = \frac{1}{2}\mathbb{V}_j\cdot\mathbb{V}_j = \frac{1}{2}\nabla\psi_j\circ\nabla\psi_j \tag{9.1}$$

Similarly, the available potential energy can be written as

$$A_j = \frac{1}{2S_j}\left(T_j - \overline{T}_j\right)^2 \tag{9.2}$$

in which we assume here that $\overline{T}_j$ has been nondimensionalized in the same manner as T_j. The local time rate of change of the quantities K_j and A_j in (9.1) and (9.2) become

$$\left.\begin{aligned} \frac{\partial K_j}{\partial t} &= \frac{1}{2}\nabla\frac{\partial\psi_j}{\partial t}\cdot\nabla\psi_j + \frac{1}{2}\nabla\psi_j\cdot\nabla\frac{\partial\psi_j}{\partial t} \\ &= \nabla\cdot\psi_j\frac{\partial\psi_j}{\partial t} - \psi_j\frac{\partial S_j}{\partial t} \\ \frac{\partial A_j}{\partial t} &= \frac{1}{S_j}\left(T_j - \overline{T}_j\right)\frac{\partial T_j}{\partial t} \end{aligned}\right\} \tag{9.3}$$

for hwich we have utilized (3.6). We also want to define horizontal mean values for (9.1) - (9.3) on the unit sphere as

$$\left.\begin{aligned} \overline{K}_j &= \frac{1}{4\pi}\int_S K_j\,ds \\ &= \frac{1}{8\pi}\int_S \cancelto{0}{\nabla\cdot\psi_j\nabla\psi_j}\,ds - \frac{1}{8\pi}\int_S \psi_j S_j\,ds \\ \overline{A}_j &= \frac{1}{4\pi}\int_S A_j\,ds = \frac{1}{8\pi S_j}\int_S \left(T_j - \overline{T}_j\right)^2 ds \end{aligned}\right\}. \tag{9.4}$$

$$\left.\begin{aligned}
\dot{\overline{K}}_j &= \frac{1}{4\pi}\int_S \frac{\partial K_j}{\partial t}\,ds \\
&= \frac{1}{4\pi}\int_S \cancelto{0}{\nabla\cdot\psi_j\nabla\frac{\partial\psi_j}{\partial t}}\,ds - \frac{1}{4\pi}\int_S \psi_j\frac{\partial S_j}{\partial t}\,ds \\
\dot{\overline{A}}_j &= \frac{1}{4\pi}\int_S \frac{\partial A_j}{\partial t}\,ds \\
&= \frac{1}{4\pi S_j}\int_S (T_j-\overline{T}_j)\frac{\partial T_j}{\partial t}\,ds
\end{aligned}\right\} \quad (9.4\text{ cont.})$$

Finally, integrating vertically, the total values for each of the energy types are defined

$$\left.\begin{aligned}
K &= \sum_{j=1}^{J-1}(r-1)P_j\overline{K}_j = -\frac{1}{8\pi}\sum_{j=1}^{J-1}(r-1)P_j\int_S \psi_j S_j\,ds \\
A &= \sum_{j=2}^{J-1}\Delta z_j P_j\overline{A}_j = \frac{1}{8\pi}\sum_{j=2}^{J-1}\Delta z_j\frac{P_j}{S_j}\int_S (T_j-\overline{T}_j)^2\,ds \\
\dot{K} &= \sum_{j=1}^{J-1}(r-1)P_j\dot{\overline{K}}_j = -\frac{1}{4\pi}\sum_{j=1}^{J-1}(r-1)P_j\int_S \psi_j\frac{\partial S_j}{\partial t}\,ds \\
\mathring{A} &= \sum_{j=2}^{J-1}\Delta z_j P_j\dot{\overline{A}}_j = \frac{1}{4\pi}\sum_{j=2}^{J-1}\Delta z_j\frac{P_j}{S_j}\int_S (T_j-\overline{T}_j)\frac{\partial T_j}{\partial t}\,ds
\end{aligned}\right\}. \quad (9.5)$$

In order to demonstrate the energy conversion properties of our model we consider only the time rate of change equations of (9.4) and (9.5). Substituting from the vorticity prediction equation (3.9) into the third equation of (9.4) we have

$$\dot{K}_j = \frac{1}{4\pi}\int_S \psi_j \cancelto{0}{J(\psi_j, S_j + \mu)}\, ds \; +$$

$$+\frac{1}{4\pi}\int_S \psi_j \nabla\cdot\left\{\mu\nabla\mathcal{L}\left[\left(\frac{\Omega}{\Omega-1}\right)W_{j+1} - \left(\frac{1}{\Omega-1}\right)W_j\right]\right\} ds$$

$$-\frac{1}{4\pi}\left(\frac{\Omega}{\Omega-1}\right)\int_S \psi_j F_{j+1}\, ds + \frac{1}{4\pi}\left(\frac{1}{\Omega-1}\right)\int_S \psi_j F_j\, ds$$

$$= \frac{1}{4\pi}\int_S \mathcal{L}\left[\left(\frac{\Omega}{\Omega-1}\right)W_{j+1} - \left(\frac{1}{\Omega-1}\right)W_j\right]\nabla\cdot\mu\nabla\psi_j\, ds -$$

$$-\frac{1}{4\pi}\left(\frac{\Omega}{\Omega-1}\right)\int_S \psi_j F_{j+1}\, ds + \frac{1}{4\pi}\left(\frac{1}{\Omega-1}\right)\int_S \psi_j F_j\, ds \,. \qquad (9.6)$$

Similarly, substitution of the thermal equation (3.19) into the fourth of (9.4) gives

$$\dot{A}_j = -\frac{1}{8\pi S_j}\int_S (T_j - \bar{T}_j)\cancelto{0}{J(\psi_j + \psi_{j-1}, T_j)}\, ds -$$

$$-\frac{1}{4\pi}\int_S (T_j - \bar{T}_j) W_j\, ds + \frac{1}{4\pi S_j}\left(\frac{R}{c_p 8\Omega^3 a^2}\right)\int_S (T_j - \bar{T}_j) q_j\, ds \,. \qquad (9.7)$$

Then, using (9.6) and (9.7) in the third and fourth equations of (9.5), we have for the total time rate of change of kinetic and available potential energies,

$$\dot{K} = \frac{1}{4\pi}\sum_{j=1}^{J-1} P_j \int_S \mathcal{L}\left[\Omega W_{j+1} - W_j\right]\nabla\cdot\mu\nabla\psi_j\, ds -$$

$$-\frac{1}{4\pi}\sum_{j=1}^{J-1} P_j\, \Omega \int_S \psi_j F_{j+1}\, ds + \frac{1}{4\pi}\sum_{j=1}^{J-1} P_j \int_S \psi_j F_j\, ds$$

$$\dot{K} = -\frac{1}{4\pi} P_1 \int_S \cancelto{0}{W_1 \nabla\cdot\nu\nabla\psi_1}\, ds + \frac{1}{4\pi}\sum_{j=2}^{J-1} P_j \int_S \ell W_j\, \nabla\cdot\nu\nabla(\psi_{j-1}-\psi_j)\, ds +$$

$$+\frac{1}{4\pi} P_J \int_S W_J \nabla\cdot\nu\nabla\psi_{J-1}\, ds - \frac{1}{4\pi}\sum_{j=1}^{J-1} P_j \int_S \psi_j (rF_{j+1}-F_j)\, ds .$$

But, from (3.18) we know that for j = 2, 3, 4,..., J-1,

$$\nabla\cdot\nu\nabla(\psi_j-\psi_{j-1}) = -\Delta Z_1 \nabla^2 T_j$$

and thus

$$\dot{K} = \frac{1}{4\pi}\sum_{j=2}^{J-1} P_j \int_S \ell W_j \Delta Z_1 \nabla^2 T_j\, ds + \frac{1}{4\pi} P_J \int_S W_J \nabla\cdot\nu\nabla\psi_{J-1}\, ds$$

$$-\frac{1}{4\pi}\sum^{J-1} P_j \int_S \psi_j (rF_{j+1}-F_j)\, ds$$

$$= \frac{\Delta Z_1}{4\pi}\sum_{j=2}^{J-1} P_j \int_S W_j T_j\, ds + \frac{1}{4\pi} P_J \int_S W_J \nabla\cdot\nu\nabla\psi_{J-1}\, ds$$

$$-\frac{1}{4\pi}\sum_{j=1}^{J-1} P_j \int_S \psi_j (rF_{j+1}-F_j)\, ds \qquad (9.8)$$

and,

$$\dot{A} = -\frac{\Delta Z_1}{4\pi}\sum_{j=2}^{J-1} P_j \int_S (T_j-\overline{T}_j) W_j\, ds +$$

$$+\frac{\Delta Z_1}{4\pi}\left(\frac{R}{C_p\delta\Omega^3a^2}\right)\sum_{j=2}^{J-1}\frac{P_j}{S_j}\int_S (T_j-\overline{T}_j) q_j\, ds$$

$$= -\frac{\Delta Z}{4\pi}\sum_{j=2}^{J-1} P_j \int_S T_j W_j\, ds +$$

$$+\frac{\Delta Z_1}{4\pi}\left(\frac{R}{C_p 8\Omega^3a^2}\right)\sum_{j=2}^{J-1}\frac{P_j}{S_j}\int_S (T-\overline{T}_j) q_j\, ds \quad . \qquad (9.9)$$

We see that in (9.8) and (9.9), the terms involving $W_j T_j$ represent conversions between kinetic and available potential energies. Addition of these two equations yields the correct relationship for the time rate of change of total energy, E,

$$
\begin{aligned}
\mathring{E} &= \mathring{K} + \dot{A} \\
&= \frac{1}{4\pi} P_J \int_S W_J \nabla \cdot \mu \nabla \Psi_{J-1} \, ds - \\
&\quad - \frac{1}{4\pi} \sum_{j=1}^{J-1} P_j \int_S \Psi_j (r F_{j+1} - F_j) \, ds + \\
&\quad + \frac{\Delta z_1}{4\pi} \left(\frac{R}{c_p 8 \Omega^3 a^2} \right) \sum_{j=2}^{J-1} \frac{P_j}{\sigma_j} \int_S (T_j - \overline{T}_j) q_j \, ds \qquad (9.10)
\end{aligned}
$$

in which the first term on the right side of (9.10) represents energy changes at the bottom level due to orography, and the other two terms are respectively the disappation of kinetic energy due to frictional stress and the generation of available potential energy due to diabatic heating.

Appendix A. Spectral form of Jacobian terms and evaluation of the associated nonlinear interaction coefficients.

Consider on the unit sphere the Jacobian of arbitrary horizontal global scales A and B where

$$J(A,B)=\frac{\partial A}{\partial \lambda}\frac{\partial B}{\partial \mu}-\frac{\partial A}{\partial \mu}\frac{\partial B}{\partial \lambda} \tag{A.1}$$

and λ is longitude while μ is the sine of latitude. Expanding A and B in terms of spherical harmonics, we have for solutions

$$\left.\begin{aligned} A &= \sum_{\alpha} a_\alpha Y_\alpha(\lambda,\mu), \\ B &= \sum_{\alpha} b_\alpha Y_\alpha(\lambda,\mu), \\ \alpha &= n_\alpha + i\,l_\alpha \end{aligned}\right\} \tag{A.2}$$

in which the special properties of the orthonormal spherical functions $Y_\alpha(\lambda,\mu)$ are outlined in (7.3) - (7.8). Inserting solutions (A.2) into (A.1), transforming the result to insure symmetry with respect to vector indices α and β, and writing in terms of a single nonredundant sum (for details of these developments, see Baer and Platzman, 1961) we arrive at

$$J(A,B)=-i\sum_{\substack{\alpha,\beta\\ n_\beta\geq n_\alpha}}\left(1-\frac{E_{\alpha,\beta}}{2}\right)\left(a_\alpha b_\beta-a_\beta b_\alpha\right)\times \\ \times e^{i(l_\alpha+l_\beta)\lambda}\left(l_\beta P_\beta\frac{dP_\alpha}{d\mu}-l_\alpha P_\alpha\frac{dP_\beta}{d\mu}\right) \tag{A.3}$$

for which we define through use of the Kronecker delta, $\delta_{i,j}$,

$$E_{\alpha,\beta}\equiv\delta_{n_\alpha,n_\beta}\,\delta_{|l_\alpha|,|l_\beta|}\ . \tag{A.4}$$

The term $\left(1-\frac{E_{\alpha,\beta}}{2}\right)$ is necessary because the two conjugate interactions for the case $n_\beta = n_\alpha$ and $|\ell_\beta| = |\ell_\alpha|$, assumed in the symmetric reduction of J(A,B) to the form of (A.3), are not unique and one of them must be ignored.

We now multiply (A.3) through with any arbitrary member of the orthogonalizing set, say $Y_\gamma^*/4\pi$, and integrate over the unit sphere to get

$$G_\gamma = \frac{1}{4\pi}\int_0^{2\pi}\int_{-1}^{1} J(A,B)\,Y_\gamma^*(\lambda,\mu)\,d\mu\,d\lambda$$

$$= -i \sum_{\substack{\alpha,\beta \\ \left\{ n_\beta \geq n_\alpha \atop \ell_\gamma = \ell_\alpha + \ell_\beta \right\}}} \left(1-\frac{E_{\alpha,\beta}}{2}\right)(a_\alpha b_\beta - a_\beta b_\alpha)\,K_{\gamma,\beta,\alpha} \tag{A.5}$$

and the interaction coefficient, $K_{\gamma,\beta,\alpha}$ is obtained from

$$K_{\gamma,\beta,\alpha} \equiv \frac{1}{2}\int_{-1}^{1}\left(\ell_\beta P_\beta \frac{dP_\alpha}{d\mu} - \ell_\alpha P_\alpha \frac{dP_\beta}{d\mu}\right) P_\gamma\, d\mu\,. \tag{A.6}$$

Since we intend to evaluate $K_{\gamma,\beta,\alpha}$ using the "transform" method with integration by exact Gaussian quadrature (see, for example, Eliasen et al., 1970), a time saving simplification can be obtained by noting that the integral in (A.6) can be nonzero only if the integrand possesses an even parity with respect to the equator. For this condition we can reduce (A.6) to

$$K_{\gamma,\beta,\alpha} = \int_0^1 \left(\ell_\beta P_\beta \frac{dP_\alpha}{d\mu} - \ell_\alpha P_\alpha \frac{dP_\beta}{d\mu}\right) P_\gamma\, d\mu\,. \tag{A.7}$$

In order to evaluate (A.7) numerically let us define

$$\left.\begin{aligned} f_\alpha(\mu) &\equiv l_\alpha P_\alpha(\mu) \\ g_\alpha(\mu) &\equiv \frac{dP_\alpha(\mu)}{d\mu} \end{aligned}\right\} \tag{A.8}$$

where g_α can be determined from the Legendre differential relationships in the form

$$\left.\begin{aligned} g_\alpha(\mu) &\equiv \frac{dP_\alpha(\mu)}{d\mu} \\ &= \frac{(n_\alpha+1)\mu P_\alpha}{(1-\mu^2)} - \frac{(2n_\alpha+1)}{(1-\mu^2)}\left[\frac{(n_\alpha+l_\alpha+1)(n_\alpha-l_\alpha+1)}{(2n_\alpha+1)(2n_\alpha+3)}\right]^{1/2} P_{\alpha+\epsilon}, \\ \epsilon &\equiv 1 + i0 \end{aligned}\right\} . \tag{A.9}$$

we now let

$$\begin{aligned} H_{\beta,\alpha}(\mu) &= l_\beta P_\beta \frac{dP_\alpha}{d\mu} - l_\alpha P_\alpha \frac{dP_\beta}{d\mu} \\ &= f_\beta g_\alpha - f_\alpha g_\beta \end{aligned} \tag{A.10}$$

which can be expanded in the form

$$H_{\beta,\alpha}(\mu) = \sum_\delta h_{\delta,\beta,\alpha} P_\delta(\mu) . \tag{A.11}$$

from (A.10) and (A.11) we see that (A.7) can be replaced with

$$\left.\begin{aligned} K_{\gamma,\beta,\alpha} &= \int_0^1 \left[H_{\beta,\alpha}(\mu)\right] P_\gamma \, d\mu \\ &= \sum_\delta h_{\delta,\beta,\alpha} \int_0^1 P_\delta P_\gamma \, d\mu \\ &= h_{\gamma,\beta,\alpha} \end{aligned}\right\} . \tag{A.12}$$

However, if we represent $H_{\beta,\alpha}(\mu)$ at N discrete points μ_k where k = 1, 2,....,N, then an exact quadrature analog for (A.12) is obtained in the form (see Eliasen et al., 1970)

$$K_{\gamma,\beta,\alpha} = \sum_{k=1}^{N} W_k \left[H_{\beta,\alpha}(\mu_k)\right] P_\gamma(\mu_k)$$

$$= \sum_{k=1}^{N} W_k \left[f_\beta(\mu_k) g_\alpha(\mu_k) - f_\alpha(\mu_k) g_\beta(\mu_k)\right] P_\gamma(\mu_k) \qquad \text{(A.13)}$$

provided

$$\left.\begin{aligned} &N = (K+1)/2 \\ &K \geq l_{max} + \frac{3}{2}(n_{max} - l_{max}) + \frac{1}{2} \end{aligned}\right\} \qquad \text{(A.14)}$$

(N and K must be intergers) and the latitudes μ_k are located at the Northern Hemisphere zeroes of the Legendre polynomial $P_k^0(\mu)$ (including the equator if K is odd). In (A.13) the W_k represent the Gaussian weights required to maintain orthogonalization of the discrete set of Legendre polynomials used in (A.13) such that

$$\sum_{k=1}^{N} W_k P_\alpha(\mu_k) P_\beta(\mu_k) = \delta_{\alpha,\beta} \,. \qquad \text{(A.15)}$$

A discussion of the evaluation of these Gaussian weights is contained in Appendix D.

References

Baer, R., and G.W. Platzman, 1961: A procedure for numerical integration of the spectral vorticity equation. J. Meteor., 18, 393-401.

Eliasen, E., B. Mackenhauer and E. Rasmussen, 1970: On a numerical method for integration of the hydrodynamical equations with a spectral representation of the horizontal fields. Report No. 2, Institut for Teoretisk Meteorologi, Kobenhavns Universitet, 37 pp.

Appendix B. Spectral representation of divergence terms of the general form $\nabla\cdot\mu\nabla A$.

In terms of spherical operators on the unit sphere in which λ is longitude and μ is the sine of latitude we have

$$\begin{aligned}\nabla\cdot\mu\nabla A &= \nabla\mu\cdot\nabla A + \mu\nabla^2 A\\ &= (1-\mu^2)\frac{\partial A}{\partial\mu} + \mu\nabla^2 A\end{aligned} \tag{B.1}$$

in which A is an arbitrary horizontal global scaler expandable in the form

$$A = \sum_\alpha a_\alpha Y_\alpha(\lambda,\mu) \quad . \tag{B.2}$$

Properties of the orthonormal spherical functions $Y_\alpha(\lambda,\mu)$ are outlined in (7.3) - (7.8). Insertion of solutions (B.2) into (B.1) yields

$$\left.\begin{aligned}\nabla\cdot\mu\nabla A &= (1-\mu^2)\sum_\alpha a_\alpha e^{il_\alpha\lambda}\frac{dP_\alpha(\mu)}{d\mu} - \mu\sum_\alpha c_\alpha a_\alpha e^{il_\alpha\lambda}P_\alpha(\mu)\\ &= \sum_\alpha a_\alpha e^{il_\alpha\lambda}\left[(1-\mu^2)\frac{dP_\alpha}{d\mu} - \mu c_\alpha P_\alpha\right],\\ c_\alpha &= n_\alpha(n_\alpha+1)\end{aligned}\right\} . \tag{B.3}$$

But, if we define

$$\left.\begin{aligned}N_\alpha &= \left[\frac{(2n_\alpha+1)\,(n_\alpha-l_\alpha)!}{(n_\alpha+l_\alpha)!}\right]^{1/2}\\ \epsilon &= 1+i\,0\end{aligned}\right\} \tag{B.4}$$

then we know from the Legendre differential and recurrence relations (for example, see Jahnke and Emde, 1945) that

$$(1-\nu^2)\frac{dP_\alpha}{d\nu} = -n_\alpha \nu P_\alpha + (n_\alpha + l_\alpha)\frac{N_\alpha}{N_{\alpha-\epsilon}} P_{\alpha-\epsilon}$$

and

$$\nu P_\alpha = \frac{(n_\alpha - l_\alpha + 1)}{(2n_\alpha+1)}\frac{N_\alpha}{N_{\alpha+\epsilon}} P_{\alpha+\epsilon} + \frac{(n_\alpha + l_\alpha)}{(2n_\alpha+1)}\frac{N_\alpha}{N_{\alpha-\epsilon}} P_{\alpha-\epsilon} \qquad \text{(B.5)}$$

Then, using (B.5), we can show that

$$(1-\nu^2)\frac{dP_\alpha}{d\nu} - \nu C_\alpha P_\alpha = \frac{(1-n_\alpha^2)(n_\alpha+l_\alpha)}{(2n_\alpha+1)}\frac{N_\alpha}{N_{\alpha-\epsilon}} P_{\alpha-\epsilon} - \frac{n_\alpha(n_\alpha+2)(n_\alpha-l_\alpha+1)}{(2n_\alpha+1)}\frac{N_\alpha}{N_{\alpha+\epsilon}} P_{\alpha+\epsilon}\,. \qquad \text{(B.6)}$$

We now insert (B.6) into (B.3), multiply through using $Y_\gamma^*/4\pi$, and integrate over the unit sphere to get

$$\frac{1}{4\pi}\int_0^{2\pi}\int_{-1}^{1}(\nabla\cdot\nu\nabla A)Y_\gamma^*\,d\nu\,d\lambda =$$

$$= \sum_{\substack{\alpha \\ l_\alpha = l_\gamma}} a_\alpha\left[\frac{(1-n_\alpha^2)(n_\alpha+l_\alpha)}{(2n_\alpha+1)}\frac{N_\alpha}{N_{\alpha-\epsilon}}\right]\frac{1}{2}\int_{-1}^{1} P_{\alpha-\epsilon}P_\gamma\,d\nu -$$

$$- \sum_{\substack{\alpha \\ l_\alpha = l_\gamma}} a_\alpha\left[\frac{n_\alpha(n_\alpha+2)(n_\alpha-l_\alpha+1)}{(2n_\alpha+1)}\frac{N_\alpha}{N_{\alpha+1}}\right]\frac{1}{2}\int_{-1}^{1} P_{\alpha+\epsilon}P_\gamma\,d\nu$$

$$= (1-n_\gamma^2)\left[\frac{(n_\gamma+l_\gamma)(n_\gamma-l_\gamma)}{(2n_\gamma-1)(2n_\gamma+1)}\right]^{1/2} a_{\gamma-\epsilon} -$$

$$- n_\gamma(n_\gamma+2)\left[\frac{(n_\gamma+l_\gamma+1)(n_\gamma-l_\gamma+1)}{(2n_\gamma+1)(2n_\gamma+3)}\right] a_{\gamma+\epsilon}$$

$$= D_\gamma a_{\gamma-\epsilon} - E_\gamma a_{\gamma+\epsilon} \qquad \text{(B.7)}$$

where we have defined

$$\left.\begin{aligned} D_\gamma &\equiv (1-n_\gamma^2)\left[\frac{(n_\gamma+l_\gamma)(n_\gamma-l_\gamma)}{(2n_\gamma-1)(2n_\gamma+1)}\right]^{1/2} \\ E_\gamma &\equiv n_\gamma(n_\gamma+2)\left[\frac{(n_\gamma+l_\gamma+1)(n_\gamma-l_\gamma+1)}{(2n_\gamma+1)(2n_\gamma+3)}\right]^{1/2} \end{aligned}\right\} . \qquad (B.8)$$

A special case of (B.7) occurs when we consider scaler B in which

$$B = \nabla^2 A \qquad (B.9)$$

where similar to (B.2) we can expand B in the form

$$B = \sum_\alpha b_\alpha Y_\alpha(\lambda,\mu) \ . \qquad (B.10)$$

Then, from (7.6), we know that

$$b_\alpha = -c_\alpha a_\alpha \qquad (B.11)$$

and, in terms of coefficients b_α, (B.7) becomes

$$\begin{aligned} \frac{1}{4\pi}\int_0^{2\pi}\int_{-1}^{1}(\nabla\cdot\mu\nabla A)Y_\gamma^* d\mu\, d\lambda &= -\frac{D_\gamma}{c_{\gamma-\epsilon}} b_{\gamma-\epsilon} + \frac{E_\gamma}{c_{\gamma+\epsilon}} b_{\gamma+\epsilon} \\ &= \mathcal{D}_\gamma b_{\gamma-\epsilon} - \mathcal{E}_\gamma b_{\gamma+\epsilon} \end{aligned} \qquad (B.12)$$

in which we have defined

$$\mathcal{D}_\gamma = -\frac{D_\gamma}{c_{\gamma-\epsilon}} \ , \quad \mathcal{E}_\gamma = -\frac{E_\gamma}{c_{\gamma+\epsilon}} \qquad (B.13)$$

provided that in (B.12) we ignore terms in which $c_{\gamma-\epsilon}=0$ (ie, $n_{\gamma-\epsilon}=0$). Further, for both (B.7) and (B.13) we must stipulate that all terms calling for any $a_{\gamma-\epsilon}$, $a_{\gamma+\epsilon}$, $b_{\gamma-\epsilon}$ or $b_{\gamma+\epsilon}$ outside the r~~e~~ange of the particular spectral truncation chosen must also be ignored.

Reference

Jahnke, E. and F. Emde, 1945: Tables of Functions. Dover, New York, 306 pp. plus tables.

Appendix C. Solution of a tridiagonal set of equations.

Suppose we have an equation set of the form

$$\left.\begin{aligned} a_\gamma X_{\gamma-1} + b_\gamma X_\gamma + c_\gamma X_{\gamma+1} &= R_\gamma \\ \gamma = 1, 2, 3, \cdots, \Gamma & \end{aligned}\right\} \tag{C.1}$$

where we must have

$$\left.\begin{aligned} a_1 &= 0 \\ c_\Gamma &= 0 \end{aligned}\right\} . \tag{C.2}$$

That is, in matrix form we can write (C.1) as

$$A X = R \tag{C.3}$$

with A being tridiagonal of the form

$$A = \begin{pmatrix} b_1 & c_1 & 0 & \cdots & \cdots & 0 \\ a_2 & b_2 & c_2 & & & \vdots \\ \vdots & \ddots & \ddots & \ddots & & \vdots \\ 0 & & a_r & b_r & c_r & \vdots \\ \vdots & & & \ddots & \ddots & \ddots \\ 0 & \cdots & \cdots & 0 & a_\Gamma & b_\Gamma \end{pmatrix} . \tag{C.4}$$

For solutions we define

$$\left.\begin{aligned} G_1 &= 1/b_1 \\ G_r &= 1/(b_r - a_r c_{r-1} G_{r-1}) ; \quad 2 \le r \le \Gamma \\ D_r &= -c_r G_r \end{aligned}\right\} \tag{C.5}$$

and let

$$\left.\begin{aligned} B_1 &= G_1 R_1 \\ B_r &= G_r (R_r - a_r B_{r-1}) ; \\ & \qquad 2 \le r \le \Gamma \end{aligned}\right\} . \tag{C.6}$$

Then, the solutions appear as

$$\left.\begin{aligned} X_\Gamma &= B_\Gamma \\ X_\gamma &= D_\gamma X_{\gamma+1} + B_\gamma\,; \\ &\qquad \gamma = \Gamma-1, \Gamma-2, \ldots, 1 \end{aligned}\right\} \qquad \text{(C.7)}$$

provided all G_γ in (C.5) are finite. That is, if

$$\left.\begin{aligned} b_1 &\neq 0 \\ b_\gamma &\neq a_\gamma c_{\gamma-1} G_{\gamma-1} \end{aligned}\right\} . \qquad \text{(C.8)}$$

Appendix D. Computation of the weight functions for Gauseian quadrature.

We consider the set of complete orthogonal Legendre polynomials; $P_n^l(\mu)$, in which $l = 0, \pm1, \pm2, \cdots$ and $n = 0, 1, 2, \cdots$. We define this set, according to (7.8), to be normalized such that

$$\int_{-1}^{1} P_n^l(\mu)\, P_{n'}^l(\mu)\, d\mu = 2\,\delta_{n,n'} \tag{D.1}$$

where μ is the sine of latitude or equivalently, the cosine of colatitude, ϕ. Now in order to expand an arbitrary functin of latitude, say $f(\mu)$, in terms of the set of Legendre polynomials we let

$$f(\mu) = \sum_l \sum_n f_n^l P_n^l(\mu) \tag{D.2}$$

from which the coefficients, f_n^l, are obtained through application of (D.1) such that

$$\begin{aligned} f_n^l &= \frac{1}{2} \sum_l \sum_n f_{n'}^l \int_{-1}^{1} P_{n'}^l(\mu)\, P_n^l(\mu)\, d\mu \\ &= \frac{1}{2} \int_{-1}^{1} f(\mu)\, P_n^l(\mu)\, d\mu \quad . \end{aligned} \tag{D.3}$$

However, to be able to transform at will between spectral and grid point space, it is necessary to represent $f(\mu)$ at a number of discrete points, μ_k, in which k = 1, 2, 3,..., N with N being the total number of points lying within $-1 < \mu < 1$. Thus at each latitude point, (D.2) becomes

$$f(\mu_k) = \sum_l \sum_n f_n^l P_n^l(\mu_k) \quad . \tag{D.4}$$

This means that in order to determine coefficients f_n^l we must evaluate the integrals in (D.3) numerically and at the same time maintain the orthogonality properties of the discrete polynomial representation in (D.4). For this purpose, integrating by quadratures, we introduce a set of Gaussian weight functions, w_k, such that

$$\sum_{k=1}^{N} w_k P_n^l(\mu_k) P_{n'}^l(\mu_k) \equiv \int_{-1}^{1} P_n^l(\mu) P_{n'}^l(\mu)\, d\mu \tag{D.5}$$

and the numerical analog for (D.3) becomes

$$\begin{aligned} f_n^l &= \frac{1}{2} \sum_{l} \sum_{n} f_{n'}^l \sum_{k=1}^{N} w_k P_{n'}^l(\mu_k) P_n^l(\mu_k) \\ &= \frac{1}{2} \sum_{k=1}^{N} w_k f(\mu_k) P_n^l(\mu_k) \quad . \end{aligned} \tag{D.6}$$

The remainder of this Appendix is devoted to the method of evaluation of the Gaussian weights, w_k.

Because we know that any given Legundre polynomial, $P_n^l(\mu)$, can be represented by a finite series in μ of at most degree n, we can expand

$$\left.\begin{aligned} &P_n^l(\mu) P_{n'}^l(\mu) = \sum_{i=0}^{n+n'} b_i \mu^i \\ \text{or} \quad &P_n^l(\mu_k) P_{n'}^l(\mu_k) = \sum_{i=0}^{n+n'} b_i [\mu_k]^i \end{aligned}\right\} \tag{D.7}$$

and thus,

$$\int_{-1}^{1} P_n^l(\mu) P_{n'}^l(\mu)\, d\mu = \sum_{i=0}^{n+n'} b_i \int_{-1}^{1} \mu^i\, d\mu \, . \tag{D.8}$$

Integrating (D.8) by quadratures using (D.5),

$$\begin{aligned}\int_{-1}^{1} P_n^{\ell}(\nu)\,P_{n'}^{\ell}(\nu)\,d\nu &= \sum_{k=1}^{N} w_k\, P_n^{\ell}(\nu_k)\,P_{n'}^{\ell}(\nu_k) \\ &= \sum_{k=1}^{N} w_k \sum_{i=0}^{n+n'} b_i\,[\nu_k]^i \quad . \end{aligned} \tag{D.9}$$

Equating (D.8) and (D.9) we have

$$\sum_{i=0}^{n+n'} b_i \int_{-1}^{1} \nu^i\,d\nu = \sum_{k=1}^{N} w_k \sum_{i=0}^{n+n'} b_i\,[\nu_k]^i \tag{D.10}$$

and thus for any i such that $0 \le i \le n+n'$ it must hold that

$$\int_{-1}^{1} \nu^i\,d\nu = \sum_{k=1}^{N} w_k\,[\nu_k]^i \quad . \tag{D.11}$$

We see from (D.11) that if we choose the number of latitude points, N, such that $N-1 = n+n'$ then utilizing all $i = 0, 1, 2, \cdots, n+n'$ we can form a set of N equations containing N unknown quantities, w_k, for inversion. However, in terms of colatitude, ϕ , for which we can show that any $\cos j\phi$ (j is an integer) can be expanded in the form

$$\left.\begin{aligned}\cos j\phi &= \sum_{m=0}^{j/2} a_{2m}\,\nu^{2m} \\ &= a_j\,\nu^j + \sum_{m=0}^{j/2-1} a_{2m}\,\nu^{2m} \\ \text{and}\qquad \cos j\phi_k &= a_j\,[\nu_k]^j + \sum_{m=0}^{j/2-1} a_{2m}\,[\nu_k]^{2m}\end{aligned}\right\} . \tag{D.12}$$

Then, inserting (D.12) into (D.11),

$$\frac{1}{a_i}\int_{-1}^{1}\cos i\phi\, d\nu - \frac{1}{a_i}\sum_{m=0}^{i/2-1} a_{2m}\int_{-1}^{1}\nu^{2m}\, d\nu =$$

$$= \frac{1}{a_i}\sum_{k=1}^{N} w_k \cos i\phi_k - \frac{1}{a_i}\sum_{m=0}^{i/2-1} a_{2m}\sum_{k=1}^{N} w_k [\nu_k]^{2m} \tag{D.13}$$

or

$$\sum_{k=1}^{N} w_k \cos i\phi_k = \int_{-1}^{1}\cos i\phi\, d\nu$$

$$= \int_{0}^{\pi}\cos i\phi \sin\phi\, d\phi$$

$$= \left\{\begin{array}{l} 0 \text{ for } i \text{ odd} \\ \frac{-2}{i^2-1} \text{ for } i \text{ even} \end{array}\right\}, \quad i = 0, 1, 2, \ldots, n+n' \tag{D.14}$$

where we have made use of (D.11) to eliminate the second term on each side of (D.13). Again, as for (D.11), we see that if we take $N-1 = n+n'$, we can invert (D.14) to obtain the Gaussian weights.

As an example, consider N=3 where we select $\phi_1 = 30^\circ$, $\phi_2 = 90^\circ$, and $\phi_3 = 150^\circ$. Then, from (D.14) we can construct the set (using $i = 0, 1, 2$)

$$\left\{\begin{array}{l} w_1 + w_2 + w_3 = 2 \\ \frac{\sqrt{3}}{2} w_1 - \frac{\sqrt{3}}{2} w_3 = 0 \\ \frac{1}{2} w_1 - w_2 + \frac{1}{2} w_3 = -2/3 \end{array}\right\} \tag{D.15}$$

with solutions

$$\left.\begin{aligned} w_1 = w_3 &= 4/9 \\ w_2 &= 10/9 \end{aligned}\right\} . \tag{D.16}$$

We note that the solutions (D.16) are symmetric in w_k about the equator. If we assume such symmetry <u>a priori</u> then all equations in (D.14) involving odd values of i become redundant and we can write (D.14) over the integration interval from $\phi = 0$ to $\phi = \pi/2$ as

$$\left.\begin{aligned} \sum_{k=1}^{\frac{N+1}{2}} w_k \cos 2i\phi_k &= \int_0^{\pi/2} \cos 2i\phi \sin\phi \, d\phi \\ &= -\frac{1}{4i^2-1} , \\ i = 0, 1, 2, \ldots, \frac{n+n'}{2} &, \quad N-1 = n+n' \end{aligned}\right\} . \tag{D.17}$$

Again, using the example used above in which N=3, $\phi_1 = 30^\circ$, and $\phi_2 = 90^\circ$ we have $\frac{N+1}{2} = 2$ and $\frac{N-1}{2} = 1$ giving the set

$$\left\{\begin{aligned} w_1 + w_2 &= 1 \\ \tfrac{1}{2} w_1 - w_2 &= -1/3 \end{aligned}\right\}$$

with solutions

$$\left.\begin{aligned} w_1 &= 4/9 \\ w_2 &= 5/9 \end{aligned}\right\} . \tag{D.18}$$

Furthermore, if we want to obtain w_k's for the entire pole to pole integration, we need only make use of the symmetry property

$$w_{N+1-k} = w_k + \delta_{\phi_k, \pi/2} w_k \tag{D.19}$$

which gives for our example

$$\left.\begin{aligned} w_1 = w_3 &= 4/9 \\ w_2 = 5/9 + 5/9 &= 10/9 \end{aligned}\right\} . \tag{D.20}$$

Solutions (D.20) are identical with those of (D.16).