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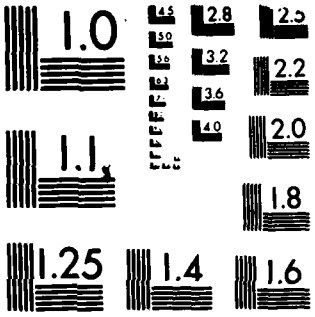

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A THREE-DIMENSIONAL DYNAMICAL-CHEMICAL MODEL OF THE MESOSPHERE AND LOWER THERMOSPHERE FOR UPPER ATMOSPHERIC RESEARCH

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20 January 1984

Final Report
18 May 1981 - 30 September 1983

Approved for public release; distribution unlimited

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~~Unclassified~~
SECURITY CLASSIFICATION OF THIS PAGE

REPORT DOCUMENTATION PAGE

1a. REPORT SECURITY CLASSIFICATION Unclassified	1b. RESTRICTIVE MARKINGS
2a. SECURITY CLASSIFICATION AUTHORITY	3. DISTRIBUTION/AVAILABILITY OF REPORT Approved for public release; distribution unlimited
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE	
4. PERFORMING ORGANIZATION REPORT NUMBER(S)	5. MONITORING ORGANIZATION REPORT NUMBER(S) AFGL-TR-84-0070
6a. NAME OF PERFORMING ORGANIZATION Georgia Institute of Technology School of Geophysical Sciences 6b. OFFICE SYMBOL (If applicable)	7a. NAME OF MONITORING ORGANIZATION Air Force Geophysics Laboratory
6c. ADDRESS (City, State and ZIP Code) Atlanta, Georgia 30332	7b. ADDRESS (City, State and ZIP Code) Hanscom AFB, Massachusetts 01731 Monitor/Thomas J. Keneshea/LKB
8a. NAME OF FUNDING/SPONSORING ORGANIZATION 8b. OFFICE SYMBOL (If applicable)	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER F19628-81-K-0045
8c. ADDRESS (City, State and ZIP Code)	10. SOURCE OF FUNDING NOS.

PROGRAM ELEMENT NO.	PROJECT NO.	TASK NO.	WORK UNIT NO.
62101F	6690	07	AH

11. TITLE (Include Security Classification)
(over)

12. PERSONAL AUTHOR(S)
Alyea, Fred N.

13a. TYPE OF REPORT	13b. TIME COVERED	14. DATE OF REPORT (Yr., Mo., Day)	15. PAGE COUNT
Final Report	FROM ~~5-18-81~~ TO ~~9-30-83~~	20 January 1984	86

16. SUPPLEMENTARY NOTATION

17. COSATI CODES			18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
FIELD	GROUP	SUB. GR.	atmospheric modeling, mesosphere, thermosphere, atmospheric dynamics

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

The recent appearance of new observational data from specialized satellites and rocket probes has led to increased interest in upper atmospheric processes. The work to be reported herein is of the current status of a limited three-dimensional model of the dynamical and important chemical processes which are known to take place in the mesosphere and lower thermosphere to an altitude of about 400 km above the earth's surface.

The modeling approach taken was to make use of the dynamical schemes and simplified chemical treatments embodied in our three-dimensional Stratospheric Circulation Model (SCM) developed for the study of stratospheric ozone (see Cunnold et al., 1975). The basic strategy in the modeling effort was to use the modified SCM codes to specify the large scale dynamical properties of the upper atmospheric region and for the integration of the time dependent, three-dimensional mass continuity equations for the chemically active species. Development of the chemical and sub-scale transport properties of the model were to be (over)

20. DISTRIBUTION/AVAILABILITY OF ABSTRACT UNCLASSIFIED/UNLIMITED ☒ SAME AS RPT. ☒ DTIC USERS ☐	21. ABSTRACT SECURITY CLASSIFICATION Unclassified
22a. NAME OF RESPONSIBLE INDIVIDUAL Thomas J. Keneshea/LKB	22b. TELEPHONE NUMBER (Include Area Code) 22c. OFFICE SYMBOL LKB

DD FORM 1473, 83 APR EDITION OF 1 JAN 73 IS OBSOLETE.

Unclassified
SECURITY CLASSIFICATION OF THIS PAGE

Block 11 (Contd)

A THREE-DIMENSIONAL DYNAMICAL-CHEMICAL MODEL OF THE MESOSPHERE AND LOWER THERMOSPHERE FOR UPPER ATMOSPHERIC RESEARCH

Block 19 (Contd)

undertaken by the AFGL group under the direction of Dr. S. P. Zimmerman. Thus, the complete modeling program was devised to be a cooperative venture between Georgia Tech and AFGL.

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0. Introduction and Accomplishments

Introduction

The recent appearance of new observational data from specialized satellites and rocket probes has led to increased interest in upper atmospheric processes. The work to be reported herein is of the current status of a limited three-dimensional model of the dynamical and important chemical processes which are known to take place in the mesosphere and lower thermosphere to an altitude of about 400 km above the earth's surface. Unfortunately, funds for the program were cut off prior to its completion and thus the model codes have not been finalized. It is hoped that this program can be picked up again in the near future.

The modeling approach taken was to make use of the dynamical schemes and simplified chemical treatments embodied in our three-dimensional Stratospheric Circulation Model (SCM) developed for the study of stratospheric ozone (see Cunnold, et al., 1975). This model has been running on the now defunct ILLIAC-4 vector computer at NASA's Ames Research Center in California. In addition to large changes required in the existing dynamics and chemistry to reform the model for thermospheric and mesospheric levels, it was also necessary to revise the code structure to accommodate the shift from the ILLIAC machine to the AFGL CDC-660 computer. Much of this work was accomplished on the NASA machines prior to the availability, through special modems and telephone connections, of the AFGL CDC-6600. Since that time the programs have been transferred to AFGL and, while not completed, tests of the model dynamics on that machine have been undertaken.

The basic strategy in the modeling effort was to use the modified SCM codes to specify the large scale dynamical properties of the upper atmospheric region

and for the integration of the time dependent, three-dimensional mass continuity equations for the chemically active species. Development of the chemical and sub-scale transport properties of the model were to be undertaken by the AFGL group under the direction of Dr. S. P. Zimmerman. Thus, the complete modeling program was devised to be a cooperative venture between Georgia Tech and AFGL.

Accomplishments.

The program's goal was to create a three-dimensional model of the mesosphere and lower thermosphere over a three-year period with limited funds. The model was to incorporate simplified dynamics and interactive chemistry. A "first" run of a single simulation experiment with the completed model was anticipated late in the third year. Thus, intermediate results of a scientifically viable nature could not be expected prior to completion of the program. While the program has been cut short before these goals could be attained, substantial progress has been made, particularly in the modification of the dynamical portions of the model codes and the changes required to run the model on the AFGL CDC-6600 machine.

A. Model heating

One of the principal needs of the upper atmospheric model is the incorporation of realistic heat forcing processes for the 40-400 km regions of interest. Considerable thought, therefore, has been given to this problem.

The existing Dynamical/Chemical Stratospheric Circulation Model (SCM), which is being revised for the present work to include mesospheric and lower thermospheric levels, currently uses heating codes applicable to altitudes below $\sim$ 80 km. Since a number of quite different physical processes lead to atmospheric heating in the thermosphere, new model codes will have to be developed for these thermospheric levels. For this, however, we must keep in mind that such codes must be considerably simplified because of time and size limitations which must be imposed on the already large three-dimensional calculations.

Some of the heating processes we have considered include:

(1) Direct solar absorption

It is convenient to divide the solar spectrum into several large wavelength segments according to their absorption characteristics and treat each of these segments separately.

a. 2050 - 3000 Å region.

Heating is due to absorption by both O_2 and O_3 in this region and is most important at the lowest thermospheric and mesospheric levels (i.e., < 100 km). Model treatment for this region can be essentially the same as was devised for the SCM (see Cunnold, et al., 1975). For example, for O_3, the rate of temperature change due to O_3 absorption is approximated by the linear law

$$\left(\frac{\partial T}{\partial t}\right)_{O_3} = \frac{\chi_{O_3}}{M} Q(N\sec\zeta)$$

where χ_{O_3} is the number mixing ratio of O_3, M the mass of an average air molecule, $Q(N\sec\zeta)$ the heating rate due to absorption by one molecule of O_3, N is the number of O_3 molecules in the cm^2 vertical column above the point of heating, and ζ is the solar zenith angle. In the SCM calculations the heating rate, Q, is approximated by a finite sum over a number of small spectral intervals centered on wavelengths λ_i in the form

$$Q(N\sec\zeta) = \sum_i \alpha_{O_3}(\lambda_i)\, F(\lambda_i)\, \frac{1}{\lambda_i} \exp(-\, N\sec\zeta)$$

in which $\alpha_{O_3}(\lambda_i)$ is the absorption coefficient of O_3 and $F(\lambda_i)$ is the solar flux of photons integrated over each λ_i interval. In the calculations, tables of α_{O_3}, F, and the exponential functions are maintained for a wide range of likely values.

b. 1027 - 1300 Å and 1750 - 2050 Å (Schumann-Runge bands) regions.

Absorption by O_2 in these two banded regions is comparatively large below about 120 km altitude but can probably be safely neglected above this level. As in the 2050 - 3000 Å region we can estimate the heating rates by summing over the important absorption bands using band averages as tabulated by Hudson and Mahle (1972) for the 1750 - 2050 Å region (although the apparent temperature dependence of the cross sections is a complication) and by Adams (1974) for the 1027 - 1300 Å region.

c. 1300 - 1750 Å (Schumann-Runge continuum) regions.

For this O_2 absorption region, the absorption cross sections are quite consistent and we should be able to treat this region as a single band. Heating by absorption in this region is most important to total heating at levels between ∿ 100 and 130 km.

d. 40 - 1027 Å (EUV) region.

Nearly all photons in this frequency range are absorbed by photoionization of N_2, O_2, and O which leads to very complicated ionization and photoelectric processes. These processes are particularly dominant above ∿ 110 km but are replaced by heating through collisional processes above ∿ 300 km. It may be possible to estimate the magnitude of the heating resulting from photon absorption in the 40 - 1027 Å region by using a simple electron density model such as that of Ching and Chiu (1973) to infer photon absorption quantities and apply a heating efficiency factor of ∿ 30 - 35% (Stolarski, et al., 1975). Such a model is currently being tested.

(2) Atomic oxygen recombination and deactivation

Atomic oxygen produced at high model altitudes does not recombine (and thus release its chemical energy of recombination) above $\sim$ 120 km. Two processes, $O + O + M \rightarrow O_2 + M$ and $O + O_2 + M \rightarrow O_3 + M$ may be important here. A simple estimate for heating by these processes may be possible by assuming (Adams, 1974) that the lifetime of an oxygen atom goes from $\sim$ 5000 years at 150 km to $\sim$ 2 hours at 80 km. Clearly, model vertical transports will play a large role here.

The process of deactivation of $O(^1D)$ is somewhat uncertain but potent .ly important to heating in the lower thermosphere. Whatever the mechanism ($O(^1D) + M \rightarrow O(^3P) + M + KE$ is the prime candidate), the reaction takes place very fast and, since there is no known large source for $O(^1D)$ at night, is confined to sunlit hours. A possible estimate for $O(^1D)$ deactivation in the model may be obtained by using the results of Adams (1974, pg. 97) with suitable adjustments for diurnal and latitudinal variations.

3. Molecular thermal conduction

The flux of heat across a horizontal surface, F_Z, is usually parameterized using

$$F_Z = -K \frac{\partial T}{\partial Z}$$

where here K represents a thermal conduction coefficient. This is a fairly simple process to represent computationally but the selection of the proper K's will be done in consultation with the AFGL group.

4. 15μ CO_2 and 62μ O radiational cooling

Various authors have estimated cooling rates for these two frequencies

and the model parameterization will make use of a simplified version of one of these. The 62μ O band is particularly effective above ∿ 110 km while the 15μ CO_2 band seems to dominate below that level.

5. Other heating processes

Thermal heating by the dissipation of tidal and gravity waves may be important to the thermosphere. In three dimensional models, such as we are working with here, these heat quantities will be realized through the thermal and dynamic dissipation terms built into the model equations.

Joule heating and non-thermal emissions may also play a role in total thermospheric heating but their magnitudes are usually thought to be small and will thus be neglected in the current work.

B. Model lower boundary conditions

The Stratospheric Circulation Model (SCM) has been reconfigured in its vertical structure to incorporate the region $\sim$ 40 km - 400 km in its 26 vertical levels. As required by the model, mean global temperatures ($\bar{T}$) and stability quantities ($\frac{d\bar{T}}{dZ} - \frac{R}{C_p}\bar{T}$) at each level were obtained from the U.S. Standard Atmosphere. The quantities will be discussed and displayed in some detail in later sections. However, we want to point out that the new Mesospheric and Lower Thermospheric Model (MTM) overlaps the height range of the SCM over the MTM's lowest six levels. Thus, it will be possible to "drive" the lower boundary of the MTM using values computed from annual runs of the SCM. To this end, a special run of the SCM for a two year integration period was performed on the machine at NASA's Ames Research Center. From these results, we have obtained for transference to AFGL:

(1) A set of lower boundary conditions for temperature (T), vertical motion (W) and ozone (χ). A complete one-year cycle of these quantities for the model's 70 horizontal degrees of freedom were collected at four-hour intervals. Thus, we have tabulated (on a computer tape) the required lower boundary conditions to drive the MTM as functions of both time and space. This involves more than 1/2 million values.

(2) Twelve sets of initial conditions, one for each month of the year, were generated by the SCM runs and tabulated on tape files. This data includes values for the model temperatures, vertical motions and ozone mixing ratios in the region of overlap between the SCM and the MTM. In addition, a set of time dependent total heating values from the SCM have been collected for the one year cycle for use in driving the MTM during early dynamical tests. These functions

will be replaced by internally derived heating quantities in the MTM's final form.

All of the data fields described in (1) and (2) have been transferred (in ASCII codes) to the AFGL 6600 disk system and are available for use in the model although some may not have been rewritten in binary form as required by the MTM input scheme.

To incorporate these lower boundary conditions, the MTM codes have been extensively rewritten and tested. Furthermore, new codes have been generated to allow for the introduction of additional minor species into the model calculation in fully predictive form (through the species continuity equations). Details of the chemical production and loss terms, however, are to be added later in cooperation with the AFGL research group.

C. Dynamical tests

A considerable problem arises in working with large, non-linear numerical models concerning the viability of the final computer codes. That is, how can one feel confident that the code is correctly performing the numerical integrations originally envisioned? Even changing a working program from machine to machine frequently introduces computational errors which cannot always be detected by simple model runs. It is necessary, therefore, to subject such model codes to rigorous testing procedures whenever the codes are modified or transported to other machines. Such a procedure was undertaken and completed for the dynamical portion of the MTM subsequent to introduction of the model changes outlined in sections A and B above. Similar checks were underway for the version transferred to the AFGL CDC 6600 at the time of the stoppage of work on the model.

Of particular concern is the performance of the non-linear terms in the dynamical sections of the MTM. We thus make use of known conservative properties of the model to test for "correctness" of solutions under various model circumstances. Some care, however, has to be taken in this procedure since it is frequently very difficult to distinguish true model or programming errors from normal numerical or machine induced inaccuracies.

One series of tests which have been completed for the MTM involves running the model with the heating, frictional dissipation and lower boundary vertical motion terms all set to zero. Thus, the quasi-geostrophic set of dynamical equations reduce to the form

$$\frac{\partial \nabla^2 \psi}{\partial t} = -2\Omega \frac{\partial \psi}{\partial \lambda} - J(\psi, \nabla^2 \psi) - \nabla \cdot f \nabla \left(\frac{\partial X}{\partial P}\right)$$

$$\frac{\partial T'}{\partial t} = -J(\psi, T') - \frac{\sigma}{P} \nabla^2 X \qquad (0.1)$$

$$R \nabla^2 T = \nabla \cdot f \nabla \left(\frac{\partial \psi}{\partial Z}\right)$$

and we can show, for example, that total energy (kinetic plus available potential) must be preserved (for details of the model, see the following sections). Table 0.1 contains the results of several runs under varying conditions. As a base case, Run "A" was computed using the normal N-cycle scheme of Lorenz (1971) with N = 4 and an internal time step δt = 1 hour. We see from the table that $\sim$ 0.06% of the initial model energy has been lost after one day of computations and $\sim$ 0.19% at the end of two days. Thus, the energy has not been preserved (which, of course, is not unexpected) and we must ascertain whether the inaccuracy is due to our numerical approximations or results from some more important physical or computational problem.

Run "B" is similar to "A" but we have removed the non-linear Jacobian terms from (0.1). For this case, the table shows that the energy conserves much better during the first two days, losing only $\sim$ 0.014%. From these results it appears that the Jacobian terms generate the major inaccuracies in the model runs but it is still not certain whether this can be attributed to model errors or to numerical approximations. One possibility would be to change the N-cycle routine from four to eight cycles per step as an attempt to generate a more accurate solution. This can be of help, particularly for the linear parts of the Jacobian calculations. Still maintaining δt = 1 hour for the internal time intervals, Run "C" repeats the calculation of "A" for N = 8 with no improvement

Table 0.1: Total energy as a percent of the initial total energy for days 0, 1, and 2 of test Runs "A" through "F". The conditions for each run are described below the table.

Day	Run "A"*	Run "B"*	Run "C"*	Run "D"*	Run "E"*	Run "F"*
0	100.000	100.000	100.000	100.000	100.000	100.000
1	99.943	99.993	99.942	99.999	99.478	99.299
2	99.812	99.986	99.797	99.996	99.962	99.719

* All the Runs make use of the Lorentz N-cycle time stepping scheme and, unless otherwise indicated below, the friction, heating, and lower boundary vertical motion terms are all zero. The specific conditions for each run are:

Run "A": Uses the 4-cycle scheme with internal time steps $\delta t = 1$ hour.

Run "B": Same as "A" but the non-linear Jacobian (advection) terms in (0.1). are zero.

Run "C": Same as "B" but uses 8-cycles.

Run "D": Same as "A" but $\delta t = 0.2$ hours.

Run "E": Same as "A" but the lower boundary vertical motion (W_{Bot}) is forced using the results of a Stratospheric Circulation Model (SCM) computation.

Run "F": Same as "E" but heating from the SCM computation has been added.

in the accuracy of the solutions (as seen in the table). On the other hand, when we repeat the calculation of Run "A" (4 cycle) but with internal time step intervals reduced to 12 minutes (δt = 0.2 hours), the accuracy greatly improves (Run "D") with an energy loss of only $\sim$ 0.004% during the first two days. Clearly, the small energy losses observed over the first two days of the model test runs are due to numerical inaccuracies in the time stepping scheme rather than to coding errors in the Jacobian terms.

To get an idea of the relative importance of the numerical errors detected above, we ran two more experimental tests. The first of these was computed under the conditions of Run "A" but with the vertical motion at the lower boundary of the model introduced from the results of previous runs of the SCM. For the second test we added the computed heating values from the SCM to the lower levels of the MTM. The results, shown as Runs "E" and "F" in Table 0.1, show that the energy changes introduced by these physical terms in the model are at least as large as the uncertainties created by the numerical procedures used. Thus, reductions in the time step increments used for the model to improve the accuracy of the non-linear terms are not justified since they would be masked by the forcing and boundary terms.

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

$$\left.\begin{aligned} P &= p \div (100 \text{ cbar}) \\ Z &= -\ell n P, \; P = e^{-Z} \end{aligned}\right\} . \tag{1.1}$$

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

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

The vertical levels will be separated by a uniform value of ∇Z. To the extent that the temperature T is approximately uniform at near surface values, a change of one in Z corresponds to a height change of the order of 7 km. The bottom of the atmosphere, but not necessarily of the model, 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 dynamical system not only assumes hydrostatic balance, but also a "quasi-geostrophic blance" 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:

$$f = 2\Omega \sin\phi$$
$$\Omega = 7.292 \times 10^{-5} \text{ rad sec}^{-1} \tag{1.3}$$

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:

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

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

$$\left.\begin{aligned} u &= a \cos\phi \frac{d\lambda}{dt} = -\frac{1}{a}\frac{\partial\psi}{\partial\phi} - \frac{1}{a\cos\phi}\frac{\partial\chi}{\partial\lambda} \\ v &= a\frac{d\phi}{d\tau} = \frac{1}{a\cos\phi}\frac{\partial\psi}{\partial\lambda} - \frac{1}{a}\frac{\partial\chi}{\partial\phi} \end{aligned}\right\} . \tag{1.5}$$

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

$$\zeta = \hat{k} \cdot \text{curl } \vec{v} = \nabla^2\psi; \text{ div } \vec{v} = -\nabla^2\chi \tag{1.6}$$

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

The condition of the quasi-geostrophic balance is

$$\nabla \cdot f\nabla\psi = g\nabla^2 z \tag{1.7}$$

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

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

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":

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

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

The continuity equation (conservation of mass) is

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

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

$$X = -\int_{p_{top}}^{p}\chi dp, \; \chi = -\frac{\partial X}{\partial P} \quad . \tag{1.12}$$

Equation (1.10) can then be rewritten as

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

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

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

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

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

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

$$PW = \nabla^2 x \quad . \tag{1.16}$$

Boundary conditions on W are that W vanishes at Z_{top} and that it is given from external sources at the bottom:

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

$$Z = Z_{bot}: W = W_0(t,\lambda,\phi) \text{ as given.} \tag{1.17a}$$

Since Z_{bot} is some distance above the actual earth's surface, we must also specify the bottom dynamical and thermodynamical conditions. For this purpose, we will make use of previous runs of the model version which includes the surface as its bottom boundary. The results from such a computation will be used to specify the bottom boundary temperature field (in space and time) for the present upper level model. Thus, we have

$$Z = Z_{bot}: T = T_0(t,\lambda,\phi) \text{ as given.} \tag{1.17b}$$

The bottom streamfunction field will then be given through the thermal wind equation.

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 $\nabla\cdot\vec{F}r\times\hat{k} = \frac{\partial}{\partial p}\,[\nabla\cdot(\frac{-g}{p_0}\vec{\tau}\times\hat{k})]$. We set $\vec{\tau} = \rho K_m\,\partial(\hat{k}\times\nabla\psi)/\partial z$, giving

$$\nabla\cdot(\frac{-g}{p_0}\vec{\tau}\times\hat{k}) = \nabla\cdot[\frac{g^2\rho^2}{p_0^2}K_m\frac{\partial\nabla\psi}{\partial p}]$$

Using the "scale height"

$$H_0 = \frac{RT_0}{g}\,, \tag{1.18}$$

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

$$\nabla\cdot[\frac{-g}{p_0}\vec{\tau}\times\hat{k}] = -\frac{K_m}{H_0^2}\,P\,\frac{\partial\nabla^2\psi}{\partial Z}\,.$$

To summarize the friction term we can write

$$\left.\begin{aligned} &\nabla\cdot\vec{F}r\times\hat{k} = \frac{\partial}{\partial P}(PF) \\ &Z>0:\ F = \frac{K_m}{H_0^2}\,P\,\frac{\partial\nabla^2\psi}{\partial Z} \end{aligned}\right\}\,. \tag{1.19}$$

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

$$C_p\,\frac{d}{dt}\,[\ell n(Tp^{-\kappa})] = \frac{q}{T}\ ;\ \kappa = \frac{R}{C_p} = \frac{2}{7} \tag{1.20}$$

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

of T, this becomes

$$\frac{\partial T}{\partial t} = -(\hat{k}x\nabla\psi - \nabla\chi) \cdot \nabla T - W\frac{\partial T}{\partial Z} - \kappa WT + \frac{q}{C_p} \tag{1.21}$$

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

$$\left.\begin{aligned} T &= \overline{T}(p,t) + T'(\lambda,\phi,p,t) \\ \overline{T} &= \frac{1}{4\pi a^2}\int_{-\pi/2}^{\pi/2} \cos\phi d\phi \int_0^{2\pi} T d\lambda;\ \overline{T'} = 0 \end{aligned}\right\} \tag{1.22}$$

[This definition of $(\overline{\ })$ and $(\ )'$ will be applicable to any variable.] This greatly simplifies the computations, and is reasonably accurate because $\nabla\psi >> \nabla\chi$ and $\partial T'/\partial Z + \kappa T'$ is generally small compared to $\partial\overline{T}/\partial Z + \kappa\overline{T}$. The result is

$$\frac{\partial T}{\partial t} = -\hat{k}x\nabla\psi \cdot \nabla T - W(\frac{d\overline{T}}{dZ} + \kappa\overline{T}) + q/C_p \quad . \tag{1.23}$$

However, this simplification has the result that we can no longer interpret (1.23) as forecasting $\overline{T}$, the horizontally averaged T; this is because the horizontal average of (1.23) gives simply

$$\frac{\partial\overline{T}}{\partial t} = \overline{q}/C_p$$

whereas the horizontal average of the exact equation (1.21) gives

$$\frac{\partial\overline{T}}{\partial t} = \frac{\overline{q}}{C_p} - \kappa\overline{W'T'} - \frac{1}{P}\frac{\partial}{\partial Z}(P\overline{W'T'}), \tag{1.24}$$

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 discussed separately.]

In passing, we note that

$$\begin{aligned} \frac{\partial T}{\partial Z} + \kappa T &= \frac{RT}{g}\left(\frac{\partial T}{\partial z} + \frac{g}{C_p}\right) \\ &= T\frac{\partial}{\partial Z}\left[\ln(Tp^{-\kappa})\right] \\ &= \frac{N^2}{R}\left(\frac{RT}{g}\right)^2 \end{aligned} \tag{1.25}$$

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

$$x_i = n_i \div n_m \tag{1.26}$$

where n_i is the number density of the i-th trace substance, n_m is the total number density. For levels below $\sim$ 110 km we use

$$\begin{aligned} n_m &\cong p/kT \\ k &= \text{Boltzman constant} = 1.380\times10^{-26} \text{ kilojoules deg}^{-1} \end{aligned} \tag{1.27}$$

Above $\sim$ 110 km, $n_m = \sum_i n_i$.

The equation for dx_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 photochemical generation of the substance (number per unit volume per unit time) and K_d is the vertical eddy-diffusion coefficient [with dimensions length)^2 ÷ time]. K_d will vary only with P.

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

$$\frac{\partial}{\partial P}\left[K_d\left(\frac{gP}{RT}\right)^2\frac{\partial \chi_i}{\partial P}\right] \approx \frac{\partial}{\partial P}\left[-\frac{K_d}{H_0^2}P\frac{\partial \chi_i}{\partial Z}\right] \tag{1.28}$$

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

$$\frac{\partial \chi_i}{\partial t} = -(\hat{k}\times\nabla\psi-\nabla\chi) \cdot \nabla\chi_i - W\frac{\partial \chi_i}{\partial Z} + \frac{1}{n_m}\left(\frac{dn_i}{dt}\right)_c + \frac{\partial}{\partial P}\left[-\frac{K_d}{H_0^2}P\frac{\partial \chi_i}{\partial Z}\right] \tag{1.29}$$

or

$$\frac{\partial \chi_i}{\partial t} = -\frac{1}{P}\left[\nabla\cdot(P\vec{v}\chi_i) + \frac{\partial(PW\chi_i)}{\partial z}\right] + \frac{1}{n_m}\left(\frac{dn_i}{dt}\right)_c + \frac{\partial}{\partial P}\left[-\frac{K_d}{H_0^2}P\frac{\partial \chi_i}{\partial Z}\right] \tag{1.30}$$

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

The rate of change of $\bar{\chi}_i$ (the horizontal average) is obtained from the horizontal average of (1.30):

$$\frac{\partial \bar{\chi}_i}{\partial t} = \frac{\partial}{\partial P}[P\ \overline{W'\chi_i'}] + [\overline{\frac{1}{n_m}\left(\frac{dn_i}{dt}\right)_c}] + \frac{\partial}{\partial P}[-\frac{K_d}{H_0^2} P \frac{\partial \bar{\chi}_i}{\partial Z}] \tag{1.31}$$

The rate of change of χ_i' will, however, be obtained from a simplified form of (1.29), much as was done in the thermodynamic equation (1.23):

$$\begin{aligned}\frac{\partial \chi_i'}{\partial t} = &- \hat{k}x\nabla\psi \cdot \nabla\chi_i' - W\frac{\partial \bar{\chi}_i}{\partial Z} \\ &+ [\frac{1}{n_m}\frac{dn_i}{dt}]_c' + \frac{\partial}{\partial P}[-\frac{K_d}{H_0^2} P \frac{\partial \chi_i'}{\partial Z}]\end{aligned} \tag{1.32}$$

In contrast to $\bar{T}$, where we are for the most part content to take $\bar{T}$ as given, we must predict $\bar{\chi}_i$ as well as χ_i'. Equation (1.31) will therefore be used as well as (1.32).

[Presumably (1.33) need not be applied every time step in the numerical integration, $\bar{\chi}_i$ 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.]

A special treatment of the minor species equation will be necessary at certain levels. As an example, Lindzen and Goody (J. Atmos. Sci., 1965, P. 341) show that the photodissociation of ozone is extremely rapid at heights above 45 km, with a time constant becoming less than 1 hour. (They presumably use typical values of incident solar radiation). The conventional methods of "time-

stepping) equations such as (1.32) require a computational time step no longer than the characteristic physical times associated with terms on the right side of (1.32). Since the advective time scale is of the order of an hour or so, we must consider replacing (1.31) and (1.32) at these levels by the <u>equilibrium condition</u>.

$$\chi_i = (\chi_i)_{equil} \iff \frac{dn_i}{dt} = 0 \tag{1.33}$$

2. Choice of vertical levels.

We obtain equal intervals in $Z = -\ell n P$ (P = pressure : 100 cb) by defining

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

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

$$Z = \frac{Z_1}{J-1} = \frac{Z_{top}}{J-1} \quad .$$

A convenient choice is obtained by choosing

$$\begin{aligned} e^{\Delta Z} &= r, \quad r = 2.12472 \\ \Delta Z &= \ell n r = 0.753640 \end{aligned} \tag{2.2}$$

so that

$$\begin{aligned} Z_1 &= Z_{top} = (J-1)\ell n r \\ P_1 &= r^{-(J-1)} \quad . \end{aligned} \tag{2.3}$$

Successive pressure levels are separated by (roughly) 6 km below the turbopause. The relations

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

are useful. At these levels, the following basic variables will be represented $j = 1, 2, \ldots, J$: T_j, W_j, $(\chi_i)_j$ together with the heating rate, the photochemical term, and the vertical turbulent fluxes of momentum. At the intermediate levels

the streamfunction ψ_j will be represented

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

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

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

This results in the scheme as seen in Figure 2.1.

Table 2.1 lists the values of the more basic variables for the choice $r = 2.12472$, $J = 26$. Values of $\bar{T}$ were taken from the U.S. Standard Atmosphere, 1976 (NOAA, NASA, and USAF). The static stability parameter S is defined later in equation (3.20).

Figure 2.1: Vertical levels of the model and the location on these levels of the model variables.

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

TABLE 2.1

Pressure, temperature, approximate height, and static stability for model levels.

Level	Z (= $-\ell n(p/1000mb)$)	p(mb)	$\overline{T}$(°k)	z(km)	$\frac{d\overline{T}}{dZ} + \frac{R}{c_p}\overline{T}$(°k)
1	24.92	0.15 (-7)	995.5	398.0	289.01
2	24.17	0.32 (-7)	991.0	354.3	292.70
3	23.42	0.68 (-7)	981.0	313.6	299.13
4	22.66	0.14 (-6)	962.5	275.2	308.45
5	21.91	0.31 (-6)	930.5	240.7	321.53
6	21.15	0.65 (-6)	878.5	210.0	336.53
7	20.40	0.14 (-5)	801.5	183.1	346.05
8	19.65	0.29 (-5)	702.0	161.0	345.16
9	18.89	0.62 (-5)	583.5	143.0	327.56
10	18.14	0.13 (-4)	459.5	129.0	288.16
11	17.39	0.28 (-4)	347.0	118.9	233.47
12	16.63	0.60 (-4)	257.0	111.4	162.65
13	15.88	0.13 (-3)	212.5	106.0	100.51
14	15.13	0.27 (-3)	197.0	101.0	71.20
15	14.37	0.57 (-3)	190.0	96.6	60.91
16	13.62	0.12 (-2)	187.0	92.3	55.41
17	12.86	0.26 (-2)	187.0	88.0	50.76
18	12.11	0.55 (-2)	191.0	83.9	45.93
19	11.36	0.01	200.0	79.5	45.52
20	10.60	0.02	208.5	74.8	46.62
21	9.85	0.05	219.5	69.8	47.77
22	9.10	0.11	231.0	64.7	49.07
23	8.34	0.24	245.0	59.3	50.08
24	7.59	0.51	261.0	53.7	59.96
25	6.84	1.07	267.0	47.8	80.58
26	6.08	2.28	254.5	41.9	88.62

Note: Levels 21-26 (between the dashed lines) are levels which overlap the Stratospheric Circulation Model.

3. Non-dimensional finite-difference equations

In this section we write the basic equations 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

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

In the last expression T (dim) is the "total" temperature in absolute degrees, $\bar{T} = \bar{T}(Z)$ is the "standard atmosphere" temperature (also in degrees) given in the table at the end of Section 2, while the quantity $(4\Omega^2 a^2/R)$ T (non-dim) is the (deviation from the horizontal mean) variable T appearing in (1.23), having a zero horizontal average. [The total T (dim) is, of course, used in all chemical computations].

$$\left.\begin{aligned}
\Omega &= 2\pi/8.64\times10^4 \text{ rad sec}^{-1} \\
a &= 6.371\times10^6 \text{ meters} \\
R &= 287 \text{ kJ ton}^{-1}\text{ deg}^{-1} \\
Cp &= (7/2)R
\end{aligned}\right\} \quad (3.2)$$

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

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

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

$$PW = \nabla^2 X \tag{3.16}$$

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

$$\left.\begin{aligned} L &\equiv \nabla^{-2} \\ X &= PLW \end{aligned}\right\} \tag{3.5}$$

We also have

$$\zeta = \nabla^2\psi\ ;\ \psi = L\zeta \tag{3.6}$$

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

$$\frac{\partial X}{\partial P} = \frac{\partial}{\partial P}[P(LW)]$$

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

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

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

The non-dimensional form of the vorticity equation (1.13), with regard to the subscript labelling defined in Section 2, together with equation (1.19) and (3.5) - (3.8) is as follows:

For j = 1, 2, ..., J-1:

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

$$+ (\frac{r}{r-1})F_{j+1} - (\frac{1}{r-1})F_j \tag{3.9}$$

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

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

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

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

$$E_j = (K_m)_j \div [H_0^2 2\Omega\Delta Z] \tag{3.14}$$

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

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

$$W_J = -J(\frac{h}{H_0}, \psi_{J-1}) \tag{3.17}$$

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

$j = 2, 3, \ldots, J-1$:

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

The non-dimensional form of the thermal equation (1.23) becomes for

$j = 2, 3, \ldots, J-1$:

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

where

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

is tabulated at the end of Section 2. Note that q_j, the rate of heating per unit mass, is still in dimensional form in (3.19).

The trace substance is, for

$j = j_o, j_o+1, \ldots, J-1$:

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

$$\left.\begin{aligned} G_j &= D_j(\chi_{j+1} - \chi_j) \; ; \quad \text{for } j = j_o, \ldots, J-2 \\ D_j &= (K_d)_{j+1/2} : (2\Omega H_0^2 \Delta Z) \end{aligned}\right\} . \tag{3.22}$$

[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 interger values of j.]

4. Spectral form of the equations

We define spectral solutions at arbitrary level j in the form

$$\left.\begin{aligned} \psi_j &= \sum_\alpha \psi_{\alpha,j} Y_\alpha(\lambda,\mu) \\ \zeta_j &= \sum_\alpha \zeta_{\alpha,j} Y_\alpha(\lambda,\mu) \\ W_j &= \sum_\alpha W_{\alpha,j} Y_\alpha(\lambda,\mu) \\ T_j &= \sum_\alpha T_{\alpha,j} Y_\alpha(\lambda,\mu) \\ q_j &= \sum_\alpha q_{\alpha,j} Y_\alpha(\lambda,\mu) \end{aligned}\right\} , \tag{4.1}$$

and for the trace substance equation

$$\left.\begin{aligned} \chi_j &= \sum_\alpha \chi_{\alpha,j} Y_\alpha(\lambda,\mu) \\ G_j &= \sum_\alpha G_{\alpha,j} Y_\alpha(\lambda,\mu) \end{aligned}\right\} . \tag{4.2}$$

In terms of longitude (λ) and latitude (μ), we have defined members of the complete set of orthogonal spherical harmonics in (4.1) and (4.2) using

$$Y_\alpha(\lambda,\mu) = e^{i\ell_\alpha \lambda} P_\alpha(\mu) \tag{4.3}$$

with

$$\alpha = n_\alpha + i\ell_\alpha \tag{4.4}$$

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

$$\int_s Y_\alpha Y_\beta^* \, ds = 4\pi\delta_{\alpha,\beta} \quad . \tag{4.5}$$

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

$$\nabla^2 Y_\alpha = -c_\alpha Y_\alpha ; \; c_\alpha = n_\alpha(n_\alpha+1) \tag{4.6}$$

The complete set of orthonormal Legendre polynomials as used in (4.3) are defined such that

$$P_\alpha^* \equiv P_\alpha \tag{4.7}$$

and all P_α have been normalized such that

$$\int_{-1}^{+1} P_\alpha P_\beta \, d\mu = 2\delta_{\alpha,\beta} \tag{4.8}$$

We now want to substitute solutions (4.1) and (4.2) 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,

$$\frac{d\zeta_{\gamma,j}}{dt} = -i\ell_\gamma \psi_{\gamma,j} - A_{\gamma,j} + \frac{D_\gamma}{c_{\gamma-\varepsilon}}\left[\left(\frac{r}{r-1}\right)W_{\gamma-\varepsilon,j+1} - \right.$$

$$\left. -\left(\frac{1}{r-1}\right)W_{\gamma-\varepsilon,j}\right] - \frac{E_\gamma}{c_{\gamma+\varepsilon}}\left[\left(\frac{r}{r-1}\right)W_{\gamma+\varepsilon,j+1} - \right. \tag{4.9}$$

$$\left. -\left(\frac{1}{r-1}\right)W_{\gamma+\varepsilon,j}\right] + \left(\frac{r}{r-1}\right)F_{\gamma,j+1} - \left(\frac{1}{r-1}\right)F_{\gamma,j}$$

in which, over the unit spherical surface s,

$$\left.\begin{aligned}
\frac{d\zeta_{\gamma,j}}{dt} &= \frac{1}{4\pi}\int_s \frac{\partial\zeta_j}{\partial t}\, Y_\gamma^*\, ds \\
i\ell_\gamma \psi_{\gamma,j} &= \frac{1}{4\pi}\int_s J(\psi_j,\mu)Y_\gamma^* ds = \frac{1}{4\pi}\int_s \frac{\partial\psi_j}{\partial\lambda}Y_\gamma^* ds \\
A_{\gamma,j} &= \frac{1}{4\pi}\int_s J(\psi_j,\zeta_j)Y_\gamma^* ds \text{ (See Appendix A)} \\
\frac{D_\gamma}{c_{\gamma-\varepsilon}}W_{\gamma-\varepsilon,j} - \frac{E_\gamma}{c_{\gamma+\varepsilon}}W_{\gamma+\varepsilon,j} &= -\frac{1}{4\pi}\int_s [\nabla\cdot\mu\nabla L(W_j)]Y_\gamma^* ds \text{ (See Appendix B)} \\
F_{\gamma,j} &= \frac{1}{4\pi}\int_s F_j Y_\gamma^* ds
\end{aligned}\right\} \tag{4.10}$$

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

$$\left.\begin{aligned}
\frac{dT_{\gamma,j}}{dt} &= -B_{\gamma,j} - S_j W_{\gamma,j} + \left[\frac{R}{C_p \beta \Omega^2 a^2}\right] q_{\gamma,j} \\
\frac{d\chi_{\gamma,j}}{dt} &= -B^{(\chi)}_{\gamma,j} - \left(\frac{d\bar{\chi}}{dZ}\right) W_{\gamma,j} + \left(\frac{r}{r-1}\right) G_{\gamma,j} - \\
&\quad -\left(\frac{1}{r-1}\right) G_{\gamma,j-1} + \frac{1}{4\pi}\int_s \frac{1}{2\Omega}\left[\frac{1}{n_m}\left(\frac{dn}{dt}\right)_c\right]_j Y^*_\gamma ds \\
\Delta Z\, c_\gamma T_{\gamma,j} &= -D_\gamma(\psi_{\gamma-\varepsilon,j-1} - \psi_{\gamma-\varepsilon,j}) + E\,(\psi_{\gamma+\varepsilon,j-1} - \psi_{\gamma+\varepsilon,j})
\end{aligned}\right\} \quad (4.11)$$

where, for example,

$$\left.\begin{aligned}
\frac{dT_{\gamma,j}}{dt} &= \frac{1}{4\pi}\int_s \frac{\partial T_j}{\partial t} Y^*_\gamma ds \\
\frac{d\chi_{\gamma,j}}{dt} &= 4\pi\int_s \frac{d\chi_j}{dt} Y^*_\gamma ds \\
c_\gamma T_{\gamma,j} &= \frac{1}{4\pi}\int_s (-\nabla^2 T_j) Y^*_\gamma ds \\
B_{\gamma,j} &= \frac{1}{8\pi}\int_s J(\psi_j + \psi_{j-1}, T_j) Y^*_\gamma ds \text{ (See Appendix A)} \\
B^{(\chi)}_{\gamma,j} &= \frac{1}{8\pi}\int_s J(\psi_j + \psi_{j-1}, \chi_j) Y^*_\gamma ds \text{ (See Appendix A)} \\
D_\gamma \psi_{\gamma-\varepsilon,j} - E_\gamma \psi_{\gamma+\varepsilon,j} &= -\frac{1}{4\pi}\int_s [\nabla\cdot\mu\nabla\psi_j] Y^*_\gamma ds \text{ (See Appendix B)}
\end{aligned}\right\} \quad (4.12)$$

In addition, we want to determine the spectral form of (1.6) relating the verti-

cal component of relative vorticity (ζ) and the streamfunction (ψ). It can be shown that

$$\zeta_{\gamma,j} = -c_\gamma \psi_{\gamma,j} \tag{4.13}$$

or

$$\psi_{\gamma,j} = -\frac{\zeta_{\gamma,j}}{c_\gamma} \tag{4.14}$$

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

The spectral relationships (4.9), (4.11), and (4.13) [or (4.14)] along with definitions (4.10) and (4.12) 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 determining the vertical velocity field represented by W. In order to define W, we want to alter the thermal wind relationship in (4.11) This development is contained in the next section. Furthermore, specification of the truncation limits to be used for series solutions (4.1) and (4.2) have not yet been established and will be discussed in a later section.

5. 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 (4.14) into the thermal wind equation of (4.11) and differentiate w.r.t. time to get

$$\Delta Z\, c_\gamma \frac{dT_{\gamma,j}}{dt} = \frac{D_\gamma}{c_{\gamma-\varepsilon}}\left(\frac{d\zeta_{\gamma-\varepsilon,j-1}}{dt} - \frac{d\zeta_{\gamma-\varepsilon,j}}{dt}\right) - \frac{E_\gamma}{c_{\gamma+\varepsilon}}\left(\frac{d\zeta_{\gamma+\varepsilon,j-1}}{dt} - \frac{d\zeta_{\gamma+\varepsilon,j}}{dt}\right) \tag{5.1}$$

for all levels $j = 2,3, \ldots, J-1$. We note that (5.1) does not apply for the cases $\gamma = 0+i0$. Furthermore, for notational purposes, we will stipulate that in (5.1) and all future relationships, terms which require $\gamma-\varepsilon = 0+i0$ or $n_{\gamma-\varepsilon} < \ell_{\gamma-\varepsilon}$ do not exist. This applies equally to cases in which $\gamma+\varepsilon$ is not contained within the specified model truncation limits.

Let us now define

$$a_{\gamma,j} \equiv -i\ell_\gamma(\psi_{\gamma,j-1} - \psi_{\gamma,j}) - A_{\gamma,j-1} + A_{\gamma,j} - \left(\frac{1}{r-1}\right)F_{\gamma,j-1} + \left(\frac{r+1}{r-1}\right)F_{\gamma,j} - \left(\frac{r}{r-1}\right)F_{\gamma,j+1} \tag{5.2}$$

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

such that using (4.9) we can write

$$\frac{d\zeta_{\gamma,j-1}}{dt} - \frac{d\zeta_{\gamma,j}}{dt} = a_{\gamma,j} - \frac{1}{(r-1)} \frac{D_\gamma}{c_{\gamma-\varepsilon}} [W_{\gamma-\varepsilon,j-1} - (r+1)W_{\gamma-\varepsilon,j} +$$

$$+ rW_{\gamma-\varepsilon,j+1}] + \frac{1}{(r-1)} \frac{E_\gamma}{c_{\gamma+\varepsilon}} [W_{\gamma+\varepsilon,j-1} - \tag{5.3}$$

$$- (r+1)W_{\gamma+\varepsilon,j} + rW_{\gamma+\varepsilon,j+1}]$$

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

$$\frac{dT_{\gamma,j}}{dt} = b_{\gamma,j} - S_j W_{\gamma,j} \quad . \tag{5.4}$$

Inserting solutions (5.3) and (5.4) into (5.1) has the effect of eliminating the time dependence of (5.1) and at any given time we have

$$\Delta Z\, c_\gamma b_{\gamma,j} - \Delta Z\, c_\gamma S_j W_{\gamma,j} = \frac{D_\gamma}{c_{\gamma-\varepsilon}} a_{\gamma-\varepsilon,j} - \frac{E_\gamma}{c_{\gamma+\varepsilon}} a_{\gamma+\varepsilon,j} -$$

$$- \frac{1}{(r-1)} \frac{D_{\gamma-\varepsilon} D_\gamma}{c_{\gamma-2\varepsilon} c_{\gamma-\varepsilon}} [W_{\gamma-2\varepsilon,j-1} - (r+1)W_{\gamma-2\varepsilon,j} + rW_{\gamma-2\varepsilon,j+1}] +$$

$$+ \frac{1}{(r-1)} \left(\frac{E_{\gamma-\varepsilon} D_\gamma}{c_{\gamma-\varepsilon} c_\gamma} + \frac{E_\gamma D_{\gamma+\varepsilon}}{c_\gamma c_{\gamma+\varepsilon}} \right) [W_{\gamma,j-1} - (r+1)W_{\gamma,j} + rW_{\gamma,j+1}] -$$

$$- \frac{1}{(r-1)} \frac{E_\gamma E_{\gamma+\varepsilon}}{c_{\gamma+\varepsilon} c_{\gamma+2\varepsilon}} [W_{\gamma+2\varepsilon,j-1} - (r+1)W_{\gamma+2\varepsilon,j} + rW_{\gamma+2\varepsilon,j+1}]$$

or, if we define

$$
\left.
\begin{aligned}
\tau_{\gamma,j} &\equiv (r-1)\left[\frac{D_\gamma}{c_{\gamma-\varepsilon}c_\gamma}\, a_{\gamma-\varepsilon,j} - \frac{E_\gamma}{c_\gamma c_{\gamma+\varepsilon}}\, a_{\gamma-\varepsilon,j} - \Delta Z\, b_{\gamma,j}\right] \\
f_\gamma^{(1)} &\equiv \frac{D_{\gamma-\varepsilon}D_\gamma}{c_{\gamma-2\varepsilon}c_{\gamma-\varepsilon}c_\gamma} \\
f_\gamma^{(2)} &\equiv -\frac{1}{c_\gamma^2}\left(\frac{E_{\gamma-\varepsilon}D_\gamma}{c_{\gamma-\varepsilon}} + \frac{E_\gamma D_{\gamma+\varepsilon}}{c_{\gamma+\varepsilon}}\right) \\
f_\gamma^{(3)} &\equiv \frac{E_\gamma E_{\gamma+\varepsilon}}{c_\gamma c_{\gamma+\varepsilon}c_{\gamma+2}} \\
\sigma_j &\equiv (r-1)\Delta Z\, S_j
\end{aligned}
\right\} \quad (5.5)
$$

the W-equation can be compacted to

$$
\begin{aligned}
&[f_\gamma^{(1)}W_{\gamma-2\varepsilon,j-1} + f_\gamma^{(2)}W_{\gamma,j-1} + f_\gamma^{(3)}W_{\gamma+2\varepsilon,j-1}] - \\
&- (r+1)\,[f_\gamma^{(1)}W_{\gamma-2\varepsilon,j} + f_\gamma^{(2)}W_{\gamma,j} + f_\gamma^{(3)}W_{\gamma+2\varepsilon,j}] + \\
&+r[f_\gamma^{(1)}W_{\gamma-2\varepsilon,j+1} + f_\gamma^{(2)}W_{\gamma,j+1} + f_\gamma^{(3)}W_{\gamma+2\varepsilon,j+1}] - \\
&- \sigma_j W_{\gamma,j} = \tau_{\gamma,j}
\end{aligned}
\quad (5.6)
$$

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

$$
\left.
\begin{aligned}
&W_{\gamma,1} = 0 \\
&W_{\gamma,J} = W_{\gamma,J}\,(t,\lambda,\mu) \\
&\quad \text{as given from external sources.}
\end{aligned}
\right\} \quad (5.7)
$$

To prepare (5.6) 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 (5.6) 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 others 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 (5.6) by first denoting a maximum planetary wave number, L, for a given spectral truncation as

$$L = \ell_\gamma)_{max} \tag{5.8}$$

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

$$k = 1, 2, 3, \ldots, K; \; K = 2(L+1). \tag{5.9}$$

For a given matrix set we will determine k by designating

$$k = \begin{Bmatrix} 2\ell_\gamma + 1 \text{ for even vector sets} \\ 2(\ell_\gamma + 1) \text{ for odd vector sets} \end{Bmatrix} . \tag{5.10}$$

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

$$b_k = 1, 2, 3, \ldots, B_k \; . \tag{5.11}$$

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

$$N_k = n_k)_{max} \tag{5.12}$$

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

$$\left.\begin{aligned} b_k &= \frac{n_k - \ell_k + 2}{2} - \delta_{\ell_k,0} \\ B_k &= \frac{N_k - \ell_k + 2}{2} - \delta_{\ell_k,0} \end{aligned}\right\} \tag{5.13}$$

where we ignore values of b_k outside the range indicated in (5.11); 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 (5.1) in which $\gamma = 0+i0$ [see comments following (5.1)].

Similarily,

(2) For k even (odd vectors) let

$$N_k = n_k)_{max} \tag{5.14}$$

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

$$\left.\begin{aligned} b_k &= \frac{n_k - \ell_k + 1}{2} \\ B_k &= \frac{N_k - \ell_k + 1}{2} \end{aligned}\right\} \tag{5.15}$$

At this point we want to note an additional property inherent in the spectral W-equations represented by (5.6). That is, from definitions contained in

(5.5) and Appendix B we can show that for any given k,

$$f^{(3)}_{b_k} = \frac{E_{\gamma_k} \; E_{\gamma_k \pm \varepsilon}}{c_{\gamma_k} \; c_{\gamma_k \pm \varepsilon} \; c_{\gamma_k \pm 2\varepsilon}}$$

$$\equiv \frac{D_{\gamma_k \pm \varepsilon} \; D_{\gamma_k \pm 2\varepsilon}}{c_{\gamma_k} \; c_{\gamma_k \pm \varepsilon} \; c_{\gamma_k \pm 2\varepsilon}} \equiv f^{(1)}_{b_k \pm 1} \tag{5.16}$$

We are now prepared to convert (5.6) to matrix form. To do this we first define tridiagonal matrices $\mathcal{D}_k$ as

$$\mathcal{D}_k = \begin{bmatrix} f^{(2)}_1 & f^{(3)}_1 & 0 \cdots\cdots & 0 \\ f^{(3)}_1 & f^{(2)}_2 & f^{(3)}_2 & \vdots \\ \vdots & \ddots & \ddots & \ddots \\ 0 & f^{(3)}_{b_k-1} & f^{(2)}_{b_k} & f^{(3)}_{b_k} \\ \vdots & & \ddots & \ddots \\ 0 & \cdots\cdots & f^{(3)}_{B_k-1} & f^{(2)}_{B_k} \end{bmatrix}_k \tag{5.17}$$

where we have made use of (5.8) - (5.16). We note from (5.17) 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 (5.6) to matrix form we define vectors

$$W_{k,j} = \begin{pmatrix} W_{1,j} \\ W_{2,j} \\ \vdots \\ W_{b_k,j} \\ \vdots \\ W_{B_k,j} \end{pmatrix}_k ; \quad R_{k,j} = \begin{pmatrix} r_{1,j} \\ r_{2,j} \\ \vdots \\ r_{b_k,j} \\ \vdots \\ r_{B_k,j} \end{pmatrix}_k \tag{5.18}$$

such that (5.6) can be written in the matrix form

$$\begin{gathered} \mathcal{D}_k W_{k,j-1} - (r+1)\mathcal{D}_k W_{k,j} + r\mathcal{D}_k W_{k,j+1} - \sigma_j W_{k,j} = R_{k,j} \quad ; \\ j = 2, 3, 4, \ldots, J-1 \text{ for each } k = 1, 2, 3, \ldots, K \end{gathered} \tag{5.19}$$

We wish to modify (5.19) through diagonalization of each $\mathcal{D}_k$. However, since each tridiagonal $\mathcal{D}_k$ is <u>real</u>, <u>symmetric</u> and <u>positive definite</u>, we know that <u>all eigenvalues of $\mathcal{D}_k$</u> are <u>real</u> and <u>positive</u>. Also, the sets of <u>eigenvectors</u> associated with these eigenvalues are <u>orthonormal</u>. Thus, if $\mathcal{D}_k$ is an MxM matrix, 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 the set $(\lambda_k)_p$ and matrix $\mathcal{D}_k$, we have

$$Q_k = \begin{pmatrix} q_{11} & q_{12} & \cdots & q_{1s} & \cdots & q_{1m} \\ q_{21} & q_{22} & \cdots & q_{2s} & \cdots & q_{2m} \\ \vdots & \vdots & & \vdots & & \vdots \\ q_{p1} & q_{p2} & \cdots & q_{ps} & \cdots & q_{pm} \\ \vdots & \vdots & & \vdots & & \vdots \\ q_{m1} & q_{m2} & \cdots & q_{ms} & \cdots & q_{mm} \end{pmatrix}_k \tag{5.20}$$

such that

$$Q_k\tilde{Q}_k = \tilde{Q}_kQ_k = I \tag{5.21}$$

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

$$\Lambda_k = \begin{bmatrix} (\lambda_k)_1 & 0 & \cdots & 0 \\ 0 & (\lambda_k)_2 & & \vdots \\ \vdots & & \ddots & \vdots \\ \vdots & & & (\lambda_k)_p \\ 0 & \cdots & \cdots & (\lambda_k)_m \end{bmatrix} \tag{5.22}$$

where then we know

$$\left.\begin{aligned} \mathcal{D}_kQ_k &= Q_k\Lambda_k \\ \text{and} \qquad & \\ \tilde{Q}_k\mathcal{D}_kQ_k &= \tilde{Q}_kQ_k\Lambda_k = \Lambda_k \end{aligned}\right\} . \tag{5.23}$$

We now want to expand the vector $W_{k,j}$ in (5.19) in the form

$$W_{k,j} = Q_kV_{k,j} \; ; \; V_{k,j} = \tilde{Q}_kW_{k,j} \tag{5.24}$$

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

Inserting solutions (5.24) into (5.19) and multiplying through with $\tilde{Q}_k$ gives

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

or, from (5.23), we can write

$$\Lambda_k V_{k,j-1} - [(r+1)\,\Lambda_k + \sigma_j]\, V_{k,j} + r\Lambda_k V_{k,j+1} = \tilde{Q}_k R_{k,j} \tag{5.25}$$

Now, we know that there exists an inverse

$$\Lambda_k^{-1} = \begin{bmatrix} 1/(\lambda_k)_1 & 0 \cdots\cdots & & & 0 \\ 0 & 1/(\lambda_k)_2 & & & \vdots \\ \vdots & & \ddots & & \vdots \\ \vdots & & & 1/(\lambda_k)_p & \vdots \\ \vdots & & & & \ddots \\ 0 & \cdots\cdots & & & 1/(\lambda_k)_m \end{bmatrix} \tag{5.26}$$

such that

$$\Lambda_k^{-1}\Lambda_k = I\ . \tag{5.27}$$

Thus, if we multiply (5.25) through with Λ_k^{-1}, (5.25) reduces to the form

$$V_{k,j-1} - [(r+1)I + \sigma_j\Lambda_k^{-1}]\, V_{k,j} + rV_{k,j+1} = \Lambda_k^{-1}\tilde{Q}_k R_{k,j} \tag{5.28}$$

where for each $k = 1, 2, 3, \ldots, K$ we have $j = 2, 3, 4, \ldots, j-1$. We now let

$$\left.\begin{aligned} S_{k,j} &\equiv -[(r+1)I + \sigma_j\Lambda_k^{-1}] \\ \text{and} \quad R_{k,j} &\equiv \begin{cases} \Lambda_k^{-1}\tilde{Q}_k R_{k,2} - V_{k,1} & (\text{for } j = 2) \\ \Lambda_k^{-1}\tilde{Q}_k R_{k,j} & (\text{for } 3 \le j \le J-2) \\ \Lambda_k^{-1}\tilde{Q}_k R_{k,J-1} - rV_{k,j} & (\text{for } j = J-1) \end{cases} \end{aligned}\right\} \tag{5.29}$$

Using (5.29), (5.28) transforms to the set

$$\left.\begin{aligned} S_{k,2}V_{k,2} + r\,V_{k,3} &= R_{k,2} && (\text{for } j = 2) \\ V_{k,j-1} + S_{k,j}V_{k,j} + r\,V_{k,j+1} &= R_{k,j} && (3 \le j \le J-2) \\ V_{k,J-2} + S_{k,J-1}V_{k,J-1} &= R_{k,J-1} && (\text{for } j = J-1) \end{aligned}\right\} \tag{5.30}$$

in which from (5.24) and the boundary conditions of (5.7) we see that in (5.29)

$$\left.\begin{aligned} V_{k,1} &= 0 \\ V_{k,J} &= \tilde{Q}_k W_{k,J} \end{aligned}\right\} . \tag{5.31}$$

We see that for each k the system (5.30) is tridiagonal in j and thus submits readily to solution provided certain provisions are met (see Appendix C for details). Briefly, to invert (5.30) we first define

$$\left.\begin{aligned} u_{k,2} &\equiv S_{k,2}^{-1} && (\text{for } j = 2) \\ u_{k,j} &\equiv (S_{k,j} - r\,u_{k,j-1})^{-1} && (\text{for } 3 \le j \le J-1) \\ v_{k,j} &\equiv -\,r\,u_{k,j} && (2 \le j \le J-1) \end{aligned}\right\} \tag{5.32}$$

and then let

$$\left.\begin{aligned} y_{k,2} &= u_{k,2}\,R_{k,2} && (\text{for } j = 2) \\ y_{k,j} &= u_{k,j}\,(R_{k,j} - y_{k,j-1}) && (\text{for } 3 \le j \le J-1) \end{aligned}\right\} . \tag{5.33}$$

Solutions to (5.30) thus appear as

$$\left.\begin{aligned} V_{k,J-1} &= y_{k,J-1} \qquad (\text{for } j = J-1) \\ V_{k,j} &= v_{k,j}V_{k,j+1} + y_{k,j} \quad (\text{for } j = J-2,\ J-3,\ \ldots,\ 2) \end{aligned}\right\} \tag{5.34}$$

provided all $u_{k,j}$ in (5.23) exist and are finite. Vectors $W_{k,j}$ are then obtained from (5.24).

6. The model codes

The model consists of four separate programs, three of which are preliminary and need to be executed only once. The names of the four programs are ITCOF1, ITCOF2, MESOS1, and MESOS2. A brief description of each of these follows.

ITCOF1, ITCOF2

ITCOF1 and ITCOF2 are used consecutively to generate and store on the system disk a set of non-linear interaction coefficients for use in computing the non-linear Jacobians in the model. The definition and method used for the computation of the interaction coefficients are contained in Appendix A.

To run ITCOF1, use file RUNIC1 (see Figure 6.1). This routine requires disk files INTCOEF1 and STRAT1 as input and creates a file named IC1OUT as output. IC1OUT is used as input by ITCOF2.

The program RUNIC2 (Figure 6.2) drives ITCOF2 and requires files INTCOEF2, STRAT1, and IC1OUT as input. ITCOF2 creates a file IC2OUT on output which contains the interaction coefficient and instruction fields required by the model.

MESOS1

MESOS1 is an initializing program which creates and stores all constants, truncation parameters, transform parameters, and fixed fields required for the particular model configuration to be run. This program must be run prior to the beginning of a particular model experiment and, in general, calculates everything that can be done for the model in advance outside of the main iterative loop.

MESOS1 is driven by the file MESOSBEG (Figure 6.3) and requires input files STRAT1 and IC2OUT. On output, the file MESOS1Ø will contain all of the input

fields required by the model except for the model's initial conditions. In addition, a set of data which includes horizontal mean temperatures and stabilities is required as input as shown in Figure 6.3.

MESOS2

MESOS2 represents the central loop of the model. It is called into action by the file MESOSSTART (Figure 6.4) which requires input files STRAT2, MESOS1Ø, INITDEC, BNDFILE, and HEATFILE. The last three of these are data files which include the initial conditions file, the lower boundary conditions file, and the temporary heating file respectively. MESOS1Ø is as described above under MESOS1.

On output, the file MESOUT11 contains the complete history of the model run. The model can be restarted as often as required from this history file and the subsequent output is appended onto the file. The first records on MESOUT11 contain fixed model parameters. Subsequent records are each made up of a time step number, the spectral vorticity coefficients, the spectral vertical velocity coefficients and, if applicable, the spectral ozone mixing ratio coefficients for the particular time step.

An additional file is provided in the program to include the spectral coefficient values for all the non-linear terms in the model at each time step. This is assigned to "TAPE13" but is currently not being retained by the model as a permanent file.

The first pages of the listings for the model programs ITCOF1, ITCOF2, MESOS1, and MESOS2 are shown in Figures 6.5 - 6.8 for purposes of reference.

```
*** PROGRAM RUNIC1 ***

RICF1,T59,CM120000.
ATTACH(OLDPL,INTCOEF1,ID=ALYEA)
UPDATE(F,P=OLDPL)
RETURN(OLDPL)
FTN(L=0,I=COMPILE)
ATTACH(OLDPL,STRAT1,ID=ALYEA)
UPDATE(F,P=OLDPL,Q)
FTN(L=0,I=COMPILE,B=LOG)
REQUEST(TAPE9,*PF)
LOAD(LGO,LOG)
EXECUTE.
CATALOG(TAPE9,IC1OUT,ID=ALYEA,RP=999)
■/*EOR CDC END-OF-RECORD
■/*EOR CDC END-OF-RECORD
*IDENT COMPAK
*DELETE COMPACK.5
         USE    /PKBLK/
*COMPILE COMPACK
■/*EOR CDC END-OF-RECORD
J(A,B) -- EVEN + ODD
    2     6     6     3
■/*EOF CDC END-OF-FILE
```

Figure 6.1: Program RUNIC1.

```
*** PROGRAM RUNIC2 ***

RICF2,T59,CM120000.
ATTACH(OLDPL,INTCOEF2,ID=ALYEA)
UPDATE(F,P=OLDPL)
RETURN(OLDPL)
FTN(L=0,I=COMPILE)
ATTACH(OLDPL,STRAT1,ID=ALYEA)
UPDATE(F,P=OLDPL,Q)
FTN(L=0,I=COMPILE,B=LOG)
ATTACH(TAPE9,IC1OUT,ID=ALYEA)
REQUEST(TAPE10,*PF)
LOAD(LGO,LOG)
EXECUTE.
CATALOG(TAPE10,IC2OUT,ID=ALYEA,RP=999)
■/*EOR CDC END-OF-RECORD
■/*EOR CDC END-OF-RECORD
*IDENT COMPAK
*DELETE COMPACK.5
        USE    /PKBLK/
*COMPILE COMPACK
■/*EOR CDC END-OF-RECORD
    0    6    0
■/*EOF CDC END-OF-FILE
```

Figure 6.2: Program RUNIC2.

```
*** PROGRAM MESOSBEG ***                                          PAGE    1

INIT1,T59,CM267100.
ATTACH(OLDPL,STRAT1,ID=ALYEA)
ATTACH(TAPE10,IC2OUT,ID=ALYEA)
UPDATE(F,P=OLDPL)
RETURN(OLDPL)
FTN(L=0,T,I=COMPILE)
RETURN(COMPILE)
REQUEST(TAPE12,*PF)
LDSET(PRESET=ZERO)
LGO.
CATALOG(TAPE12,MESOS10,ID=ALYEA,RP=999)
■/*EOR CDC END-OF-RECORD
*IDENT APR
*DELETE STRAT1.2
      PROGRAM MESOS1(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE10,
*DELETE STRAT1.4
*DELETE STRAT1.10
*DELETE STRAT1.32
C     CALL VDIST(XIBAR,1,NVERT,0)
*DELETE STRAT1.33
C     CALL HDIST(H,1,NVERT,2)
*DELETE STRAT1.34
C     CALL ZONTS
*DELETE STRAT1.35
C     CALL EDDYTS
*DELETE STRAT1.36
C     CALL OVRLAP
*DELETE STRAT1.39
C     CALL DIFFK(1,DIFFM)
*DELETE STRAT1.40
C     CALL DIFFK(2,DIFFX)
*DELETE STRAT1.49
C     CALL XO3EQU
*DELETE ZLEV.6
      DATA NV26,R26,Z0/26,2.12472,6.08205/
*INSERT ZLEV.8
      ZTOP=ZTOP+Z0
*DELETE ZLEV.28
      WRITE(6,900) DZ,RVERT,Z0
*DELETE ZLEV.29
  900 FORMAT(1H0,14X,*DZ = *,F10.6,*  RVERT = *,F10.6,
     1 *  Z0 = *,F10.6)
*DELETE INITAL.1,APROXJ.33
■/*EOR CDC END-OF-RECORD
    3    6   26    1
                          HORIZONTAL MEAN TEMPERATURE DATA
    1   26          995.5                991.0                981.0
962.5               930.5                878.5                801.5
702.0               583.5                459.5                347.0
257.0               212.5                197.0                190.0
187.0               187.0                191.0                200.0
208.5               219.5                231.0                245.0
261.0               267.0                254.5
```

Figure 6.3: Program MESOSBEG.

```
*** PROGRAM MESOSBEG ***                                                    PAGE   2

                                HORIZONTAL MEAN STABILITY DATA
    1    26            289.01              292.70              299.13
308.45                 321.53              336.53              346.05
345.16                 327.56              288.16              233.47
162.65                 100.51               71.20               60.91
 55.41                  50.76               45.93               45.52
 46.62                  47.77               49.07               50.08
 59.96                  80.58               88.62
NLON,NLAT=    16    15
■/*EOF CDC END-OF-FILE
```

Figure 6.3 continued.

```
*** PROGRAM MESOSSTART ***

START,T50,CM210100,EC155.
ATTACH(OLDPL,STRAT2,ID=ALYEA)
UPDATE(F)
RETURN(OLDPL)
FTN(L=0,T,I=COMPILE)
RETURN(COMPILE)
ATTACH(TAPE10,MESOS10,ID=ALYEA)
ATTACH(TAPE12,INITDEC,ID=ALYEA)
ATTACH(TAPE14,BNDFILE,ID=ALYEA)
ATTACH(TAPE15,HEATFILE,ID=ALYEA)
REQUEST(TAPE11,*PF)
REQUEST(TAPE13,*PF)
LGO.
CATALOG(TAPE11,MESOUT11,ID=ALYEA,RP=999)
AUDIT,ID=ALYEA.
■/*EOR CDC END-OF-RECORD
■/*EOR CDC END-OF-RECORD
    0    4
    4  1.0 -110
RUN 34    AMES TEST RUN WITH NOX,OH.STARTS DEC.1
    1    0
■/*EOF CDC END-OF-FILE
```

Firgure 6.4: Program MESOSSTART.

```
*DECK ICOF1
      PROGRAM ITCOF1(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE9)
      DOUBLE PRECISION ZEROR,ZEROI,Z,COEF,WORK,AR,W,D,ARG,DLAT,P,PLN,
     1 AP,BP,PPLN
C
      COMMON ZEROR(50),ZEROI(50),Z(50),COEF(50),AR(50),W(50),D(30),
     1 ARG(50),DLAT(50),P(50),PLN(169,19),AP(156,19),BP(156,19),KMAX,
     2 KP1,IERR,LP1,IH
      DIMENSION PPLN(13,13,19),WORK(50),JCOEF(10)
C
      READ(5,890) JCOEF
  890 FORMAT(10A4)
      READ(5,900) IH,LR,NZON,ITERM
  900 FORMAT(16I5)
C
C     FOR ITERM DEFINITION SEE NOTE AT THE BEGINNING
C
      JUMP=MOD(IH,2)
      NR=NZON
      LP1=NR+1
      GO TO (3,4,5,6,7,8),ITERM
C
    3 KMAX=NZON+LR+1
      GO TO 10
    4 KMAX=LR+1.5*NZON+.5000000001
      GO TO 10
    5 KMAX=LR+1.5*NZON+.5000000001
      GO TO 10
    6 KMAX=NZON+1
      GO TO 10
    7 KMAX=1.5*NZON+1.0001
      GO TO 10
    8 KMAX=1.5*NZON+.50001
C
   10 CONTINUE
      CALL GAUSWT(ICOUNT,WORK)
      WRITE(6,997) ICOUNT
  997 FORMAT(1H ,10X,*SUB. GAUSWT,ICOUNT=*,I3)
      IF(IERR.GT.0) GO TO 2
      KMAX=ICOUNT
C
C     COMPUTATION OF LEGENDRE POLYNOMIAL VALUES
C
      ICOUNT=0
      IJP=2
      IF(IH.EQ.2) IJP=1
      DO 30 L=1,LP1
      LL=L-1
      NP1=LL+NZON+2
      DO 30 NN=L,NP1,IJP
      N=NN-1+JUMP
      ICOUNT=ICOUNT+1
   34 CALL KUGELU(LL,N,KMAX,AR,P,WORK)
```

Figure 6.5: First page of Program ITCOF1.

```
*DECK ICOF2
      PROGRAM ITCOF2(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE9,
     1 TAPE10)
      DOUBLE PRECISION COEF,W,P,AP,BP,C
      COMMON W(50),P(156,19),AP(156,19),BP(156,19),C(180),KMAX
      COMMON /PKBLK/ NS,N1,N2,N3,N4,LS,L1,L2,L3,L4
      DIMENSION INST(40,20),COEF(2000),IS(1000),KD(180,6),MTYPE(10)
C
      ICK=0
      DO 5 I=1,40
      DO 5 J=1,20
    5 INST(I,J)=0
C
      READ(9) MTYPE
      WRITE(6,9001) MTYPE
      READ(9) JH,LR,NR,ITERM,ICOUNT,KMAX,LR1,NR1,IJP,(W(I),I=1,KMAX),
     1 ((P(I,J),J=1,KMAX),I=1,ICOUNT),((AP(I,J),J=1,KMAX),I=1,ICOUNT),
     2 ((BP(I,J),J=1,KMAX),I=1,ICOUNT)
C
      READ(5,1) LBEG,LSTP,ISKIP
      WRITE(6,1230) LR,NR,LBEG,LSTP,ISKIP
      IF(LBEG.EQ.0) WRITE(10) MTYPE,LR,NR
      LBEG=LBEG+1
      LSTP=LSTP+1
      L=LR+1
      N=NR+1
      I=0
      DO 10 L2=1,L
      LL=L2
      NN=LL+N-1
      DO 10 L1=LL,NN
      I=I+1
   10 INST(L1,L2)=I
      WRITE(6,9000)
      WRITE(6,9001) LR,NR
      WRITE(6,9002)
      NN=L+N-1
      DO 20 I=1,NN
      I2=NN-I+1
      I21=I2-1
      WRITE(6,9003) I21,(INST(I2,J),J=1,L)
   20 CONTINUE
      DO 25 I=1,L
   25 IS(I)=I-1
      WRITE(6,9004) (IS(I),I=1,L)
      LL=2*L-1
      ITOT=0
      ISTOT=0
      DO 800 LGI=LBEG,LSTP
      INDEX=0
      INS=0
      LG=LGI-1
      DO 700 LBI=1,LL
```

Figure 6.6: First page of Program ITCOF2.

```
STRAT1    *DECK STRAT1                                                    STRAT1     1    A
STRAT1          PROGRAM MESOS1(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE10,  APR       1    A
STRAT1         1TAPE12)                                                    STRAT1     3    A
STRAT1          DOUBLE PRECISION A                                         STRAT1     5    A
STRAT1          COMMON A(700),IN(300),CTYPE(10),XDMP1(8500)                STRAT1     6    A
STRAT1          COMMON /COFBLK/ C(3800),IS(1500)                           STRAT1     7    A
STRAT1          COMMON /CONSTS/ INDEX,NR,LR,INS,INSZ,KINT,ILEV1,ILEV2,NVERT, STRAT1   8    A
STRAT1         1NRTP,LRTP,NTYPE,NVECT,NVREAL,NVZON,NCYC,DT                 STRAT1     9    A
STRAT1          COMMON /PKBLK/ NS,N1,N2,N3,N4,LS,L1,L2,L3,L4               STRAT1    11    A
STRAT1          COMMON /CGBLK/ KD(43),CG(43),NCOMP(12),LWAVE(12),NV(43),LV(43) STRAT1 12 A
STRAT1          COMMON /DEBLK/ DG(43),EG(43),DGCG(43),EGCG(43)             STRAT1    13    A
STRAT1          COMMON /EIGBLK/ EVECT(126),XLIVET(126),EVAL(42),NRK(14),K  STRAT1    14    A
STRAT1          COMMON /VHTBLK/ ZVAL(26),PVAL(26),VWT(26),DZ,RVERT         STRAT1    15    A
STRAT1          COMMON /BARBLK/ TBAR(26),SIGMA(26),XIBAR(26),DIFFM(26),DIFFX(26) STRAT1 16 A
STRAT1         1, DIFFMB(26),DIFFXB(26),JBM1,JBM2,JBX1,JBX2               STRAT1    17    A
STRAT1          COMMON /FTCST/ NLON,NLAT,NGRID,ARSP(30),XDMP2(30)          STRAT1    18    A
STRAT1          COMMON /HEATBK/ H(26),TSZON(104),TSEDDY(16),I1TSZ,I2TSZ,I1TSW, STRAT1 19 A
STRAT1         1 I2TSW,MERGE1,MERGE2,ZWT1(5),ZWT2(5),Q3WR(5)               STRAT1    20    A
STRAT1          COMMON /UVBLK/ U(1092),V(1092)                             STRAT1    21    A
STRAT1          COMMON /FFT/ WP(7,7,15),WW(2,7),NTRANS(16),NNN,NN,LR1,NLATHF, STRAT1 22 A
STRAT1         1 NCPAR(7),LOGN                                             STRAT1    23    A
STRAT1          COMMON /GLOP/ PNL(7,7,15),WT(50),AR(50)                    STRAT1    24    A
STRAT1          DIMENSION FX(26),X(26),B(26)                               STRAT1    25    A
STRAT1          CALL TRUNC                                                 STRAT1    26    A
STRAT1          CALL DGEG                                                  STRAT1    27    A
STRAT1          CALL EIGSOL                                                STRAT1    28    A
STRAT1          CALL ZLEV                                                  STRAT1    29    A
STRAT1          CALL VDIST (TBAR,1,NVERT,1)                                STRAT1    30    A
STRAT1          CALL VDIST (SIGMA,1,NVERT,1)                               STRAT1    31    A
STRAT1    C     CALL VDIST(XIBAR,1,NVERT,0)                                APR       2    A
STRAT1    C     CALL HDIST(H,1,NVERT,2)                                    APR       3    A
STRAT1    C     CALL ZONTS                                                 APR       4    A
STRAT1    C     CALL EDDYTS                                                APR       5    A
STRAT1    C     CALL OVRLAP                                                APR       6    A
STRAT1          ILEV1=1                                                    STRAT1    37    A
STRAT1          ILEV2=NVERT-1                                              STRAT1    38    A
STRAT1    C     CALL DIFFK(1,DIFFM)                                        APR       7    A
STRAT1    C     CALL DIFFK(2,DIFFX)                                        APR       8    A
STRAT1          ILEV2=NVERT-1                                              STRAT1    41    A
STRAT1          ILEV1=2                                                    STRAT1    42    A
STRAT1          ILEV2=NVERT-1                                              STRAT1    43    A
STRAT1          CALL UVMAT                                                 STRAT1    44    A
STRAT1          READ (5,1000) NLON,NLAT                                    STRAT1    45    A
STRAT1     1000 FORMAT (10X,14I5)                                          STRAT1    46    A
STRAT1          NGRID=NLON*NLAT                                            STRAT1    47    A
STRAT1          CALL FFTINT                                                STRAT1    48    A
STRAT1    C     CALL XO3EQU                                                APR       9    A
STRAT1          WRITE (6,1010) NLON,NLAT,NGRID                             STRAT1    50    A
STRAT1     1010 FORMAT (1H0,10X,*NLON = *,I3,*,  NLAT = *,I3,*,  NGRID = *,I6,*.*) STRAT1 51 A
STRAT1          CALL WRT12                                                 STRAT1    52    A
STRAT1          STOP                                                       STRAT1    53    A
STRAT1          END                                                        STRAT1    54    A
```

Figure 6.7: First page of Program MESOS1

```
STRAT2    *DECK STRAT2                                                    STRAT2    1    A
STRAT2          PROGRAM MESOS2(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE9,  SEP83    1    A
STRAT2         1 TAPE10,TAPE11,TAPE12,TAPE13,TAPE14,TAPE15)                SEP83    2    A
STRAT2    C     PROGRAM MESOS2                                             SEP83    3    A
STRAT2          LEVEL 3,C,HTSVE,IS,QSV,TOPO,TMPGRD,DUM2,CHDUM,XO3SV,DXO3DT STRAT2    5    A
STRAT2          COMMON PSI(2060),ZETA(2060),Z1(2060),T(2060),Z2(2060),XOX(2060), STRAT2    6    A
STRAT2         1 Z3(2060)                                                  STRAT2    7    A
STRAT2          COMMON /COFBLK/ C(3800),IS(1500)                           STRAT2    8    A
STRAT2          COMMON /CONSTS/ INDEX,MR,LR,INS,INSZ,KINT,ILEV1,ILEV2,NVERT,NRTP, STRAT2    9    A
STRAT2         1 LRTP,NTYPE,NVECT,NVREAL,NVZON,NCYC,DT,YRLAG,TIME          STRAT2   10    A
STRAT2          COMMON /CGBLK/ KD(43),CG(43),NCOMP(12),LWAVE(12),NV(43),LV(43) STRAT2   11    A
STRAT2          COMMON /DEBLK/ DG(43),EG(43),DGCG(43),EGCG(43)             STRAT2   12    A
STRAT2          COMMON /EIGBLK/ EVECT(126),XLIVET(126),EVAL(42),NRK(14),KNR STRAT2   13    A
STRAT2          COMMON /VRTBLK/ ZVAL(26),PVAL(26),VWT(26),DZ,RV            STRAT2   14    A
STRAT2          COMMON /DERIV/ VDERIV(2366),TDERIV(2366),W(2366)           STRAT2   15    A
STRAT2          COMMON /BARBLK/ TBAR(26),SIGMA(26),XIBAR(26),DIFFM(26),DIFFX(26) STRAT2   16    A
STRAT2          COMMON /HEATBK/ H(26),TSZON(104),TSEDDY(16),I1TSZ,I2TSZ,I1TSW, STRAT2   17    A
STRAT2         1 I2TSW,MERGE1,MERGE2,ZWT1(5),ZWT2(5),Q3WR(5)               STRAT2   18    A
STRAT2          COMMON /OROGRA/ TOPO(91),QSV(105),HTSVE(2060)              STRAT2   19    A
STRAT2          COMMON/WORKBK/WORK(7920),OPO(91),SHIRK(10709)              STRAT2   20    A
STRAT2          COMMON/QJBLK/NZJ,L103,COLO3(26),LEVPCM,LEVDYN              STRAT2   21    A
STRAT2          COMMON /TEMPBK/ ADVSV(182)                                 STRAT2   22    A
STRAT2          COMMON /CHEM/ TMPGRD(5280)                                 STRAT2   23    A
STRAT2          COMMON /SPECIE/ DUM2(19866)                                STRAT2   24    A
STRAT2          COMMON /FTCST/ NLON,NLAT,NGRID,MORE(30),XDMP2(30)          STRAT2   25    A
STRAT2          COMMON /O3OX/ CHDUM(5590)                                  STRAT2   26    A
STRAT2          COMMON /PREDIC/A,B,N,TIMSV(135)                            STRAT2   27    A
STRAT2          COMMON /GENER/ DXO3DT(2366)                                STRAT2   28    A
STRAT2    C                                                                SEP83    4    A
STRAT2          COMMON/BND/TBOUND(79),WBOUND(79),XOXBND(79)                SEP83    5    A
STRAT2          COMMON/STHEAT/SQ(474)                                      SEP83    6    A
STRAT2    C                                                                SEP83    7    A
STRAT2          DIMENSION XO3SV(790)                                       STRAT2   29    A
STRAT2          EQUIVALENCE (CHDUM(2401),XO3SV(1))                         STRAT2   30    A
STRAT2          DIMENSION SPACE(2400),DATAIM(6240),X3SPC(790)              STRAT2   31    A
STRAT2          EQUIVALENCE (WORK(1),SPACE(1)),(DATAIM(1),SHIRK(1))        STRAT2   32    A
STRAT2          EQUIVALENCE (WORK(2401),X3SPC(1))                          STRAT2   33    A
STRAT2          DATA NWRT /2/                                              STRAT2   34    A
STRAT2          L103=2                                                     STRAT2   35    A
STRAT2          DO 10 I=1,2060                                             STRAT2   36    A
STRAT2          PSI(I)=0.0                                                 STRAT2   37    A
STRAT2          ZETA(I)=0.0                                                STRAT2   38    A
STRAT2          T(I)=0.0                                                   STRAT2   39    A
STRAT2          Z1(I)=0.0                                                  STRAT2   40    A
STRAT2          Z2(I)=0.0                                                  STRAT2   41    A
STRAT2          Z3(I)=0.0                                                  STRAT2   42    A
STRAT2          W(I)=0.0                                                   STRAT2   43    A
STRAT2       10 CONTINUE                                                   STRAT2   44    A
STRAT2    C     CALL READ3                                                 SEP83    8    A
STRAT2          CALL READ10                                                STRAT2   46    A
STRAT2    C     CALL NLNADJ                                                SEP83    9    A
STRAT2    C                                                                SEP83   10    A
```

Figure 6.8: First page of Program MESOS2.

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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 scalars 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

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

in which the special properties of the orthonormal spherical functions $Y_{\alpha}(\lambda,\mu)$ are outlined in (4.3) - (4.8). 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 sun (for details of these developments, see Baer and Platzman, 1961) we arrive at

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

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

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

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) with any arbitrary member of the orthogonalizing set, say $Y^*_\gamma/4\pi$, and integrate over the unit sphere to get

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

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

$$\left\{\begin{array}{l} n_\beta \geq n_\alpha \\ \ell_\gamma = \ell_\alpha + \ell_\beta \end{array}\right\}$$

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

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

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

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

We now let

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

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

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

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)

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

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

provided

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

(N and κ must be intergers) and the latitudes μ_k are located at the Northern Hemisphere zeroes of the Legendre polynomial $P_\kappa^0(\mu)$ (including the equator if κ 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

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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 scalar 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 (4.3) - (4.8). Insertion of solutions (B.2) into (B.1) yields

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

But, if we define

$$\begin{aligned} N_\alpha &= \left[\frac{(2n_\alpha+1)(n_\alpha-\ell_\alpha)!}{(n_\alpha+\ell_\alpha)!}\right]^{1/2} \\ \epsilon &= 1 + i0 \end{aligned} \tag{B.4}$$

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

$$\left.\begin{aligned}(1-\mu^2)\frac{dP_\alpha}{d\mu} &= -n_\alpha \mu P_\alpha + (n_\alpha+\ell_\alpha)\frac{N_\alpha}{N_{\alpha-\varepsilon}} P_{\alpha-\varepsilon} \\ \text{and} \\ \mu P_\alpha &= \frac{(n_\alpha-\ell_\alpha+1)}{(2n_\alpha+1)} \frac{N_\alpha}{N_{\alpha+\varepsilon}} P_{\alpha+\varepsilon} + \frac{(n_\alpha+\ell_\alpha)}{(2n_\alpha+1)} \frac{N_\alpha}{N_{\alpha-\varepsilon}} P_{\alpha-\varepsilon}\end{aligned}\right\} . \quad (B.5)$$

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

$$(1-\mu^2)\frac{dP_\alpha}{d\mu} - \mu c_\alpha P_\alpha = \frac{(1-n_\alpha^2)(n_\alpha+\ell_\alpha)}{(2n_\alpha+1)} \frac{N_\alpha}{N_{\alpha-\varepsilon}} P_{\alpha-\varepsilon} - \frac{n_\alpha(n_\alpha+2)(n_\alpha-\ell_\alpha+1)}{(2n_\alpha+1)} \frac{N_\alpha}{N_{\alpha+\varepsilon}} P_{\alpha+\varepsilon}. \quad (B.6)$$

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

$$\begin{aligned}\frac{1}{4\pi}\int_0^{2\pi}\int_{-1}^{1}(\nabla\cdot\mu\nabla A)Y_\gamma^* d\mu d\lambda = &\sum_{\substack{\alpha \\ \ell_\alpha=\ell_\gamma}} a_\alpha\left[\frac{(1-n_\alpha^2)(n_\alpha+\ell_\alpha)}{(2n_\alpha+1)} \frac{N_\alpha}{N_{\alpha-\varepsilon}}\right]\frac{1}{2}\int_{-1}^{1} P_{\alpha-\varepsilon}P_\gamma d_\mu - \\ &- \sum_{\substack{\alpha \\ \ell_\alpha=\ell_\gamma}} a_\alpha\left[\frac{n_\alpha(n_\alpha+2)(n_\alpha-\ell_\alpha+1)}{(2n_\alpha+1)} \frac{N_\alpha}{N_{\alpha+1}}\right]\frac{1}{2}\int_{-1}^{1} P_{\alpha+\varepsilon}P_\gamma d\mu\end{aligned}$$

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

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

$$= D_\gamma a_{\gamma-\varepsilon} - E_\gamma a_{\gamma+\varepsilon} \quad . \tag{B.7}$$

where we have defined

$$D_\gamma \equiv (1-n_\gamma^2)\left[\frac{(n_\gamma+\ell_\gamma)(n_\gamma-\ell_\gamma)}{(2n_\gamma-1)(2n_\gamma+1)}\right]^{1/2}$$

$$E_\gamma \equiv n_\gamma(n_\gamma+2)\left[\frac{(n_\gamma+\ell_\gamma+1)(n_\gamma-\ell_\gamma+1)}{(2n_\gamma+1)(2n_\gamma+3)}\right]^{1/2} \tag{B.8}$$

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

$$B = \nabla^2 A \tag{B.9}$$

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

$$B = \sum_\alpha b_\alpha Y_\alpha(\lambda,\mu). \tag{B.10}$$

Then, from (4.6), we know that

$$b_\alpha = -c_\alpha a_\alpha \tag{B.11}$$

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

$$\frac{1}{4\pi}\int_0^{2\pi}\int_{-1}^{1}(\nabla\cdot\mu\nabla A)Y_\gamma^* d\mu d\lambda = -\frac{D_\gamma}{c_{\gamma-\varepsilon}}b_{\gamma-\varepsilon} + \frac{E_\gamma}{c_{\gamma+\varepsilon}}b_{\gamma+\varepsilon}$$

$$= \mathcal{D}_\gamma b_{\gamma-\varepsilon} - \mathcal{E}_\gamma b_{\gamma+\varepsilon} \tag{B.12}$$

in which we have defined

$$\mathcal{D}_\gamma = -\frac{D_\gamma}{c_{\gamma-\varepsilon}},\ \mathcal{E}_\gamma = -\frac{E_\gamma}{c_{\gamma+\varepsilon}} \tag{B.13}$$

provided that in (B.12) we ignore terms in which $c_{\gamma-\varepsilon} = 0$ (i.e., $n_{\gamma-\varepsilon} = 0$). Further, for both (B.7) and (B.13) we must stipulate that all terms calling for any $a_{\gamma-\varepsilon}$, $a_{\gamma+\varepsilon}$, $b_{\gamma-\varepsilon}$ or $b_{\gamma+\varepsilon}$ outside the range 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

$$a_\gamma X_{\gamma-1} + b_\gamma X_\gamma + c_\gamma X_{\gamma+1} = R_\gamma \qquad \gamma = 1, 2, 3, \ldots, \Gamma \tag{C.1}$$

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

$$AX = R \tag{C.3}$$

with A being tridiagonal of the form

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

For solutions we define

$$\left.\begin{aligned} C_1 &= 1/b_1 \\ C_\gamma &= 1/(b_\gamma - a_\gamma c_{\gamma-1} C_{\gamma-1}); \quad 2 \le \gamma \le \Gamma \\ D_\gamma &= -\, c_\gamma C_\gamma \end{aligned}\right\} \tag{C.5}$$

and let

$$\left.\begin{aligned} B_1 &= C_1 R_1 \\ B_\gamma &= C_\gamma (R_\gamma - a_\gamma B_{\gamma-1}); \; 2 \leq \gamma \leq \Gamma \end{aligned}\right\}. \tag{C.6}$$

Then, the solutions appear as

$$\begin{aligned} X_\Gamma &= B_\Gamma \\ X_\gamma &= D_\gamma X_{\gamma+1} + B_\gamma; \; \gamma = \Gamma-1, \Gamma-2, \ldots, 1 \end{aligned} \tag{C.7}$$

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

$$\left.\begin{aligned} b_1 &\neq 0 \\ b_\gamma &\neq a_\gamma c_{\gamma-1} C_{\gamma-1} \end{aligned}\right\}. \tag{C.8}$$

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

We consider the set of complete orthogonal Legendre polynomials, $P_n^\ell(\mu)$, in which $\ell = 0, \pm 1, \pm 2, \ldots$ and $n = 0, 1, 2, \ldots$. We define this set, according to (4.8), to be normalized such that

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

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

$$f(\mu) = \sum_{\ell}\sum_{n} f_n^\ell P_n^\ell(\mu) \tag{D.2}$$

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

$$f_n^\ell = \frac{1}{2} \sum_{\ell}\sum_{n} f_{n'}^\ell \int_{-1}^{1} P_{n'}^\ell(\mu) P_n^\ell(\mu) d\mu = \frac{1}{2} \int_{-1}^{1} f(\mu) P_n^\ell(\mu) d\mu \ . \tag{D.3}$$

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 $k = 1, 2, 3, \ldots, N$ with N being the total number of points lying within $-1<\mu<1$. Thus at each latitude point, (D.2) becomes

$$f(\mu_k) = \sum_{\ell}\sum_{n} f_n^\ell P_n^\ell(\mu_k) \ . \tag{D.4}$$

This means that in order to determine coefficients f_n^ℓ we must evaluate the inte-

grals in (D.3) numerically and at the same time maintain the orthogonality properties of the discrete polynomials representation in (D.4). For this purpose, integrating by quadratures, we introduce a set of Gaussian weight functions, w_k, such that

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

and the numerical analog for (D.3) becomes

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

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

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

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

and thus,

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

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

$$\int_{-1}^{1} P_n^{\ell}(\mu)P_{n'}^{\ell}(\mu)d\mu = \sum_{k=1}^{N} w_k P_n^{\ell}(\mu_k)P_{n'}^{\ell}(\mu_k)$$

$$= \sum_{k=1}^{N} w_k \sum_{i=0}^{n+n'} b_i[\mu_k]^i \quad . \tag{D.9}$$

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

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

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

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

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

$$\left.\begin{aligned} \cos j\phi &= \sum_{m=0}^{j/2} a_{2m}\mu^{2m} = a_j\mu^j + \sum_{m=0}^{(j/2)-1} a_{2m}\mu^{2m} \\ &\text{and} \\ \cos j\phi_k &= a_j[\mu_k]^j + \sum_{m=0}^{(j/2)-1} a_{2m}[\mu_k]^{2m} \end{aligned}\right\} \quad . \tag{D.12}$$

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

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

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

or

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

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

$$= \begin{cases} 0 \text{ for } i \text{ odd} \\ \dfrac{-2}{i^2-1} \text{ for } i \text{ even} \\ i = 0, 1, 2, \ldots, n+n' \end{cases} , \tag{D.14}$$

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 $\phi_1=30°$, $\phi_2=90°$, and $\phi_3=150°$. Then, from (D.14) we can construct the set (using i = 0, 1, 2)

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

with solutions

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

We note that the solutions (D.16) are symmetric in w_k about the equator. If we assume such symmetry a priori 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

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

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

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

with solutions

$$\left.\begin{aligned} w_1 &= \frac{4}{9} \\ w_2 &= \frac{5}{9} \end{aligned}\right\} . \qquad (D.18)$$

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

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

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