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Transport Processes and Trace Constitutents in the Stratosphere

Progress Report

for the period

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The research program has been subdivided into three tasks:

(I) a numerical model

(i1) a stratospheric climatological data analysis(i11) the effect of trace constituents on heating rates

During the first contract period less progress was made than was originally anticipated because of the difficulty encountered in freeing researchers from prior committments and because of the departure from M. I. T. of several research personnel. At the present time a replacement for Dr. Boerwho was to be involved with Task (II) - has not yet been found; otherwise no other personnel difficulties are anticipated during the remainder of the current contract term. The principal investigator has been working full time on the project since June 1, 1972. As a result progress sufficient to merit discussion was confined to Task (I) and to the details of the development of the numerical model.

In preparation for the actual programming of the numerical dynamical model by F. Alyea (who has begun work on September 1), the basic framework of the model has been written in considerable detail. This write-up is enclosed as the appendix to this progress report. It includes the choice of vertical levels, and the associated mean state parameters, the non-dimensional finite-difference equations, details of the simplest photochemical model, and a new efficient procedure for solving the spherical quasi-geostrophic equations (Chapter 6 in the appendix). An important change in computation is represented by our decision that, at each time step, the ozone and temperature field will be first transferred to physical space, where heating and chemical computation will be made, and then transferred back to spherical harmonic space. As mentioned elsewhere this will allow more accurate computation of ultraviclet absorption and of the temperature-dependent chemical reactions. This has opened up the possibility of more accurate infrared heating computation than originally envisaged. It is for this reason that the projected Chapter 5 on heating is incomplete at the present time.

In August Dr. Cunnold attended the Arosa Symposium on Atmospheric Ozone. At this meeting observations of the global distribution of ozone in the natural stratosphere and troposphere were presented. Observations such as these form a basis ageinst which cur model results will be compared. Predictions of the perturbing effects on the stratosphere of a fleet of SSTs were also made with the use of very simple dynamical models and the latest chemical reaction schemes relating to the atmospheric ozone distribution were discussed.

During September Drs. Cunnold and Alyea attended a CIAP workshop in Gaithersburg, Maryland. The interrelationships of the various phases of the CIAP program were discussed and the type of results to be expected during the short time space of the program were outlined.

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Appendix

Dynamical-photochemical Model of the Ozone Layer

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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

$$P = p \div (100 \, cbar)$$

$$Z = -lm P, P = e^{-Z}$$
(1.1)

From the hydrostatic relation dp = -pg dz and p = p/RT, we have $dZ = -\frac{dp}{p} = \frac{g}{RT} dz$ (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 = O, 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:

I.

$$f = 2.2 \sin \phi$$
 (1.3)
 $\Omega = 7.292 \times 10^{-5} \text{ rad sec}^{-1}$

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

$$\vec{v} = k \times \nabla \psi - \nabla \chi \tag{1.4}$$

If the eastward and northward components of \mathcal{N} are represented by \mathcal{M} and \mathcal{N} and \mathcal{Q} is the radius of the earth, this is equivalent to

$$m = \alpha \cos \varphi \frac{d\lambda}{dt} = -\frac{i}{a} \frac{\partial \psi}{\partial \varphi} - \frac{i}{a} \frac{\partial \chi}{\partial \lambda} \qquad (1.5)$$

$$N = \alpha \frac{d\psi}{dt} = \frac{i}{a \cos \varphi} \frac{\partial \psi}{\partial \lambda} - \frac{i}{a} \frac{\partial \chi}{\partial \varphi}$$

The vertical component of relative vorticity, $\mathcal S$, and the horizontal divergence of $\widetilde{\mathcal W}$ are related to $\mathcal Y$ and χ by

$$S = \hat{h} \cdot curl \vec{v} = \nabla^2 \psi$$
; $div \vec{v} = -\nabla^2 \chi$ (1.6)

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

The condition of quasi-geostrophic balance is

$$\nabla \cdot f \nabla \psi = g \nabla^2 \mathcal{F}$$
 (1.7)

where \mathcal{G} is gravity and \mathcal{G} is the height of a constant pressure surface. [Unless noted otherwise, all partial derivatives with respect to \mathcal{A} , \mathcal{G} , and \mathcal{L} (time) are carried out at constant pressure (or \mathbb{Z})]. The hydrostatic relation,

2.

3.

$$9\frac{\partial 3}{\partial p} = -\frac{i}{p} = -\frac{RT}{p}$$

$$q\frac{\partial 3}{\partial z} = RT$$
(1.8a)
(1.8a)
(1.8b)

enables (1.7) to be rewritten as

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

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":

$$\nabla^{2} \frac{\partial \Psi}{\partial t} = -\hat{h}_{X} \nabla \Psi \cdot \nabla (f + \nabla^{2} \Psi) + \nabla \cdot f \nabla \chi + \nabla \cdot (\vec{F}_{X} \times \vec{h}) \quad (1.10)$$
where \vec{F}_{X} is the horizontal frictional force per unit mass.

The continuity equation (conservation of mass) is

$$\frac{\partial}{\partial P}\left(\frac{dP}{dt}\right) = \frac{\partial}{\partial P}\left(\frac{dP}{dt}\right) = -\nabla\cdot\overline{v} = \nabla^{2}\chi \qquad (1.11)$$

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

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

Equation (1.10) can then be rewritten as

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

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

$$W = \frac{dZ}{dt} = -\frac{I}{P} \frac{dP}{dt}$$
(1.14)

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

$$\nabla \cdot P \vec{\sigma} + \partial (P W) / \partial \chi = 0 \tag{1.15}$$

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

$$\mathcal{P} \mathcal{W} = \nabla^2 \chi \tag{1.16}$$

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

$$Z = Z_{TOP} : W = 0 \tag{1.17}$$

$$=0: W \approx \frac{Pq w}{P} = \frac{1}{H_0} v_q \cdot Vh$$

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

$$H_o = \frac{RT_o}{g} = 7 \, \text{km} \tag{1.18}$$

is a constant.

Friction will be represented by a vertical Austausch, $\vec{F}_n = \frac{1}{p} \frac{\partial \vec{E}}{\partial \beta}$ = $-g \frac{\partial \vec{E}}{\partial p}$. Thus $\nabla \cdot \vec{F}_n \times \vec{k} = \frac{\partial}{\partial p} \left[\nabla \cdot \left(-\frac{q}{p_0} \vec{E} \times \vec{k} \right) \right]$

In the interior regions of the model (but not at the ground) we set $\overline{z} = \rho K_m \partial (\overline{h} \times \nabla 4) / \partial \gamma$. giving

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

Replacing ρ by $\frac{1}{R}$ and replacing $\frac{g}{RT}$ by $\frac{1}{H_0}$ w

we get

4.

$$\nabla \cdot \left[-\frac{g}{P_0} \vec{z} \cdot \vec{h} \right] = -\frac{K_m}{H_0^2} P \frac{\partial \nabla^2 \psi}{\partial z}$$

At the ground, we can set \vec{z} equal to 0.003 $\rho_0 |\vec{w}| |\vec{w}|$, with $|\vec{w}|$ a suitable mean anemometer speed (5 m/sec⁻¹) and the anemometer vector wind \vec{w} equal to a rotated ($\alpha = 22.5$ degrees) fraction (0.5) of $\vec{h}_2 \times \nabla \psi$ at the lowest interior level at which ψ is defined

$$\overline{\mathcal{E}}_{grnd} = \left[0.003 \,\overline{p} \, 1\overline{v} \, 1 \, (0.5)\right] \left[\cos \alpha \, \widehat{b} \times \nabla \psi - \sin \alpha \, \nabla \psi\right]_{interior}^{(1.19)}$$

$$\nabla \cdot \left[-\frac{9}{p_0} \, \widetilde{c} \times \widehat{h}\right]_{grnd} = -\left\{\frac{1}{H_0} \left[-003 \, 1\overline{v} \, 1 \, (0.5) \, \cos \alpha\right]\right\} \nabla^2 \psi_{int}$$

For $H_0 = 7 \text{ km}$, $|\vec{nr}| = 5 \text{ m sec}^{-1}$ and $\cos 2 \alpha = 0.925$, the coefficient here has the value 10^{-6} sec^{-1} .

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

$$-\left\{\frac{i}{H_{o}}\sqrt{\frac{K_{m}+i}{2}}\right\} x m d \alpha = \sqrt{2} \psi \qquad (1.20)$$

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

$$\nabla \cdot \vec{F}_{x} \vec{h} = \frac{\partial}{\partial P} (PF)$$

$$Z > 0: \quad F = -\frac{K_{m}}{H_{o}^{2}} P \frac{\partial \nabla^{2} \psi}{\partial Z}$$

$$Z = 0: \quad F = -k_{p} \nabla^{2} \psi_{int}$$
(1.21)

where k_p 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 $\frac{1}{2}$ temperature. For our perfect gas system this would be

$$C_{pdt} \left[ln(T_{p}) \right] = \frac{R}{T}; \quad X = \frac{R}{C_{p}} = \frac{2}{7}$$
 (1.22)

where \mathcal{G} is the rate of heating per unit mass and \mathcal{T} the temperature. In terms of \mathcal{T} , this becomes

$$\frac{\partial T}{\partial t} = -(kx04 - 0\chi) \cdot 0T - W \frac{\partial T}{\partial \chi} - \chi WT + \frac{\varphi}{\zeta_p}$$
(1.23)

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

$$T = \overline{T}(p,t) + T'(\lambda, \theta, p,t)$$

$$\overline{T} = \frac{1}{4\pi a^2} \int_{-\pi/2}^{\pi/2} \cos \theta \, d\phi \int_{-\pi/2}^{2\pi} \overline{T}' = 0 \qquad (1.24)$$

6.

and () will be applicable to any variable.] ()[This definition of

This greatly simplifies the computations, and is reasonably accurate because

 $\nabla \psi >> \nabla \chi$ and $\partial T'/\partial \chi + \chi T'$ is generally small compared to $\partial \overline{T} / \partial Z + \chi \overline{T}$. The result is

$$\frac{\partial T}{\partial t} = -\hat{h} \times \nabla \psi \cdot \nabla T - W \left(\frac{dT}{dZ} + \kappa \overline{T} \right) + \frac{\partial}{\partial c_{p}} \qquad (1.25)$$

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

$$\frac{\partial T}{\partial t} = \overline{g}/c_p$$

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

$$\frac{\partial \overline{T}}{\partial t} = \frac{\overline{g}}{C_p} - \kappa \overline{W'T'} - \frac{i}{\overline{p}} \frac{\partial}{\partial \overline{z}} (P \overline{W'T'}), \quad (1.26)$$

showing the effect of vertical transports of entropy by the motion. We expect little change in $\overline{\mathcal{T}}$ from the observed annual average $\overline{\mathcal{T}}(Z)$, 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

$$\frac{\partial T}{\partial z} + \kappa T = \frac{RT}{q} \left(\frac{\partial T}{\partial z} + \frac{q}{c_{p}} \right)$$
$$= T \frac{\partial}{\partial z} \left[l_{n} \left(T_{p}^{-\kappa} \right) \right] \qquad (1.27)$$
$$= \frac{N^{2}}{R} \left(\frac{RT}{q} \right)^{2}$$

where N is the budyancy . Stequency.

Finally, we describe the basic form of the equation for the (number density) mixing ratio of a trace substance such as O_2 . Define

$$\mathcal{N}_{i} = \mathcal{M}_{i} \stackrel{\cdot}{\cdot} \mathcal{M}_{m} \tag{1.28}$$

where \mathcal{M}_{i} is the number density of the *i*-th trace substance, \mathcal{M}_{m} is the total number density, assumed to be equivalent to the "normal" constituents \mathcal{N}_{2} , \mathcal{O}_{2} and \mathcal{CO}_{2} since \mathcal{M}_{i} is very small. $\mathcal{M}_{m} \cong p/kT$

$$h = Boltzman constant = 1.380 \times 10^{-26} kilojoulos deg^{-1} (1.29)$$

The equation for d_{χ_c}/dt (the rate of change following the motion) is

$$\frac{dY_i}{dt} = \frac{\partial Y_i}{\partial t} + (\hat{k} \times \nabla \psi - \nabla \chi) \cdot \nabla Y_i + W \frac{\partial Y_i}{\partial Z}$$
$$= \frac{1}{m} \left(\frac{dm_i}{dt} \right)_c + \frac{1}{p} \frac{\partial}{\partial Z} \left(p K_d \frac{\partial Y_i}{\partial Z} \right)$$

where $(dM_i/dt)_c$ 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 (length)² \div time]. K_d will vary only with P.

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

$$\frac{\partial}{\partial P} \left[K_d \left(\frac{q}{RT} \right)^2 \frac{\partial K_c}{\partial P} \right] \approx \frac{\partial}{\partial P} \left[-\frac{K_d}{H^2} P \frac{\partial K_c}{\partial Z} \right]$$
(1.30)

where we have again absorbed the variation of density with T into H_o 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 \mathcal{H}_i is now $\mathcal{P} = \begin{bmatrix} K_d \ D & \mathcal{H}_i \end{bmatrix}$

$$\frac{\partial \mathcal{K}_{i}}{\partial t} = -\left(h_{X}\nabla\psi - \nabla\chi\right) \cdot \nabla \mathcal{K}_{i} - W \frac{\partial \mathcal{K}_{i}}{\partial z} + \frac{1}{m} \left(\frac{dm_{i}}{dt}\right) \qquad (1.31)$$

7.

$$\partial \mathcal{L} \qquad \frac{\partial \mathcal{K}_{i}}{\partial t} = -\frac{1}{P} \left[\nabla \cdot \left(P \vec{v} \cdot \mathcal{K}_{i} \right) + \frac{\partial \left(P W \mathcal{K}_{i} \right)}{\partial z} \right] \\ + \frac{1}{M_{m}} \left(\frac{d M_{i}}{d t} \right)_{c} + \frac{\partial}{\partial P} \left[-\frac{K_{d}}{H_{o}^{2}} P \frac{\partial \mathcal{K}_{i}}{\partial z} \right]$$
(1.32)

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

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

$$\frac{\partial \bar{k_i}}{\partial t} = \frac{\partial}{\partial P} \left[P W' k_i' \right] + \left[\frac{1}{m_m} \left(\frac{d M_i}{d t_c} \right) \right] + \frac{\partial}{\partial P} \left[\frac{-\kappa_d}{H_o^2} \frac{P \partial \bar{k_i}}{\partial Z_1} \right]$$

The rate of change of \mathcal{H}_{c}^{\prime} will however be obtained from a simplified form of (1.31), much as was done in the thermodynamic equation (1.25):

$$\frac{\partial k_{i}}{\partial t} = -\vec{b} \times \nabla \psi \cdot \nabla k_{i}' - W \frac{\partial k_{i}}{\partial z} + \left[\frac{1}{m_{m}} \frac{d m_{i}}{dt} \right]' + \frac{\partial}{\partial P} \left[-\frac{K_{d}}{H_{0}^{2}} P \frac{\partial \psi}{\partial z} \right]^{(1.34)}$$

In contrast to \overline{T} , where we are for the most part content to take \overline{T} as given, we must predict $\overline{\mathcal{A}_{c}}$ as well as \mathcal{A}_{c} . 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, $\overline{\mathcal{H}_c}$ being a slowly changing function of time. However, the term $\overline{\mathcal{W}'\mathcal{H}_c'}$ must be put equal to zero at P=1 to ensure no net creation of \mathcal{H}_c by the large-scale motion.

The form of $(d_{\gamma_c}/dt)_c$ 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

8.

that in the very lowest layer the vertical flux (over land) of ozone is proportional to the ground concentration

$$K_d \frac{\partial N}{\partial 3} \approx \frac{K_d}{H_0} \frac{\partial N}{\partial Z} = d \mathcal{R}_{grad}$$
 (1.35)

(the surface destruction of ozone being proportional to \mathcal{O}_3). The coefficient \mathcal{A} has a value of about 1 cm sec⁻¹. We will apply this formulation to the lowest layer in our model ($\mathcal{O} \leq Z \leq \mathcal{A}Z$). Values of \mathcal{K} are defined at the top of the layer ($Z = \mathcal{A}Z$, j = J - l) and at the ground ($Z = \mathcal{O}_j = J$). Thus (dropping the *i*-subscript on \mathcal{K}),

$$\left(\frac{K_d}{H_o}\frac{\partial_{\mathcal{H}}}{\partial^2 Z}\right)_{J-I_2} = \left(\frac{K_d}{H_o}\Delta Z\right)_{J-I_2} \left(\mathcal{N}_{J-1} - \mathcal{N}_{J}\right) = d\mathcal{N}_{J}$$
(1.36)

whence

$$\mathcal{K}_{f} = \mathcal{K}_{f-1} \div \left[1 + \frac{dH_{o}\delta Z}{K_{d}} \right]_{f-1/2}^{(1.37)}$$

and

$$\left(\frac{K_{0}}{H_{0}\delta Z}\right)\left(N_{J-1}-N_{J}\right) = \frac{dN_{J-1}}{1+(dH_{0}\delta Z/K_{d})} (1.38)$$

Galbally cites values of the vertical number flux of ozone molecules over land in the range 1 to 6 x 10^{''} mol cm⁻² sec⁻¹. Aldaz (J. Geo. Res., 1969, P. 6943) estimates a global average of 1 to 1.7 x 10^{''} mol cm⁻² sec⁻¹. Pickinga representative value of 2 x 10^{''} mol cm⁻² sec⁻¹ and equating this to $\mathcal{M}_m \notin \partial \mathcal{M}/\partial \mathcal{J}$, we find, for $\mathcal{M}_m = 4.55 \times 10^{19} \text{ cm}^{-3}$ and $\mathcal{K} = 10^5 \text{ cm}^2 \text{ Sec}^{-1}$, that a vertical gradient of ozone number mixing ratio of

$$\frac{\partial N}{\partial \gamma} \sim 0.5 \times 10^{-13} \text{ cm}^{-1} = \frac{5 \times 10^{-8}}{10 \text{ km}}$$
(1.39)

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

9,

 $5 \times 10^{\prime\prime} \div 4.5 \times 10^{\prime 9} \sim 10^{-8}$. The typical inferred downward flux of ozone observed near the ground is compatible then with a tropospheric K of $10^5 \text{ cm}^2 \text{ sec}^{-1}$ and a tropopause (10km) value for γ of 6×10^{-8} or a $10^{-k}m$ value for \mathcal{M}_3 of $(6 \times 10^{-8}) \times (8 \times 10^{18})$ $\sim 50 \times 10^{10} \text{ cm}^{-3}$. 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.

$$N_i = (N_i)_{equil} \iff \frac{dM_i}{dt} = 0$$

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

$$N_{i} = \int_{m_{i}}^{\infty} dz = \int_{m_{i}}^{\infty} n_{m} dz = \int_{m_{i}}^{\infty} \frac{R}{k} \rho dz$$
$$= \frac{R p_{0}}{g k} \int_{m_{i}}^{p} \chi_{i} dP$$

where R = 287 kj ton deg -1

is the gas constant for air.

(1,40)

This gives numerically

$$N_{i} = 2.12 \times 10^{29} \int N_{i} dP \quad in \ (meter)^{-2}$$

$$= 2.12 \times 10^{35} \int P_{i} dP \quad in \ (cm)^{-2}$$
(1.35)

In the case of molecular oxygen, \mathcal{N}_{c} is taken as uniform and equal to 0,2096, giving

$$N = 0.4444 \times 10^{25} P \text{ cm}^{-2} \quad (1.36)$$

11.

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 \div 100 cb) by defining

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

$$\Delta Z = \frac{Z_I}{J-I} = \frac{Z_{TOP}}{J-I}$$

A convenient choice is obtained by choosing

$$e^{\Delta Z} = \lambda$$
, $\lambda = \frac{3}{2}$
 $\Delta Z = \ln \chi = 0.40547$ (2.2)
 $J = 26$

so that

$$Z_{I} = Z_{TOP} = (J-I) lm n = 10.13675$$

$$P_{I} = n^{-(J-I)} = 3.9605 \times 10^{-5}$$
(2.3)

 P_1 corresponds to a pressure of 39.605 $dynes/cm^2$, typical of the height $3 \sim 71.5$ km. Successive pressure levels are separated by (roughly) $72/25 \sim 2.9$ km. The relations

$$P_{j} = \lambda^{-(J-j)}$$
; $P_{j+1} = \lambda P_{j}$ (2.4)

are useful.

At these levels, the following basic variables will be represented

 $j = 1, 2, \dots, T$: $T_{j}, W_{j}, (M_{i})_{j}$ together with the heating rate, the photo-chemical term, and the vertical turbulent fluxes of momentum. At the intermediate levels the streamfunction W_{i} will be represented

 $j = \frac{3}{2}, \frac{5}{2}, \dots, J - \frac{1}{2}$: \mathcal{H}_{j} For convenience in notation, however, \mathcal{H} 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.

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

The following table lists the values of the more basic variables for the ¹⁴. choice 2 = 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 Sis defined later in equation (3.20).

j.	P;	Zj	z (km (approx) 丐	M _m (cm	j ³ 5;/02
1	•0000396	10.137	71.5	211	136x10 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	877x10 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	48.2	267.5	274	277
10	•00152	6.488	45.1	261.5	421	302
11	•00228	6.082	42.0	254.5	649x10 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	33.1	237	2 ₃₆	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	855x10 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	17.0	210.5	302	194
21	.132	2.027	14.4	213	449	155
22	.198	1.622	11.8	222	646	125
23	•296	1.216	9.2	234	913x10 ¹⁶	116
24	•444	0.811	6.6	248	130×10^{17}	104
25	.667	0.405	3.4	266	182	105
26	1.000	0.0	0.1	284	455x10 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

$$\mathcal{M} = \operatorname{Rin} \varphi$$

$$\nabla(\dim) = \frac{1}{a} \quad \nabla(\operatorname{non-dim})$$

$$\nabla^{2}(\dim) = \frac{1}{a^{2}} \quad \nabla^{2}(\operatorname{non-dim})$$

$$\psi(\dim) = 2\Omega a^{2} \quad \psi(\operatorname{non-dim}) \quad (3.1)$$

$$X(\dim) = 2\Omega a^{2} \quad X(\operatorname{non-dim})$$

$$t(\dim) = \frac{1}{2\Omega} \quad t(\operatorname{non-dim})$$

$$W(\dim) = 2\Sigma \quad W(\operatorname{non-dim})$$

$$W(\dim) = 2\Sigma \quad W(\operatorname{non-dim})$$

$$T(\dim) = T(Z) \quad t(\operatorname{4-\Omega^{2}} a^{2}/R; \Delta Z) \quad T(\operatorname{non-dim})$$

In the last expression $T(\dim)$ in the "total" temperature in absolute degrees, $\overline{T}(Z)$ is the "standard atmosphere" temperature (also in degrees) given in the table at the end of section 2, while the quantity $(4\pi^2a^2/R\phi_Z)$ 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.]

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

$$\Delta t (non - d_{1in}) = 2 \mathcal{I} \left(\frac{2\pi}{\mathcal{I}} \right) = 4\pi$$
 (3.3)

The non-dimensional ∇^2 operator is

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

The relation

$$^{\mathcal{P}}W = \nabla^2 X \tag{1.16}$$

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

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

$$X = P \mathcal{L} W \qquad (3.5)$$

We also have;

$$5 = \nabla^2 \psi, \quad \Psi = \mathcal{L} \mathcal{S} \tag{3.6}$$

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

$$\frac{\partial X}{\partial P} = \frac{\partial}{\partial P} \left[P(XW) \right]$$

in the vorticity equation (1.13). We have

$$\begin{bmatrix} \frac{\partial}{\partial P} (PF) \end{bmatrix}_{j} = \frac{P_{j+1/2} F_{j+1/2} - P_{j-1/2} F_{j-1/2}}{P_{j+1/2} - P_{j-1/2}} = \begin{pmatrix} \frac{\lambda}{\lambda-1} \end{pmatrix} F_{j+1/2} - \begin{pmatrix} \frac{1}{\lambda-1} \end{pmatrix} \frac{F_{j-1/2}}{F_{j-1/2}}$$
where we have made use of (2.4).

The horizontal advection of a quantity $ar{ar{ heta}}$ can be written as the

Jacobian

$$-\vec{v}_{\psi} \cdot \nabla F = -\vec{k} \times \nabla \psi \cdot \nabla F = \frac{\partial F}{\partial \lambda} \frac{\partial \psi}{\partial \mu} - \frac{\partial \psi}{\partial \lambda} \frac{\partial F}{\partial \mu}$$
$$\equiv \int (F, \psi) \qquad (3.8)$$

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
$$j = 1, 2, ..., 5-1$$
:
 $\frac{\partial S_{j}}{\partial t} = \int (\mu + S_{j}, \psi_{j}) - \nabla \cdot \left\{ \mu \nabla \mathcal{L} \left[\left(\frac{\lambda}{\lambda - 1} \right) W_{j} - \left(\frac{\lambda}{\lambda - 1} \right) W_{j} \right] (3.9) + \left(\frac{\lambda}{\lambda - 1} \right) F_{j} + \left(\frac{\lambda}{\lambda - 1} \right) F_{j}$

$$\Psi_{.} = \chi_{5} - - - - (3.10)$$

 $E = 0 - - - (3.11)$

17.

$$F_{\rm T} = -D5_{\rm T}$$
 - - - (3.12)

$$F_{j} = E_{j}(5, -5_{j-1}) \quad (j = 2, 3, -5_{j-1}) \quad (3.13)$$

$$D = k_0 = 2R - - - - (3.15)$$

$$W_{1} = 0 - - - - - - - - (3.16)$$

$$W_{J} = - \left(\frac{h}{H_{0}}, \Psi_{J-1} \right) - - - (3.17)$$

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

$$\overline{\partial} \sigma_{j} = 2, 3, \overline{\partial} - \overline{\partial} \overline{\partial} - \overline{\partial} \overline{\partial} - \overline{\partial} \overline{\partial} = -\nabla^{2} \overline{T}.$$

$$\overline{\nabla} \sigma_{j} \mu \overline{\nabla} (\overline{\psi}_{j} - \overline{\psi}_{j-1}) = -\nabla^{2} \overline{T}.$$

$$(3.18)$$

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

$$\frac{\partial n \ j = z, 3, --, 5-1:}{\frac{\partial T_{j}}{\partial t} = \frac{i}{z} \int (T_{j}, \psi_{j} + \psi_{j-1}) - 5 \cdot W_{j} + \left[\frac{R\Delta Z}{c_{p} 8 \cdot 2^{3} a^{2}} \right] g_{j}$$
(3.19)

where

$$S_{j} = \left(\frac{R \Delta Z}{4 R^{2} a^{2}}\right) \left[\frac{d \overline{T}}{d Z} + \frac{R}{q} \overline{T}\right], \qquad (3.20)$$

is tabulated at the end of section 2 (but without the factor ΔZ). It 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

$$\begin{split} \partial or & j = j_{0}, j_{0} + j_{1} - J_{1}; \\ \frac{\partial \kappa_{j}}{\partial t} &= \frac{i}{2} \int (\chi_{j}, \psi_{j} + \psi_{j-1}) - W_{j} (\frac{d \pi}{d z}); \\ &- + (\frac{\kappa}{2 - i})G_{j} - (\frac{i}{2 - i})G_{j-1} + \frac{i}{2 - \alpha} \left[\frac{i}{m_{m}} (\frac{d \pi}{d t})_{c} \right]; \\ G_{j} &= D_{j} (\chi_{j+1} - \chi_{j}) \quad ; \partial or \quad j = j_{0}, \cdots, J - 2. \end{split}$$

$$\begin{split} D_{j} &= (\kappa_{d})_{j+1/2} \stackrel{*}{\to} (2\Omega + \eta_{0}^{2} \Delta z). \end{split}$$

$$\end{split} \tag{3.22}$$

[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

$$G = \frac{\chi_{J-1}}{\left[\frac{2\Omega H_{0}}{dt} + \frac{2\Omega H_{0}^{2} \Delta Z}{(K_{d})T_{-}^{\prime}/2}\right]}$$
(3.23)

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

Photochemistry. 4.

To begin with, the photochemistry will involve only oxygen and odd

nitrogen compounds, with the latter being specified as given functions of (or possibly pressure and latitude).

(Equations to predict the nitrogen compounds may be added later.) pressure The reactions involved are the four main Chapman reactions and reactions of and NO_2 with oxygen. (The following write-up is based on analysis ND by R. Prinn.)

Reference:

(a)
$$\begin{array}{c} 0_{2} + h\nu \rightarrow 20\\ \hline 2459 - X\\ \hline J_{0} = \int \alpha Ie^{-2}d\lambda sec^{-1}\\ \hline \end{array}$$
(4.1)

 $0 + 0_3 + iM \rightarrow 0_3 + M$ $l_1 = 1.6 \times 10^{-35} e^{-1050} T cm^6 sec^{-1}$

(c)

$$C_3 + h\nu \rightarrow D_2 + 0$$

$$J_0 = \int x_0 I e^{-X_0} d\lambda \ sec^{-1}$$

$$(4.3)$$

÷.*

$$0 + 0_3 \rightarrow 20_2 - \frac{2395}{T}$$
 (4.4)
 $k_1 = 2X10'' e^{-1} T cm^3 sec^{-1}$

(e)
$$NO + O_3 \rightarrow NO + O_2$$

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

(a)
$$NO_2 + O \rightarrow NO + O_R$$

 $h_3 = 3.2 \times 10^{-11} e^{-\frac{530}{T}} un^3 sec^{-1}$ (4.6)

(f)
$$NO_{2} + h\nu \rightarrow NO + O$$

 $J_{NO_{2}} = \int_{NO_{2}}^{3975} -X_{NO_{2}} d\lambda \quad sec^{-1}$
(4.7)

In the three radiation integrals the exponent X is

$$X_{i} = \frac{\alpha_{i}(\lambda) N_{i}}{\cos \psi}$$
(4.8)

20.

where $\alpha_{c}(\lambda)$ is the absorption cross-section, N_{c} is the number of imolecules in the \mathcal{Om}^{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.) Γ is the incident solar radiation, a function of the wavelength λ .

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: <u>Science</u>, 173, P. 517.
 Schiff, 1969: <u>Can. J. Chem.</u>, 47, P.1903.
 (*l* is an average of their values)

(c) Ackerman, 1970: As for Kockarts.
 (d) Schiff, 1969: As above.

(e) Schofield, 1967: <u>Ptanet. Space Sci</u>., 15, P. 643.

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

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NOTE ADDED Sept. 25, 1972: The CIAP newsletter dated Sept. 8, 1972 reports two revised rate constants (Davis, Herron and Huie) as follows:

k3 = (9.12±0.44) × 10⁻¹² cm³ sec⁻¹ $l_{1} = (6.19 \pm 0.50) \times 10^{-35} e^{\frac{523 \pm 19}{T}} cm^{6} sec^{-1}$

with the result that k_3 is about twice as large and l, half as large as the values cited above on page 19. Use of these new values would modify the ratio K defined in (4.19) and (4.21) below.

					Comonto
Coefficient	50	Heigh 40	: (km) 30	20	CGS units
J ₀₂	10 ⁻⁹	3x10 ⁻¹⁰	2x10 ⁻¹¹	4x10 ⁻¹⁴	day only
J ₀₂ [02]	4x10 ⁶	5x10 ⁶	1.6x10 ⁶	1.4x10 ⁴	day only(=0 at night)
∮ ₁[0 ₂][M]	0.08	1.3	32	600	same day and night
J ₀₃	8x10 ⁻³	5,5x10 ⁻³	3x10 ⁻³	1.3x10 ⁻³	day only
J ₀₃ [03]	5x10 ⁸	3x10 ⁹	7x10 ⁹	5x10 ⁹	day only
[0] (day)	9x10 ⁹	7x10 ⁸	4x10 ⁷	1.3x10 ⁶	
(night)	0	0	0	0	
[0,](day)	7x10 ¹⁰	6x10 ¹¹	2.6×10^{12}	3.8x10 ¹²	
) (night)	14x10 ¹¹	6x10 ¹¹	2.6x10 ¹²	3.8×10^{12}	
[NO](day)	7x10 ⁸	2x10 ⁹	3x10 ⁹	4x10 ⁹	
(night)	0	0	0	0	
[N0,](day)	2x10 ⁷	1x10 ⁹	8x10 ⁹	1x10 ¹⁰	
2 (night	5x10 ⁸	2x10 ⁹	6x10 ⁹	1x10 ¹⁰	
J _{NO2}	7x10 ⁻³	7x10 ⁻³	7x10 ⁻³	6x10 ⁻³	day only
k ₃ [0]	45x10 ⁻³	35x10 ⁻⁴	20x10 ⁻⁵	6.5x10 ⁻⁶	$(k_3 = 5 \times 10^{-12})$
k ₃ [0]+J _{N02}	5x10 ⁻²	1x10 ⁻²	7x10 ⁻³	6x10 ⁻³	
k ₂ [0 ₃]	7x10 ⁻⁴	6x10 ⁻³	2.6x10 ⁻²	3.8x10 ⁻²	(k ₂ =10 ⁻¹⁴)

Typical Variation of rate coefficients with height

nd from day to night based upon results in Crutzen (1971)

-

	Height (km)						
Coefficient	50	40	30	20	CGS units		
$\frac{k_{3}[0]+J_{NO_{2}}}{k_{2}[0_{3}]}$	70	2	0.3	.15	day only		
Ŧ.	267	250	231	212			
^k 1	2.5x10 ⁻¹⁵	1.4x10 ⁻¹⁵	0.6x10 ⁻¹⁵	0.2x10 ⁻¹⁵			
k ₃	0.44×10^{-11}	0.38x10 ⁻¹¹	0.32×10^{-11}	0.26x10 ⁻¹¹			
k ₁ [0 ₃]+k ₃ [NO ₂	l) 19x10 ⁻⁴	65x10 ⁻⁴	240x10 ⁻⁴	270x10 ⁻⁴			
К	2.4x10 ⁻²	5x10 ⁻³	7x10 ⁻⁴	5x10 ⁻⁴			
J ₀₂ [02]÷J ₀₃ [0	0.8×10^{-2}	1.7×10^{-3}	2.3x10 ⁻⁴	2.8x10 ⁻⁴			
				· · ·			
					·		
· ·	ł	1	1	i			

The equation for d[0]/dt (we denote temporarily number densities m_i by a square bracket) is

$$\frac{d[o]}{dt} = 2[0_2] \overline{J}_2 + [0_3] \overline{J}_{0_3} + [NO_2] \overline{J}_{NO_2} \quad (4.9)$$

- [0] { l, [0_2][M] + k, [0_3] + k_3 [NO_2] }

([M] is the neutral number density, equal to $\mathcal{M}_{\mathcal{M}}$ in the table at the end of section 2.) The term $\ell_{1} [\mathcal{O}_{2}] [\mathcal{M}]$ 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]:

$$[0] = \frac{2[0_{2}]J_{0_{2}} + [0_{3}]J_{0_{3}} + [NO_{2}]J_{NO_{2}}}{L(1+K)}$$
(4.10)

where

$$L = l_{1}[o_{2}][M]$$

$$K = \frac{k_{1}[o_{3}] + k_{3}[No_{2}]}{l_{1}[o_{2}][M]}$$
(4.11)

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

$$\frac{d[No]}{dt} = k_3[No_2][0] + J_{NO_2}[NO_2] - [NO] \{k_2[O_3]\}$$
(4.12)

where the product $k_2 \begin{bmatrix} 0_3 \end{bmatrix}$ is again large enough $(10^{-3} \text{ sec}^{-1} \text{ at } 50 \text{ km}, 04 \text{ sec}^{-1} \text{ at } 20 \text{ km})$ to allow us to assume d [N0]/dt = 0. Thus

$$[NO] = \left\{ \frac{k_{3}[O] + \int_{NO_{2}}}{k_{2}[O_{3}]} \right\} [NO_{2}]$$
(4.13)

23.

In the nightime [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; <u>Science</u>, 173, P. 517) and Crutzen (1971; <u>J. Geophy. Res.</u>, 76, P. 7311) suggest that the total odd nitrogen mixing ratio ($[NO] + [NO_2]$) $\frac{o}{r}$ [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 $[NO_2] \frac{o}{r} [M]$ 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 $[\mathcal{NO}_2]$ or $[\mathcal{NO}_2] \frac{1}{2} [\mathcal{M}]$ is a prescribed function of pressure, with $[\mathcal{NO}]$ determined from (4.13).

The equation for [\mathcal{O}_3] is

$$\frac{d[0_3]}{dt} = l[0_2][M][0] - J[0_3] - k[0][0_3] - k[N0][0_3]$$
(4.14)

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

$$\frac{d [0_3]}{dt} = \frac{1-\kappa}{1+\kappa} 2 [0_3] J_0 - \frac{2\kappa}{1+\kappa} ([0_3] J_0 + [N0_2] J_{NO_2})$$
$$= \frac{1}{1+\kappa} \begin{cases} 2 [0_3] J_0 - 2\kappa ([0_2] J_0 + [0_3] J_0 + [N0_2] J_{NO_2}) \end{cases}$$

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

$$\frac{d[0_3]}{dt} \approx R[0_2] J_0 - 2K([0_3] J_0 + [N0_2] J_{N0_2})$$
(4.16)

25.

where we have retained only the leading terms. In terms of the number mixing ratios \mathcal{H}_{i}

$$\begin{aligned}
\mathcal{H}_{O_2} &= \left[\mathcal{O}_2 \right] \stackrel{\circ}{\rightarrow} \mathcal{M}_m = 0.2096 \\
\mathcal{H}_{O_3} &= \left[\mathcal{O}_3 \right] \stackrel{\circ}{\rightarrow} \mathcal{M}_m \\
\mathcal{H}_{NO_2} &= \left[NO_2 \right] \stackrel{\circ}{\rightarrow} \mathcal{M}_m
\end{aligned}$$
(4.17)

we have $\begin{bmatrix} \frac{1}{m_{m}} & \frac{d}{dt} & \frac{m_{0}}{dt} \end{bmatrix} = 2(.2096) \int_{0}^{2} - \frac{2}{k} \left[\frac{1}{N_{0}} & \frac{1}{3} + \frac{1}{N_{0}} & \frac{1}{N_{0}} \right]^{(4.18)}$ $K = \frac{k_{1} N_{0} + k_{3} N_{0}}{(.2096) l_{1} m_{m}} = K(p, T)$ (4.19)

At constant pressure the logarithmic derivative of \mathcal{M}_{m} with T is \overline{T}^{-1} , whereas the logarithmic variation of $(\frac{k_2}{2}/l_1,)$ and $(\frac{k_2}{3}/l_1,)$ with \overline{T} is $3445/\overline{T}^2 \sim \frac{10}{\overline{T}}$ and $1580/\overline{T}^2 \sim \frac{5}{\overline{T}}$ respectively. We therefore treat \mathcal{M}_{m} as a known function of pressure $(=p/k\overline{T})$; see table at end of section 2), but will compute the exact dependence of the rate constants on \overline{T} .

A proper way to compute $|\langle$ is suggested as follows, using the particular numerical values given in (4.2), (4.4) and (4.6). We define a scaled neutral number density $\hat{\mathcal{M}}$:

$$\hat{M} = 10^{-17} m_{m} (.0136 \le \hat{m} \le 455 \text{ cm}^{-3})$$
 (4.20)

$$K = \frac{2 \times 10^{-11} e^{-\frac{3395}{T}} + 3.2 \times 10^{-11} e^{-\frac{530}{T}}}{(0.2096)(1.6 \times 10^{-35})e^{\frac{1050}{T}}(10^{17} n)}$$

$$= \frac{1}{N} \left\{ \begin{bmatrix} 5.96374 \times 10 \ e \end{bmatrix} e^{-14} \left(\frac{14}{T} - \frac{3445}{T} \right) \\ = \frac{1}{N} \left\{ \begin{bmatrix} 5.96374 \times 10 \ e \end{bmatrix} e^{-14} \left(\frac{14}{T} - \frac{3445}{T} \right) \\ = \frac{1}{N} \left\{ 49.603 \ e \end{bmatrix} e^{-14} \left(\frac{14}{T} - \frac{3445}{T} \right) \\ = \frac{1}{N} \left\{ 49.603 \ e \end{bmatrix} e^{-14} \left(\frac{14}{T} - \frac{3445}{T} \right) \\ = \frac{1}{N} \left\{ 49.603 \ e \end{bmatrix} e^{-14} \left(\frac{14}{T} - \frac{3445}{T} \right) \\ = \frac{1}{N} \left\{ 49.603 \ e \end{bmatrix} e^{-14} \left(\frac{14}{T} - \frac{3445}{T} \right) \\ = \frac{1}{N} \left\{ 49.603 \ e \end{bmatrix} e^{-14} \left(\frac{14}{T} - \frac{3445}{T} \right) \\ = \frac{1}{N} \left\{ 49.603 \ e \end{bmatrix} e^{-14} \left(\frac{14}{T} - \frac{3445}{T} \right) \\ = \frac{1}{N} \left\{ 49.603 \ e \end{bmatrix} e^{-14} \left(\frac{14}{T} - \frac{3445}{T} \right) \\ = \frac{1}{N} \left\{ \frac{14}{N} \left\{ \frac{14}{N} - \frac{3445}{T} \right\} \right\} \\ = \frac{1}{N} \left\{ \frac{14}{N} \left\{ \frac{14}{N} + \frac{3445}{T} \right\} \\ = \frac{1}{N} \left\{ \frac{14}{N} \left\{ \frac{14}{N} + \frac{3445}{T} \right\} \right\} \\ = \frac{1}{N} \left\{ \frac{14}{N} \left\{ \frac{14}{N} + \frac{3445}{T} \right\} \\ = \frac{1}{N} \left\{ \frac{14}{N} \left\{ \frac{14}{N} + \frac{3445}{T} \right\} \\ = \frac{1}{N} \left\{ \frac{14}{N} + \frac{3445}{T} \right\} \\ = \frac{1}{N} \left\{ \frac{14}{N} + \frac{14}{N} + \frac{14}{N} + \frac{14}{N} + \frac{14}{N} + \frac{14}{N} + \frac{14}{N} \right\} \\ = \frac{1}{N} \left\{ \frac{14}{N} + \frac{14}{$$

The exponents have been chosen so that the exponent in both cases has an average value — considering variations in T from 200 to 300 -- which is close to zero. They range from -3.5 to +3. T itself is computed from the last equation in (3.1).

Temporarily denoting the exponent by \mathscr{N}

fi= eti

$$N = 14 - \frac{3445}{T}$$
 or $6 - \frac{1580}{T}$

we can get e^{π} efficiently by interpretation in a stored table of $f = e^{\pi}$.

from the formula

$$\mathcal{K} = \mathcal{K} + \mathcal{Z}, \quad 0 \leq \mathcal{Z} \leq \mathcal{S}$$

$$f(\mathcal{X})_{inter} = f_{c} \left[1 + \mathcal{Z} \left(A + B \mathcal{Z} \right) \right]$$

شته و ا

(4,22)

26.

where A and B are constants depending only on $\,\mathcal{S}\,$:

27.

$$A = \frac{1}{8^{2}} \left[(6-2\delta)e^{-1} - (6+4\delta) \right] \sim 1 - \frac{1}{72}\delta^{2} + \cdots$$

$$B = \frac{3}{8^{3}} \left[2+\delta - (2-\delta)e^{-\delta} \right] \sim \frac{1}{2} + \frac{\delta}{4} + \cdots$$
(4.23)
(4.23)

 $f(x)_{int}$ agrees with f_c and f_{c+1} when $\xi = 0$ and $\xi = \delta$ and has the same mean value as f(x):

$$\int_{0}^{\delta} f_{int} d\xi = f_{i+1} - f_{i} = \int_{0}^{\pi} e^{\pi} d\mu$$

The percentage error is

-1

$$G = \frac{f_{int} - f}{f} = \left[1 + \frac{5}{A} + \frac{85}{9} \right] e^{-\frac{5}{4}} - \frac{1}{A} (A - 1) \frac{5}{4} + (B - A + \frac{1}{2}) \frac{5^{2}}{4} - \frac{5^{3}}{44}$$

= $\frac{(A - 1)^{2}}{4(B - A + \frac{1}{2})} - \frac{5^{3}}{144}$

For $\delta = 1/2$, the percentage error is at most 0.00115:

5:	•05	.1	.15	• 2	.25	.•3	•35	•4	•45
10 ⁵ ∈∶	-89	-115	-98	~55	-3	45	79	88	64

In the photochemical radiation integrals \overline{J} (and in the solar heating integrals), we have the problem of averaging over a day, during which the zenith angle varies.

where

28.

Using the relation

$$\cos \psi = \sin \phi \sin \delta + \cos \phi \cos \delta \cosh (4.25)$$

we find sunrise and sunset at h = -H and h = +H, with

$$\cos H = -\tan \phi \tan \delta$$
 (4.26)

Considering only the Northern Hemisphere ($\tan \phi \ge 0$) we have $\tan \phi \tan \delta \le -1 : H \equiv 0$ (Polar winter night) $-1 < \tan \phi \tan \delta < 0$ $0 < H < \frac{\pi}{2}$ $\tan \phi \tan \delta = 0$ $H = \frac{\pi}{2}$ (Equinox) $0 < \tan \phi \tan \delta < 1$ $\frac{\pi}{2} < H < \pi$ $1 \le \tan \phi \tan \delta$ $H \equiv \pi$ (Polar summer day)

Using the relation $\mathcal{R} = \frac{dh}{dt} dt$, the 24-hour average of I is $I_{24} = \frac{\mathcal{R}}{\partial \pi} \int I dt = \frac{1}{\partial \pi} \int I dh$ $= \frac{1}{\pi} \int I dh$

Dividing the interval O < h < H into ten portions gives

$$I_{24} = \frac{H}{10\pi} \sum_{i=1}^{10} \overline{I} \left(X = \frac{N}{\cos \psi_i} \right)$$

(co24); = sindsin S + co2d co2 S co2 $\left[\frac{H}{10} \left(\dot{c} - \frac{t}{2} \right) \right]^{(4.27)}$

This results finally in a function of latitude, declination and and N.

$$I_{24} = T(\phi, \delta, N) \qquad (4.28)$$

By symmetry, Southern Hemispheric values are given by

$$I_{24}(-\phi, \delta, N) = I_{24}(\phi, -\delta, N)$$
 (4.29)

An important practical problem is to represent the function (4.28) at each of a series of selected latitudes as a moderately simple function of \mathcal{S} (i.e., time of year) and N. Our current approach to this problem is to construct and store a table for I (X) as a function of X and then to use expression (4.27) to value I. Now this technique will only work provided that within each absorption band a single species of atom is responsible for the absorption of each incident solar photon.

Let us consider each of the photodissociation rates J_{O_2} , J_{O_3} , and J_{NO_2} . There exists a small amount of overlap between the absorption bands of O_2 and O_3 and between NO_2 and O_3 . Now the absorption by NO_2 is sufficiently weak that it does not significantly reduce the number of photons available for absorption at any altitude of the atmosphere. Thus for NO_2 , I (X) may be written as a function of the column concentration of O_3 only. The absorption bands of O_2 and O_3 overlap in the region 2000-2450 Å. For ozone strong absorption also occurs in the region 2450-3200 Å and because there is more solar energy in this portion of the spectrum than in the overlap region, absorption by O_2 only reduces \mathcal{J}_{O_3} at any altitude by a few % at most. Therefore I (X) for O_3 will be calculated as a function of the columnar concentration of O_3 only. Finally considering the photodissociation of O_2 , it is found that at low altitudes at which absorption in the range 2000-2450 Å is significant, photodissociation of O_3 is a more effective source of 0 atoms by 3 orders of magnitude. Therefore for O_2 , I (X) will be calculated as a function of the columnar concentration of O_2 atoms only with the integration over wavelength being truncated with an upper limit of 2000 Å.

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5. Heating

The heating of the atmosphere between the ground and 70 km consists of latent heat release, the absorption of short wave solar energy, and the absorption and remission of long wave radiation. The absorption of short wave radiation by ozone (including absorption in the Chappuis band) and the small contribution resulting from absorption by molecular oxygen may be treated in a straightforward manner.

$$Q_{0_3} = \left[O_3\right] \int_{2000 \text{ Å}}^{7500\text{ A}} \chi_{0_3} \text{ Tre} = \chi_{0_3} \text{ d} \text{ joules/cm}^3/see$$

where ξ is the energy of a photon. A similar expression may be written down for heating by O_2 - which makes a significant contribution to total heating only at altitudes above 50 km. It is convenient as it was in the discussion of photodissociation rates to construct a table of Q_{03} as a function of the columnar concentration of O_3 and similarly to calculate Q_{O_2} as a function of the O_4 column concentration. In these cases also the daily average values of these heating rates are needed rather than the instantaneous values; thus, by analogy with (4.27), the average value Q_{03} may be derived from

$$Q_{24} = \frac{H}{10 \text{ Tr}} \sum_{i=1}^{10} Q\left(X = \frac{\alpha N}{\cos \psi_i}\right)$$

with
$$\cos \psi_i = \sin \phi \sin \delta + \cos \phi \cos \delta \cos \left[\frac{H}{10} \left(i - \frac{i}{2}\right)\right] (5.1)$$

30.

E simple algorithm for representing infrared heating and cooling is more difficult to derive. Our current approach which will be used in initial runs of the computer model is to separate the atmosphere into two regions - above and below 30 km - and to represent these terms slightly differently in the two regions. Above 30 km we plan to use a Newtonian cooling approximation with different coefficients at each altitude of the model. Kuhn and London have kindly supplied us with their detailed results of infrared cooling by CO_2 , H_2O , and O_3 at each latitude and each altitude above 30 km. We have plotted total cooling versus temperature at each altitude and have made a linear fit to the resulting data. It has been found that straight line representations on the average account for approximately 50 % of the variance of the data points. Although absorption is the 9.6μ band of O_3 is not the major cooling source above 30 km, it makes a sufficiently large contribution that it appears desirable to relate this cooling to the concentration of ozone molecules. Possible ways of doing this are under investigation at the present time.

Below 30 km we plan to represent infrared heating and latent heat release as Trenberth (M. I. T. thesis, 1972) did by a single linear term of the form

 $h_i(T_i^*-T)$

where j refers to the altitude level j. The equilibrium temperature distribution, T*, is obtained from calculations by Manabe and Strickler (J. A. G., 21, 361, 1964) in which using

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climatogical distributions of minor constituents a value of T* corresponding to zero net heating was derived. Newell <u>et. al.</u> (RMS London, 1970) have made daily heating rate calculations including boundary layer heating and latent heat release. These computations may be used to derive values of

6. Determination of W in the dynamic equations.

Defining

$$E = \frac{n}{n-1} > 1 \quad (n = e^{\Delta Z})$$

$$M = \nabla \cdot \mu \nabla \mathcal{L}$$

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

$$S_{i} = \nabla^{2} \mathcal{U}.$$
(6.1)

the basic equations can be written as

$$j = 1, --, J - 1: \quad \frac{\partial S}{\partial t} = A_{j} - \mathcal{M}\left[\in W_{j+1} - (\epsilon - 1) W_{j} \right]$$
 (6.2)

$$j = 2, -, 5 - 1: M(5, -5, -) = -\nabla^2 T_{j}$$
 (6.3)

$$j=2, --, J-1:$$
 $\frac{\partial T_j}{\partial \tau} = -S_j W_j + B_j.$ (6.4)

where A_j and B_j symbolize the following quantities:

$$A_{j} = \int (\mu + S_{j}, \Psi_{j}) + \epsilon F_{j+1} - (\epsilon - 1)F_{j} \qquad (6.5)$$

$$B_{j} = \frac{1}{2} \int (T_{j}, \psi_{j} + \psi_{j-1}) + \int \frac{RAZ}{C_{p} 8 \Omega^{3} a^{2}} \int 8_{j}$$
(6.6)

As boundary conditions we have

$$W_{J} = - \int \left(\frac{h}{H_{o}}, \Psi_{J-1}\right)$$

$$(6.7)$$

Note that \mathcal{X} is not defined when it acts on a constant function. Considering A., B. and W_J as known (at a given time step), the problem is to solve for $\partial S./\partial t$ and W_j. We propose to eliminate $\frac{\partial S}{\partial t} = \nabla^2 \frac{\partial 4}{\partial t}$ in

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favor of W. Having found W, $\partial S/\partial t$ is determinable from (6.2) and can be used to extrapolate S in time.

In general we will represent \mathcal{S} , \mathcal{T} , \mathcal{W} as a series in spherical harmonics \mathcal{V}

$$S_{i}(\lambda,\mu,t) = \sum_{m} \sum_{m} S_{i}(t) \overline{P}_{i}^{m}(\mu) e^{im\pi m}$$

For concreteness, let us focus attention on only one longitudinal wave number \mathcal{M} , and consider only those parts of \mathcal{S} , \mathcal{T} , \mathcal{W} etc which are proportional to $\mathcal{COP} = \mathcal{M} \hat{A}$. Thus

The above sum limits hold for $M \ge l$. For M = 0 the sum will be from M = l, 2, --, L+l. Thus there will be L+l latitudinal modes for each zonal wave number M = 0, l, --. The discussion below is given primarily for $M \ge l$, with occasional comments for M = 0 where appropriate.

From Abramowitz and Stegun (pages 332-341) we have V

$$\overline{P}(\mu) = \alpha_{mm} P_{m}(\mu) \qquad (6.9)$$

$$\frac{q'_{mm} = (-1)^{m} \left[\frac{(2m+1)(m-m)}{2(m+m)!} \right]^{1/2}}{\frac{(6.10)}{2(m+m)!}}$$
(6.10)
If Trenberth uses P_{m}^{m} and T_{m}^{m} in place of $\int_{\overline{a}} \overline{P}_{m}^{m}$ and P_{m}^{m}

$$\int_{-1}^{\infty} \frac{P(\mu)}{P(\mu)} \frac{P(\mu)}{\mu} = 0 \quad \text{if } l = n \quad (6.11)$$

33.

$$(m+1-m)P_{m+1} = (2m+1)\mu P_m - (m+m)P_{m-1}$$
 (6.12)

$$(\mu^2 - 1) \frac{dP_m}{d\mu} = m\mu P_m - (m+m) P_{m-1}^{m}$$
 (6.13)

The \bigtriangledown operator introduces a coefficient -m(m+1) inside each sum. The \mathcal{M} operator is more complicated, however:

$$\mathcal{M}F = \mu F + (I - \mu^2) \frac{\partial}{\partial \mu} (\mathcal{Z}F)$$
(6.14)

Applying this to the \mathcal{W} , sum in (6.8) we get, by using (6.9) - (6.14)

$$MW_{i} = \cos m \Im \sum_{n=m}^{N} \widetilde{W}_{i} \left[\mu \overline{P}_{n}^{m} + (\mu^{2} - i) \frac{d \overline{P}_{n}^{m}}{m(m+i)} \right]$$
$$= \cos m \Im \sum_{n=m}^{N} \widetilde{W}_{i} \left[\beta \overline{P}_{n}^{m} + \Im \overline{P}_{n}^{m} \right] \overline{f}^{(6.15)}$$

where

$$\beta_{mm} = \left(\frac{m^{-1}}{m}\right) \sqrt{\frac{m^2 - m^2}{4m^2 - 1}}$$
(6.16)

$$\mathcal{Y}_{mm} = \frac{m+2}{n} B_{m+1m} \qquad (6.17)$$

$$\beta_{mm} = 0$$
, $\gamma_{m-1m} = 0$ (6.18)

34. β_{mm} and $\delta_{m-1,m} = 0$, so that \overline{P}_{m-1}^{m} Note that does not appear in (6.15). We also drop the \overline{P}_{N+1} term. Thus we have (suppressing the j -subscript) ٨/

$$\mathcal{M} W = \cos m\lambda \sum_{m=m} \left[\begin{array}{c} \mathcal{S} & \tilde{\mathcal{W}} \\ m-1m & m-1m \end{array} \right] + \left[\begin{array}{c} \mathcal{M} & \mathcal{M} \\ \mathcal{M} \end{array} \right] + \left[\begin{array}{c} \mathcal{M} \\ \mathcal{M} \end{array} \right] \right]$$
(6.19)

in which

$$m-1m = 0$$
, $W = 0$
 $N+1m$

Combining this with (6.2) and (6.8), and using the orthonormal properties of

PM we have

 $\frac{\Im \tilde{S}}{\Im t} = \tilde{A}_{,m,m} - \varepsilon \begin{bmatrix} y & W \\ m-m & j+1m-1m \end{bmatrix} + \begin{pmatrix} B & W & j+1m+1m \end{pmatrix} \int (6.20) \\ + (\varepsilon - 1) \begin{bmatrix} y & W & j+1m+1m \end{pmatrix} + \begin{pmatrix} B & W & j+1m+1m \end{pmatrix} \\ + (\varepsilon - 1) \begin{bmatrix} y & W & j+1m & m+1m \end{pmatrix} \\ m-1m & jm-1m & m+1m \end{pmatrix} \int (6.20) \\ + (\varepsilon - 1) \begin{bmatrix} y & W & j+1m+1m \end{pmatrix} \\ m-1m & jm-1m \end{pmatrix}$ Consider now the \mathcal{M} operator on \mathcal{S} in (6.3). By similarity with $\mathcal{M}W$

we get

$$M = com \lambda \sum_{n=m}^{N} \begin{bmatrix} y & \tilde{s} + \beta & \tilde{s} \\ n-im & n-im & m+im & m+im \end{bmatrix} \overline{P}_{n}$$
(6.21)

in which again

$$\gamma_{m-1m}=0$$
, $\tilde{S}_{N+1m}=0$

Combining (6.3) and (6.4) to eliminate \mathcal{T}_{i} gives

$$S_{j} \nabla^{2} W_{j} = \nabla^{2} B_{j} + \mathcal{M} \left(\frac{\partial S_{j}}{\partial t} - \frac{\partial S_{j-1}}{\partial t} \right) \qquad (6.22)$$

which in terms of the $\overline{P}_{\mathcal{M}}^{\mathcal{M}}$ series gives

$$-m(M+1)S; \widetilde{W}_{jMM} = -m(M+1)\widetilde{B}_{jMM} \qquad (6.23)$$

$$+ \mathscr{E}_{M-1M} \left[\frac{\partial \widetilde{S}}{\partial \overline{t}} - \frac{\partial \widetilde{S}}{\partial \overline{t}} \right] + \mathcal{E}_{M+1M} \left[\frac{\partial \widetilde{S}}{\partial \overline{t}} - \frac{\partial \widetilde{S}}{\partial \overline{t}} \right]$$

$$+ \mathscr{E}_{M-1M} \left[\frac{\partial \widetilde{S}}{\partial \overline{t}} - \frac{\partial \widetilde{S}}{\partial \overline{t}} \right] + \mathcal{E}_{M+1M} \left[\frac{\partial \widetilde{S}}{\partial \overline{t}} - \frac{\partial \widetilde{S}}{\partial \overline{t}} \right]$$

Equations (6.20) and (6.23) together with the boundary conditions

$$\widetilde{W}_{imm} \equiv 0$$

$$\widetilde{W}_{jmm} = known$$
(6.24)

35.

form a system of (J-1)(L+1) + (J-2)(L+1) = 294 simultaneous equations (if J=26 and L=5) for $\Im\overline{S}/\Im t$ and \widetilde{W} .

We want a less demanding solution than the straightforward matrix inversion of this system. The philosophy is suggested by the usual Cartesian "betaplane" approximations in which the $\mathcal{M} = \operatorname{Ain} \phi$ appearing explicitly in $\mathcal{M} = \nabla \cdot \mathcal{M} \nabla \mathcal{A}$ is replaced by a constant $\mathcal{M}_{\mathcal{O}}$ so that \mathcal{M} is simply $\mathcal{M}_{\mathcal{O}}$. If in that system the horizontal variation is expressed by sines and cosines, with $\nabla^2 = -h^2$, the $\partial S/\partial t$ and \mathcal{W} equations can be combined into an operator on \mathcal{W}_1 : alone

$$\nabla^2 W_{\cdot} + \frac{\mu_0^2}{5!} \left[e W_{\cdot} - (ae-1)W_{\cdot} + (e-1)W_{\cdot} \right] = F_{\cdot}$$

and, by considering each component

$$W_{j} \propto \widetilde{W}_{j \propto \beta} e^{-\lambda (d_{k} + B_{j})}$$

 $\alpha^{2} + \beta^{2} = k^{2}$

one gets

$$- \in \widetilde{W} + \left[(2E-1) + \frac{k^2 S \cdot j}{\mu_0^2} \right] \widetilde{W} - (E-1) \widetilde{W}$$

$$= \widetilde{F}_{j \times \beta} \frac{S \cdot j}{\mu_0^2}$$
(6.25)

The "elliptic" character of this one-dimensional system allows rapid inversion for $\widetilde{\mathcal{W}}_{\mathcal{J} \not\subset \mathcal{B}}$ by the method given in Richtmyer and Morton (Difference Methods for <u>Initial Value Problems</u>, P. 199). About 3J operations are needed instead of the \mathcal{J}^2 operations needed with a matrix inversion of (6.25). At this point it is convenient to change the \mathcal{M} subscript to

$$l = n - m$$
 $l = 0, 1, - -, L$ for $m > 0$ (6.26)
 $l = 1, 2, - -, L + 1$ for $m = 0$

and suppress the *M* subscript. We have

$$\begin{split} \beta_{l} &= \beta_{l+m} = \left[\frac{(m+l)^{2} - m^{2}}{4(m+l)^{2} - 1}\right] \left(\frac{l+m-1}{l+m}\right) \\ \delta_{l} &= \delta_{l+m} = \left(\frac{m+l+2}{m+l}\right) \beta_{l+1} \\ \delta_{l} &= 0, \delta_{l} = 0 \text{ for } m > 0; \quad \beta_{l} = 0, \delta_{l} = 0 \text{ for } m = 0 \end{split}$$

$$\end{split}$$
(6.27)

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We also define

$$\mathcal{V}_{l} = M(M+1) = (l+m)(l+m+1)$$
 (6.28)

Equation (6.20) yields (m > o)

$$\begin{split} \ell = o: \left(\frac{\Im\tilde{S}}{\Im t}\right)_{j} &= \tilde{A}_{j,0} - \beta_{j} \left[\in \tilde{W}_{j+1,\overline{1}} - (\epsilon-1) \tilde{W}_{j,1} \right] \\ \ell = l_{j} - j_{L-1} : \left(\frac{\Im\tilde{S}}{\Im t}\right)_{j,1} &= \tilde{A}_{j,1} - \mathcal{Y}_{L-1} \left[\in \tilde{W}_{j+1,L-1} - (\epsilon-1) \tilde{W}_{j,L-1} \right] \\ &= \beta_{J+1} \left[\in \tilde{W}_{j+1,L+1} - (\epsilon-1) \tilde{W}_{j,L+1} \right] \\ \ell = L: \left(\frac{\Im\tilde{S}}{\Im t}\right)_{j,L} &= \tilde{A}_{j,L} - \mathcal{Y}_{L-1} \left[\in \tilde{W}_{j+1,L-1} - (\epsilon-1) \tilde{W}_{j,L-1} \right] \\ \text{while (6.23) gives} \\ \ell = o: -S_{j,V} \tilde{W}_{j,0} &= -\gamma_{0} \tilde{B}_{j,0} + \beta_{1} \left[\frac{\Im\tilde{S}}{\Im t}\right]_{j,L-1} - \frac{\Im\tilde{S}}{\Im t}_{j,L-1} \right] \\ \ell = l_{j} - j_{L-1} : -S_{j,V} \tilde{W}_{j,L} &= -\gamma_{L} \tilde{B}_{j,L} + \mathcal{Y}_{L-1} \left[\frac{\Im\tilde{S}}{\Im t}\right]_{j,L-1} - \frac{\Im\tilde{S}}{\Im\tilde{t}}_{j,L-1} - \frac{\Im\tilde{S}}{\Im\tilde{t}}_{j,L-1} \right] \\ \ell = L : -S_{j,V} \tilde{W}_{j,L} &= -\gamma_{L} \tilde{B}_{j,L} + \mathcal{Y}_{L-1} \left[\frac{\Im\tilde{S}}{\Im\tilde{t}}_{j,L-1} - \frac{\Im\tilde{S}}{\Im\tilde{t}}_{j,L-1} \right] \\ \ell = L : -S_{j,V} \tilde{W}_{j,L} &= -\gamma_{L} \tilde{B}_{j,L} + \mathcal{Y}_{L-1} \left[\frac{\Im\tilde{S}}{\Im\tilde{t}}_{j,L-1} - \frac{\Im\tilde{S}}{\Im\tilde{t}}_{j,L-1} \right] \end{split}$$

Differencing (6.29) in $\frac{1}{0}$ introduces the important operator

 $\mathcal{D}()_{j} = \epsilon()_{j+1} - (2\epsilon - 1)()_{j} + (\epsilon - 1)()_{j-1}^{(6.31)}$

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and results in the following equations:

$$\begin{split} \mathcal{I} = o: \frac{\partial \tilde{J}}{\partial t_{j0}} - \frac{\partial \tilde{J}}{\partial t_{j-10}} &= \tilde{A}_{j0} - \tilde{A}_{j-10} - \mathcal{O}\left(\beta, \tilde{W}_{j1}\right) \\ \mathcal{I} = I_{j-1} \mathcal{I}^{-1} : \frac{\partial \tilde{J}}{\partial t_{j-1}} - \frac{\partial \tilde{J}}{\partial t_{j-1}} &= \tilde{A}_{j-1} \mathcal{I}^{-1} - \tilde{\mathcal{O}}\left(\beta, \tilde{W}_{j-1}\right) \\ \mathcal{I} = L: \frac{\partial \tilde{J}}{\partial t_{j-1}} - \frac{\partial \tilde{J}}{\partial t_{j-1}} &= \tilde{A}_{j-1} - \tilde{\mathcal{O}}\left(\gamma, \tilde{W}_{j-1}\right) \\ \text{Using these to eliminate } \partial \tilde{J} / \partial t \text{ in (6.30) gives us the destined system in } \tilde{W} \text{ alone:} \\ \mathcal{I} = o: \\ \mathcal{J}_{j} = \mathcal{O}\left(\gamma, \tilde{W}_{j} + \beta, \tilde{W}_{j}\right) - S_{j} \nu_{0} \tilde{W}_{j0} = -\nu_{0} \tilde{B}_{j0} + \beta_{1} \left(\tilde{A}_{j-1} - \tilde{A}_{j-10}\right) \\ \mathcal{I} = 1: \\ \mathcal{J}\left[\left(\gamma_{0}, \beta, + \gamma, \beta_{1}\right) \tilde{W}_{j}, +\beta_{2} \beta, \tilde{W}_{j3}\right] - S_{j} \nu_{0} \tilde{W}_{j}, \\ \mathcal{J} = 2, - , L^{-2:} \\ \mathcal{O}\left[\left(\gamma_{1} \mathcal{J}_{j} + \gamma, \beta_{1} - \lambda_{1} -$$

(Note the equation for l = L is not obtained from the equation for l = 2, --, L-2 by simply putting l = L with $\widetilde{A}_{j,L+1}$ and $\widetilde{W}_{j,L+2} = 0$.) We have now a system of only (J-2)(L+1) = 1444 equations for $\widetilde{W}_{j,L+2}$. We can go farther, however.

Let us concentrate on the case of odd \underline{L} . First note that equations (6.33) divide into two independent sets for $\widetilde{W}_{\mathcal{A}}$, whether \underline{L} is even or odd. For odd \underline{L}

Set I:
$$l = 0, 2, ---, L-1$$
 ($m > 0$)
Set II: $l = 1, 3, --, L$ ($m > 0$)
(6.34)

Let us define

$$G_{1} = \frac{\chi_{1}}{\chi_{l+2}} = \frac{\beta_{l+1}}{\chi_{1}} = \frac{\beta_{l+1}}{\chi_{1}} = \frac{\left[(m+l+1)^{2}-m^{2}\right]\left[(m+l+2)^{2}-m^{2}\right]\left(1-m^{2}\right]}{\left[(4(m+l+1)^{2}-l)^{2}-l^{2}\right]} = \frac{\beta_{1}}{\left[(4(m+l+1)^{2}-l)^{2}-l^{2}\right]}$$

$$H_{j} = \mathcal{Y}_{l-1} B_{j} = \frac{\mathcal{Y}_{l}}{\mathcal{Y}_{l-1}} B_{l}^{2} = \frac{\left[(l+m)^{2} - m^{2} \right] \left[(l+m)^{2} - 1 \right]}{\left[4 (l+m)^{2} - 1 \right] (l+m)^{2}}$$
(6.36)

$$v_{l} = (l+m)(l+m+1)$$
 (6.37)

$$\mu_{l} = \frac{8l}{\nu_{l+1}} = \frac{\beta_{l+1}}{\nu_{l}}$$
(6.38)

By using the relation

$$\mathcal{X}_{l} = \frac{\mathcal{Y}_{l+1}}{\mathcal{Y}_{l}} \mathcal{B}_{l+1}$$

from (6.27), equations (6.33), after division by the γ_{ℓ} appearing in each of them, can be rewritten as

1/2

39.

If we now define an index k common to both sets I and II, according to the following scheme (for M > 0),

$$k: 1 2 3 -- \frac{L+1}{2}$$

Set I, $l=2k-2: 0 2 4 -- L-1$
Set I, $l=2k-1: 1 3 5 -- L$ (6.40

we can define an (L+1)/2 square matrix A_{2k} with non-zero elements only along the main and adjacent diagonals. These are, for the two sets I and II, as follows:

40. Set II (l=ah-1) Set I (l=2k-2) Hi $\frac{1}{\nu}(H_1+H_2)$ A ,,1 G A ,,2 G Gl-2 Ge-z Ak, k-1 (6.41)A k, le $\frac{1}{\nu_{p}}(H_{\ell}+H_{\ell+1})$ $\frac{1}{20}(H_{l}+H_{l+1})$ G Ge Ak, k+1 $A_{\underline{L+1}} \underbrace{L-1}_{\underline{L-3}} \qquad G_{\underline{L-3}}$ G_1-2 $\begin{array}{c} A_{\underline{l+l}} \underbrace{L+l}_{Z, Z} \underbrace{L+l}_{Z, Z$ $\frac{1}{2}H_{L}$ We also designate \widetilde{F}_{ik} as the proper one of the \widetilde{F}_{ik} in (6.39) according to the scheme (6.40). Equations (6.39) can then be expressed as a single matrix equation, of the same symbolic form for Set I and II: $(\mathcal{A} A_{k,2} - S, S_{k,2}) \widetilde{W} = \widetilde{F}_{\cdot,k}$ (6.42) where δ_{kl} is the unit matrix. A_{kl} is symmetric and has a set of (L+1)/2 real positive eigenvalues λ_p and orthonormal eigenvectors QP [2=1,2,--, +; p=1,2,--, +].

$$A_{kr}Q_{r}^{p} = \lambda_{p}Q_{k}^{p} \qquad (6.43a)$$

$$\sum_{n=1}^{2} Q^{*} Q^{0} = \delta_{pq} \qquad (6.43b)$$

We express

(6.44)

 $\widetilde{W}_{.} = \sum_{p=1}^{N} \bigvee_{p=1}^{p} \bigvee_{n=1}^{p} \sum_{n=1}^{n} \bigvee_{n=1}^{p} \bigvee_{n=1}^{p} \sum_{n=1}^{n} \bigvee_{n=1}^{p} \bigvee_{n=$ insert this into (6.42), use (6.43a), multiply by $\mathcal{Q}_{L}^{\mathcal{F}}$ and sum over h and use (6.43b) to get 1+1

$$\lambda_q \mathcal{D} V_i^{\mathcal{B}} - 5. V_i^{\mathcal{B}} = \sum_{k=1}^{\overline{\mathcal{A}}} \mathcal{Q}_k^{\mathcal{B}} \widetilde{F}_{ik} \equiv -\lambda_g \in D_i^{\mathcal{B}}$$

(6.45)

For ease in applying the Richtmyer-Morton method we rewrite this by dividing to obtain [Refer to the definition of \mathcal{A} in (6.31)]: by $-\lambda_{g} \in$ $-V_{j+1}^{\&} + \left[\frac{2e-1}{e} + \frac{5}{e\lambda_{g}}\right]V_{j}^{\&} - \left(\frac{e-1}{e}\right)V_{j-1}^{\&} = D_{j}^{\&}$ (6.46)

With λ positive, this satisfies the requirements of the R-M.method. To use it we need for each g a pre-computed table of $E_{f}^{\mathscr{B}}$:

$$j = 2, --, J - 1: \quad E_{j}^{\&} = E \stackrel{\circ}{=} \left[(a \in -1) + \frac{S_{j}}{\lambda_{g}} - (e - 1) E_{j}^{\&} (6.47) \right]$$

$$E_{j}^{\&} = E \stackrel{\circ}{=} \left[(a \in -1) + \frac{S_{j}}{\lambda_{g}} - (e - 1) E_{j}^{\&} (6.47) \right]$$

Given these, we first compute

$$j = 1: \quad F_{j}^{\ \ \theta} = 0$$

$$j = 2, --, 5 - 1: \quad F_{j}^{\ \ \theta} = E_{j}^{\ \ \theta} \left[D_{j}^{\ \ \theta} + \left(\frac{\epsilon - 1}{\epsilon} \right) F_{j-1}^{\ \ \theta} \right]$$
(6.48)

Then, in the reverse order j = J - j J - 2, - - -, 2 we get $\forall j = by$ VJ = E WJk Qk (6.49)

$$V_{j}^{g} = E_{j}^{g} V_{j+1}^{g} + F_{j}^{g} \quad j = J - 1, - - , 2 \quad (6.50)$$

The required operations (multiplication plus addition) are 3(J-2)in number .

To compare the matrix inversion with the eigenfunction method we have (defining 1"operation" as 1 multiplication plus 1 addition), for J = 26 and 1=5:

<u>Matrix method</u>: 2 sets of equations, each set $(J-2)\begin{pmatrix} L+1\\ -2 \end{pmatrix}$ in number;

$$2(J-2)^{2}\left(\frac{L+1}{2}\right)^{2} = 10,368 \text{ operations}$$
 (6.51)

Eigenfunction method:

For each function --

"Right hand side": $(J-1)\begin{pmatrix} L+1\\ 2 \end{pmatrix}$ (includes $\bigvee_{J}^{\mathcal{B}}$)

Inversion by R.&M. method: 3(J-2)For (L+1) functions -- $(L+1)\left[(J-2)(3+\frac{L+1}{2})+\frac{L+1}{2}\right]$ (coefficients of)

(L+1) Legendre functions for $j = R_1 - r_2, 5-1$: Reanalysis into $2\left(\frac{L+1}{2}\right)^{2}(J-2)$

Total:

$$(l+1)\left[(J-2)(l+4)+\frac{l+1}{2}\right] = 1,314 \quad (6.52)$$

A factor of 7.9 ($\approx (\mathcal{T}-\mathcal{Z})/3$) is achieved in speed.

The eigenfunction method will also require storage of the $\lambda \not a$ and their associated eigenvectors. For each ML value there are $(L+1) \lambda' s$ and (L+1) eigenvectors, each of the latter having (L+1)/2components. Total storage required for each value of MM is

The above analysis is for M > 0, where M = M + l, l = 0, 1, -, L. For M=0 we have instead the indices m = l = 1, 2, -, L+1. The definitions and relations (6.34) - (6.50) are similar for M=0 except that l is increased by one

Set I: l = 2k - lSet II: l = 2k (m = 0)

The two sets for each \mathcal{M} correspond to distributions of \mathcal{W}_j which are either even or odd functions of \mathcal{M} (sine of latitude).

It is useful at this point to consider the energy integral for a wave number m. We expect the time-rate-of-change of the kinetic energy in a fixed zonal wave number m to be proportional to the m-sum of

$$(\tilde{\mathcal{F}}_{m} \supset \tilde{\mathcal{F}}_{m} / \partial t)(P_{j+1} - P_{j}) \div \mathcal{V}_{m}, \text{ since}$$

$$\frac{\partial}{\partial t} \left(\frac{1}{2} \left[\nabla \Psi\right]^{2}\right) = \nabla \cdot \Psi \nabla \frac{\partial \Psi}{\partial t} - \Psi \frac{\partial \mathcal{F}}{\partial t}.$$

By introducing

 $\tilde{\psi}_{in} = -\frac{1}{2m} \tilde{S}_{in}$

and using the relation

$$\in W_{j+1} - (\epsilon_{-1})W_{j} = (P_{j+1} - W_{j+1} - P_{j}W_{j}) \doteq (P_{j+1} - P_{j})$$

we can write the vorticity equation (6.20) as

$$\frac{(P_{j+i}-P_{j})}{2m} \underbrace{\widetilde{\mathcal{S}}_{m}}_{jm} = \underbrace{\frac{P_{j+1}-P_{j}}{2m}}_{m} \underbrace{\widetilde{\mathcal{S}}_{jm}}_{jm} + \underbrace{\mathcal{K}}_{m-1} \underbrace{\mathcal{L}}_{jm} \left(P_{j} \underbrace{W_{j}}_{j+1} - P_{j} \underbrace{W_{j}}_{jm-1}\right) + \underbrace{\mathcal{B}}_{m+1} \underbrace{\widetilde{\mathcal{L}}}_{jm} \left(P_{j+1} \underbrace{W_{j}}_{j+1} - P_{j} \underbrace{W_{j}}_{jm+1}\right)^{(6.53)}$$

[We suppress the zonal wave number index \mathcal{M}].

By defining $\widetilde{S}_{jm} = \widetilde{\Psi}_{i} - \widetilde{\Psi}_{i}$ $J^{-1}m$ $J^{-1}m$ $\widetilde{S}_{m} = \sum_{j=1}^{J-1} \left(\frac{P_{j+i}-P_{j}}{z_{m}}\right) \widetilde{S}_{jm} \frac{\partial \widetilde{S}_{im}}{\partial T}$ $\Omega_{n} = \sum_{j=1}^{J-1} \frac{P_{i}-P_{i}}{z_{m}} \widetilde{S}_{i} A_{i}, \quad \mathcal{G}_{n} = \mathcal{G}_{n} \widetilde{\Psi}_{n} \frac{W_{n}}{W_{n}} + \mathcal{B}_{n} \frac{W_{n}}{W_{n}} \frac{W_{n}}{W_{n}} + \mathcal{G}_{n} \frac{W_{n}}{W_{n}} \frac{W$

and summing over \int , we obtain

$$\mathcal{R} = \mathcal{Q} + \mathcal{I}_{m} - \mathcal{I}_{m-1} \sum_{j=2}^{J-1} \mathcal{I}_{jm-1} \sum_{jm-1}^{N} \mathcal{I}_{m} - \mathcal{I}_{m+1} \sum_{j=2}^{J-1} \mathcal{I}_{jm-1} \sum_{jm-1}^{J-1} \mathcal{I}_{m+1} \sum_{j=2}^{J-1} \mathcal{I}_{m+1} \sum_{jm-1}^{J-1} \sum_{jm-1}^{J-1} \mathcal{I}_{m+1} \sum_{jm-1}^{J-1} \mathcal{I}_{m+1} \sum_{jm-1}^{J-1} \mathcal{I}_{m+1} \sum_{jm-1}^{J-1} \mathcal{I}_{m+1} \sum_{jm-1}^{J-1} \mathcal{I}_{m+1} \sum_{jm-1}^{J-1} \sum_{jm-1}^{J-1} \mathcal{I}_{m+1} \sum_{jm-1}^{J-1} \sum_{jm-1}^{J-1} \sum_{jm-1}^{J-1} \sum_{jm-1}^{J-1} \sum_{jm-1}^{J-1} \sum$$

The "thermal wind equation" (6.3) and equation (6.21) together give

$$\frac{2}{m-1}\frac{m-1}{2}\int_{m-1}^{\infty}\frac{1}{m+1}\frac{m+1}{2}\int_{m+1}^{m+1}\int_{m+1}^{\infty}\frac{1}{m+1}=-T.$$

or, using the relation $\mathcal{V}_{M} \overset{\mathcal{Y}}{=} \mathcal{V}_{M+1} \overset{\mathcal{B}}{=} \mathcal{B}_{M+1}$ from (6.18), $\mathcal{B}_{M} \overset{\mathcal{S}}{\underset{jM-1}{\longrightarrow}} + \overset{\mathcal{S}}{\underset{jM+1}{\longrightarrow}} = -\overset{\mathcal{T}}{\underset{jM}{\longrightarrow}} \overset{\mathcal{C}}{=} -\overset{\mathcal{C}}{\underset{jM}{\longrightarrow}} \overset{\mathcal{C}}{=} -\overset{\mathcal{C}}{$

(6.55)

We also have (6.4) in the component form [see also (6.23)]

$$\widetilde{W}_{im} = -\frac{1}{S_i} \frac{\partial \overline{T}_{im}}{\partial t} + \frac{B_{jm}}{S_i}$$

Defining also

$$B_{m} = -\gamma \sum_{j=2}^{r} \frac{P_{j}}{s_{j}} \widetilde{B}_{m-1} \widetilde{S}_{jn} - B_{m+1} \sum_{j=2}^{r} \frac{P_{j}}{s_{j}} \widetilde{B}_{jm+1} \widetilde{S}_{jm}$$

allows equation (6.54) to be written as

$$\mathcal{H}_{m} = \Omega_{m} + B + J_{m} + \sum_{j=2}^{m} \frac{F_{j}}{S_{j}} \int_{jm}^{m}$$
 (6.56)

J-1

`whe**re**

$$\overline{\Gamma}_{j,m} = \frac{1}{M-1} \underbrace{\widetilde{S}_{j,m}}_{\partial T} \frac{\partial \overline{T}_{j,m-1}}{\partial T} + \underbrace{\mathcal{B}_{m+1}}_{J,m} \underbrace{\widetilde{S}_{j,m}}_{\partial T} \frac{\partial \overline{T}_{j,m+1}}{\partial T}$$
(6.57)

We now sum (6.57) over M (at fixed M) from M = M to N:

45.

$$\sum_{N=m}^{N} \overline{f_{in}} = \sum_{n=m}^{N-1} \frac{3}{N} \frac{3}{2t} + \sum_{n=m+1}^{N} \frac{3}{N} \frac{3}{N} \frac{3}{2t} + \sum_{n=m+1}^{N} \frac{3}{2t} \frac{3}{2t} + \sum_{n=m+1}^{N-1} \frac{3}{2t} + \sum_{$$

Using (6.55), with $\partial_{jm} = 0$ for M = M - 1 and M = N + 1, gives $N = \sum_{jm} \frac{1}{jm} = -\sum_{m=m} \frac{1}{m} \frac{2\overline{1}jm}{2\overline{1}}$

Using this result in the *M*-sum of (6.56) finally gives

$$\frac{1}{2} \frac{\partial}{\partial t} \sum_{n=m}^{N} \left\{ \sum_{j=1}^{J-1} \frac{(P_{j+1}-P_{j})}{\mathcal{Y}_{n}} (\overline{S}_{jn})^{2} + \sum_{j=2}^{J-1} \frac{P_{j}}{S_{j}} (\overline{T}_{jn})^{2} \right\}$$
(6.58)
$$= \sum_{n=m}^{N} (A_{n} + B_{n} + \overline{J}_{n}).$$

The left-hand side defines the time rate of change of the energy-- kinetic plus available -- associated with a single zonal wave number MM, and the right side (symbolically) represents the net addition of energy into this wave number from heating, friction, orography, and non-linear transfer from other wave numbers.