Lawrence Livermore Laboratory

Modeling of Transport in the Two-Dimensional Atmospheric Transport
and Kinetics Codes SPHERNEW and TRACER

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July 23, 1976

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M E M O R A N D U M

TO: Distribution
FROM: A. L. Edwards
SUBJECT: Errata to UCID-17203

The following additions and replacements should be made in the report, "Modeling of Transport in the Two-Dimensional Atmospheric Transport and Kinetics Codes SPHERNEW and TRACER", dated July 23, 1976.

Page 17. Add after line 6:

The value of α must be 1.0 at any zone interface with a fixed downstream concentration, to prevent unstable or unphysical results, such as negative concentrations or extremely large concentrations.

Page 18. Add after Eq. (49):

This requires that $\alpha = 1.0$ in Eq. (42), when $j = 2$.

Page 19. Replace line 7:

This requires that $\alpha = 1.0$ in Eq. (41) when $j = NV-1$. This option may also be applied at any specified altitude, r_{jfix} , requiring that $\alpha = 1.0$ in Eq. (41) when $j = jfix-1$, and in Eq. (42) when $j = jfix+1$.

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Abstract

This report describes how transport by the wind is modeled in the 2-D atmospheric transport and chemical kinetics codes SPHERNEW and TRACER. The description includes the equations for transport by a specified velocity field, the eddy diffusion approximation for short-term fluctuations in the velocity, other simplifying approximations, the geometric grid, the difference equations, and the coefficient matrix of the grid. The assumption of a constant vertical density distribution was used to derive mass-consistent forms of the difference equations. These forms eliminate the instabilities and unrealistic solutions associated with specified wind fields which are not exactly mass-consistent. An option is allowed for variable weighting between central (second-order) and upstream (first-order) forms of the spatial differencing of the advection terms, to modulate phase and amplitude errors in the advection model.

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Modeling of Transport in the Two-Dimensional Atmospheric Transport and Kinetics Codes SPHERNEW and TRACER

I. Introduction

The purpose of this report is to describe how transport by the wind is modeled in the 2-D atmospheric transport and chemical kinetics code SPHERNEW, and in a transport-only version, TRACER. Significant changes have been made in the model since earlier versions were described.^(1,2,3) The description includes the partial differential equations for transport by a specified velocity field, the eddy diffusion approximation used to account for the effects of short-term fluctuations from the mean wind, other approximations used to simplify the model, the geometric grid used in the model, the set of derived difference equations, and the resulting coefficient matrix of the equation set.

The assumption that the total air density does not change with time was used to derive mass-consistent forms of the difference equations. These forms are stable, and result in acceptable steady-state solutions, even when the specified wind field is not mass-consistent. This allows use of wind fields whose mass-consistency have been degraded by transfer from one grid to another, by various effects of averaging or interpolation in space and time, or by changes deliberately made in the directional components of the wind.

Another feature of the difference equations is the use of a single parameter which may be specified to obtain any possible combination of

central and automatic upstream differencing in the advection terms of the difference equations. This allows a compromise to be made between the stability and freedom from spurious oscillations of upstream (first-order) spatial differencing, and the better phase accuracy of central (second-order) spatial differencing.

The mass-consistent form of the advection difference equation and the variably-weighted upstream differencing option have both been used for many years in the TRUMP code for advection and diffusion.⁽⁴⁾

II. The Differential Equations for Transport

A. Transport by a Velocity Field

In a space with general coordinates x , with a specified velocity field $\underline{u}$, with directional components which are functions of time and position, and with total density ρ and concentrations of species C_i , also functions of time and position, the Divergence Theorem gives the time dependence, as follows:

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \underline{u}) \quad (1)$$

$$\frac{\partial C_i}{\partial t} = -\nabla \cdot (C_i \underline{u}) \quad , \quad (i = 1, N_S) \quad (2)$$

Equation (2) is repeated for each species. The subscript i will be dropped below. By expansion and rearrangement, Eqs. (1) and (2) may be combined to give:

$$\rho \frac{\partial}{\partial t} (C/\rho) = -\rho [\nabla (C/\rho) \cdot \underline{u}] \quad (3)$$

Additional terms are required on the right-hand sides of Eqs. (1) through (3) to represent any sources and sinks, such as those due to production and loss by chemical reactions between species and photodissociation. These terms will not be discussed here.

Boundary conditions are specified on the bounding surfaces of the space in which the velocity field is defined, of the general form:

$$p C + \underline{q} \cdot \underline{\nabla C} = f \quad (4)$$

where p , $\underline{q}$, and f are functions of time and position.

The initial conditions within the space are specified at some time t_0 .

$$C(x, t_0) = C(x) \quad (5)$$

B. The Eddy Diffusion Approximation

Concentrations and velocities may be represented by mean values averaged over some turbulence time scale, $\Delta\tau$, plus the short time deviations from the mean values:

$$C_u = (\bar{C} + C')(\bar{u} + u') = \bar{C}\bar{u} + C'\bar{u} + \bar{C}u' + C'u' = \bar{C}\bar{u} + (C_u)' \quad (6)$$

The problem is greatly simplified if the effects of concentration and velocity changes can be modeled by the use of eddy diffusion coefficients as follows:

$$(C_u)' = -\rho \underline{\underline{K}} \cdot \nabla(C/\rho) \quad (7)$$

where $\underline{\underline{K}}$ is a symmetric eddy diffusivity tensor.⁽⁵⁾ Equation (7) may be interpreted as the definition of $\underline{\underline{K}}$, which has components for each pair of coordinate directions in space.

For a two-dimensional wind field, the tensor $\underline{\underline{K}}$ has four components, K_{11} , K_{12} , K_{21} , and K_{22} . It can be shown that K_{12} and K_{21} must be equal, and that K_{12}^2 cannot exceed $K_{11}K_{22}$. It is also possible to rotate the coordinate system so that at a given point in space, the new values of K_{12} and K_{21} are zero. The new values of K_{11} and K_{22} are then the principal

diffusivities, and the new axes are the local principal axes of diffusion. Although K_{12} may be negative, the principal diffusivities must be positive everywhere.

If the deviations from the mean values of C_i can be ignored in all terms of Eqs. (1) through (3) (including terms for chemical production and losses and general sources and sinks), except for the transport term, Eqs. (6) and (7) may be substituted to obtain (dropping the $\sim$ symbol for mean values):

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \underline{u}) \quad (8)$$

$$\frac{\partial C}{\partial t} = \nabla \cdot [\rho \underline{K} \cdot \underline{\nabla}(C/\rho)] - \nabla \cdot (C \underline{u}) \quad (9)$$

$$\rho \frac{\partial}{\partial t} \left(\frac{C}{\rho} \right) = \nabla \cdot [\rho \underline{K} \cdot \underline{\nabla}(C/\rho)] - \rho [\underline{\nabla}(C/\rho) \cdot \underline{u}] \quad (10)$$

C. The Mass-Consistent Formulation

A further simplification can be made if the mean total density ρ is a function only of the spatial coordinates, and does not change with time. In this case, Eqs. (8) and (10) become:

$$\frac{\partial \rho}{\partial t} = 0 \quad (11)$$

$$\frac{\partial C}{\partial t} = \nabla \cdot [\rho \underline{K} \cdot \underline{\nabla}(C/\rho)] - \rho [\underline{\nabla}(C/\rho) \cdot \underline{u}] \quad (12)$$

Thus, either Eq. (9) or Eq. (12) may be used for the concentration change if the total density does not change with time. However, Eq. (12) has the advantage that a steady state solution exists for which $\underline{\nabla}(C/\rho)$ is zero, regardless of the nature of the velocity field. In effect, Eq. (12) behaves

as if the velocity field were mass-consistent, even if it is not, and may be called the mass-consistent formulation of the transport equation. If the velocity field is mass-consistent, Eqs. (9) and (12) are equivalent. The transport model in previous versions of SPHERNEW was based on Eq. (9).

D. Mass-Consistent Transport in 2-D Spherical Coordinates

The transport equation is to be solved in the two-dimensional spherical coordinate system representing the radial (altitude) and meridional (latitude) directions in the earth's atmosphere. It is assumed that longitudinal transport is so rapid compared to the other directions that no concentration gradients occur in that direction. In addition, it is assumed that the total density is a function only of the altitude. For this system, Eq. (12) becomes

$$\begin{aligned} \frac{\partial C}{\partial t} = & \frac{1}{r^2} \frac{\partial}{\partial r} \left[r^2 K_{rr} \left(\frac{\partial C}{\partial r} - \gamma C \right) + r K_{r\theta} \sin \theta \frac{\partial C}{\partial x} \right] \\ & + \frac{1}{r^2} \frac{\partial}{\partial x} \left[r K_{r\theta} \sin \theta \left(\frac{\partial C}{\partial r} - \gamma C \right) + K_{\theta\theta} \sin^2 \theta \frac{\partial C}{\partial x} \right] \\ & - u_r \left(\frac{\partial C}{\partial r} - \gamma C \right) - \frac{1}{r} u_\theta \sin \theta \frac{\partial C}{\partial x} \end{aligned} \quad (13)$$

where r is the geocentric radius, θ is the angle from the North polar axis, $x = -\cos \theta$, and the K 's are the components of the eddy conductivity tensor, and γ is the fractional density gradient (always negative):

$$\gamma = \gamma(r) = \frac{1}{\rho} \frac{d\rho}{dr} \quad (14)$$

In terms of the mixing ratio $S = C/\rho$, Eq. (13) becomes:

$$\begin{aligned} \frac{\partial S}{\partial t} = & \frac{1}{r^2} \frac{\partial}{\partial r} \left[r^2 K_{rr} \frac{\partial S}{\partial r} + r K_{r\theta} \sin \theta \frac{\partial S}{\partial x} \right] + \gamma \left[K_{rr} \frac{\partial S}{\partial r} + \frac{1}{r} K_{r\theta} \sin \theta \frac{\partial S}{\partial x} \right] \\ & + \frac{1}{r^2} \frac{\partial}{\partial x} \left[r K_{r\theta} \sin \theta \frac{\partial S}{\partial r} + K_{\theta\theta} \sin^2 \theta \frac{\partial S}{\partial x} \right] \\ & - u_r \frac{\partial S}{\partial r} - \frac{1}{r} u_\theta \sin \theta \frac{\partial S}{\partial x} \end{aligned} \quad (15)$$

The effect of the gradient of the total density, as expressed in the second term on the right-hand side of Eq. (15), is a tendency for spatial variations in the mixing ratio to move upward in the absence of sources and sinks, unless counteracted by downward velocities or the effects of the $K_{r\theta}$ component of eddy diffusion.

III. Grid and Zone Geometry

A. The Grid

The difference equations to be described apply to a two-dimensional grid in the meridional and radial directions, representing points in a radial shell of the earth's atmosphere from the surface to an upper altitude currently fixed at 50 km. Conditions are assumed to be constant in the longitudinal direction, due to the relatively rapid longitudinal transport compared with the other directions.

The meridional coordinates of the grid points are the set:

$$\theta_i = \theta_1, \theta_2, \dots, \theta_{N_h-1}, \theta_{N_h} \quad (16)$$

The set now used consists of 5 degree increments from the North Pole to the South Pole, so that N_h is 37.

The radial coordinates of the grid points are the set:

$$r_j = r_1, r_2, \dots, r_{N_v-1}, r_{N_v} \quad (17)$$

The set now used consists of 1 km increments from the surface to an altitude of 36 km, and 2 km increments to an altitude of 50 km, so that N_v is 44. The earth's surface is assumed to be spherical, with a radius of 6380 km, so that r_1 is 6380.

Thus the grid currently used has $37 \times 44 = 1680$ grid points. The grid point with indices (i,j) is located at (θ_i, r_j) , and really represents a complete circle around the polar axis of the earth.

B. The Zones

A finite volume element, or zone, may be associated with each grid point. These zones are bounded by the outer boundaries of the grid, and by the surfaces containing the mid-points between adjacent grid points. The meridional surfaces are the set:

$$\theta_{i\pm\frac{1}{2}} = \theta_1, \frac{1}{2}(\theta_1 + \theta_2), \dots, \frac{1}{2}(\theta_i + \theta_{i+1}), \dots, \frac{1}{2}(\theta_{N_h-1} + \theta_{N_h}), \theta_{N_h}. \quad (18)$$

The radial surfaces are the set:

$$r_{j\pm\frac{1}{2}} = r_1, \frac{1}{2}(r_1 + r_2), \dots, \frac{1}{2}(r_j + r_{j+1}), \dots, \frac{1}{2}(r_{N_v-1} + r_{N_v}), r_{N_v}. \quad (19)$$

Zone volumes $V_{i,j}$, meridional interface areas $A_{i\pm\frac{1}{2},j}$, and radial interface areas $A_{i,j\pm\frac{1}{2}}$ are given exactly by the equations:

$$V_{i,j} = \frac{2\pi}{3} (r_{j+\frac{1}{2}}^3 - r_{j-\frac{1}{2}}^3) (\cos \theta_{i-\frac{1}{2}} - \cos \theta_{i+\frac{1}{2}}) \quad (20)$$

$$A_{i\pm\frac{1}{2},j} = \pi (r_{j+\frac{1}{2}}^2 - r_{j-\frac{1}{2}}^2) \sin \theta_{i\pm\frac{1}{2}} \quad (21)$$

$$A_{i,j\pm\frac{1}{2}} = 2\pi r_{j\pm\frac{1}{2}}^2 (\cos \theta_{i-\frac{1}{2}} - \cos \theta_{i+\frac{1}{2}}) \quad (22)$$

These can be approximated, with a fractional error of about 0.001 or less for the grid spacing currently in use, by:

$$\bar{V}_{i,j} = 2\pi r_j^2 \bar{\Delta r_j} \bar{\Delta x_i} \quad (23)$$

$$\bar{A}_{i\pm\frac{1}{2},j} = \pi r_j \bar{\Delta r_j} (\sin \theta_i + \sin \theta_{i\pm 1}) \quad (24)$$

$$\bar{A}_{i,j\pm\frac{1}{2}} = \frac{1}{2}\pi (r_j + r_{j\pm 1})^2 \bar{\Delta x_i} \quad (25)$$

where $\overline{\Delta x_i}$ is given by:

$$\overline{\Delta x_i} = \begin{cases} \frac{1}{4}(\cos \theta_1 - \cos \theta_2) , & (i = 1) \\ \frac{1}{2}(\cos \theta_{i-1} - \cos \theta_{i+1}) , & (i = 2, N_h-1) \\ \frac{1}{4}(\cos \theta_{N_h-1} - \cos \theta_{N_h}) , & (i = N_h) \end{cases} \quad (26)$$

and $\overline{\Delta r_j}$ is given by:

$$\overline{\Delta r_j} = \begin{cases} \frac{1}{2}(r_2 - r_1) , & (j = 1) \\ \frac{1}{2}(r_{j+1} - r_{j-1}) , & (j = 2, N_v-1) \\ \frac{1}{2}(r_{N_v} - r_{N_v-1}) , & (j = N_v) \end{cases} \quad (27)$$

Distances between adjacent grid points in the meridional and radial directions are given by:

$$r_{j+\frac{1}{2}} = r_{j+1} - r_j \quad (28)$$

$$\Delta \theta_{i+\frac{1}{2}} = \theta_{i+1} - \theta_i \quad (29)$$

The angular distance may be approximated, with a fractional error of less than 0.001, by using the finite difference analogous to the identity $d\theta = -d(\cos \theta)/\sin \theta$.

$$\overline{\Delta \theta_{i+\frac{1}{2}}} = 2(\cos \theta_i - \cos \theta_{i+1})/(\sin \theta_i + \sin \theta_{i+1}) \quad (30)$$

Equations (23) to (30) can be used to derive the difference equations for transport from mass balances over zones.

IV. The Difference Equations for Transport

A. General Requirements

The geometric grid used in the SPHERNEW code was described in Section III above. In order to solve the governing partial differential equation for transport, Eq. (13), on this grid, the differential equation must be transformed into a set of ordinary differential equations. One such equation is required for each discrete point on the grid, expressed in terms of concentrations, velocities, and eddy diffusion coefficients defined at discrete points in space. The resulting equations are of the general form:

$$\frac{dC_{i,j}}{dt} = \sum_{m=i-1}^{i+1} \sum_{n=j-1}^{j+1} (a_{mn})_{i,j} C_{mn}, \quad (i = 1, N_h, j = 1, N_v) \quad (31)$$

with appropriate modifications at $i = 1$, $i = N_h$, $j = 1$, and $j = N_v$, depending on the choices of boundary conditions. With the addition of terms for chemical production and losses, and general sources and sinks, the set of equations (31) can be solved by general methods, for some specified initial set of concentrations, if the coefficients a_{mn} are known.

The general ordinary differential equation, or difference equation, is obtained from Eq. (13) by replacing the spatial derivatives on the right-hand side of Eq. (13) by ratios of finite differences, based on a set of 9 grid points centered around each point (i,j) . The choice of finite differences must satisfy the requirements of conservation of mass and stability of the solution, and hopefully, reasonable accuracy.

B. Methods of Obtaining the Difference Equations

The differential equation, Eq. (13) can be converted to difference form by a variety of methods, including: (a) Intuitive replacement of differentials with differences, (b) Integration by parts over the zones associated with each grid point, with various assumptions concerning the spatial dependence of the integrand within each zone, (c) Ignoring the differential equation and doing a complete mass balance over the finite volume elements of the grid, using the distances, surface areas, and volumes defined in Section III of this report. The same assumptions used to derive the differential equation must be used, and other assumptions must be made regarding the average flux over each interface between two zones. Fortunately, all three methods have been used, and lead to the same results. Method (c) above, in particular, guarantees that the difference equations conserve mass. The derivations are standard, and will not be reproduced here.

C. The Difference Equation for Interior Points

The difference equation for interior points is as follows (the superscript $n+1$, indicating that the value is at the time $t^{(n+1)}$, has been deleted from all terms on the right-hand side of the equation):

$$\begin{aligned} \frac{dC_{i,j}}{dt} = \frac{1}{r_j \Delta r_j} & \left\{ (H_{i,j+\frac{1}{2}} + \tilde{G}_{i,j+\frac{1}{2}}) [C_{i,j+1}(1 - \beta_{j+\frac{1}{2}}) - C_{i,j}(1 + \beta_{j+\frac{1}{2}})] \right. \\ & - (H_{i,j-\frac{1}{2}} - \tilde{G}_{i,j-\frac{1}{2}}) [C_{i,j}(1 - \beta_{j-\frac{1}{2}}) - C_{i,j-1}(1 + \beta_{j-\frac{1}{2}})] \\ & + \frac{1}{\Delta x_i} [E_{i,j+\frac{1}{2}}(C_{i+1,j} + C_{i+1,j+1} - C_{i-1,j} - C_{i-1,j+1}) \\ & \left. - E_{i,j-\frac{1}{2}}(C_{i+1,j-1} + C_{i+1,j} - C_{i-1,j-1} - C_{i-1,j})] \right\} \end{aligned}$$

$$\begin{aligned}
& + \frac{1}{r_j^2 \Delta x_i} \left\{ (D_{i+\frac{1}{2},j} + \tilde{F}_{i+\frac{1}{2},j})(C_{i+1,j} - C_{i,j}) - \right. \\
& - (D_{i-\frac{1}{2},j} - \tilde{F}_{i-\frac{1}{2},j})(C_{i,j} - C_{i-1,j}) \\
& + B_{i+\frac{1}{2},j} \left[\frac{1}{\Delta r_j} (C_{i,j+1} + C_{i+1,j+1} - C_{i,j-1} - C_{i+1,j-1}) \right. \\
& - (\gamma_{j-\frac{1}{2}} + \gamma_{j+\frac{1}{2}})(C_{i,j} + C_{i+1,j}) \left. \right] \\
& - B_{i-\frac{1}{2},j} \left[\frac{1}{\Delta r_j} (C_{i-1,j+1} + C_{i,j+1} - C_{i-1,j-1} - C_{i,j-1}) \right. \\
& - (\gamma_{j-\frac{1}{2}} + \gamma_{j+\frac{1}{2}})(C_{i-1,j} + C_{i,j}) \left. \right] \left. \right\}, \quad (i = 2, N_h-1, j = 2, N_v-1) \quad (32)
\end{aligned}$$

where $\overline{\Delta x_i}$ and $\overline{\Delta r_j}$ are given by Eqs. (26) and (27), and

$$\begin{aligned}
H_{i,j+\frac{1}{2}} &= r_{j+\frac{1}{2}}^2 (K_{rr})_{i,j+\frac{1}{2}} / \Delta r_{j+\frac{1}{2}} \\
&= \frac{1}{8} (r_j + r_{j+1})^2 \left[(K_{rr})_{i,j} + (K_{rr})_{i,j+1} \right] / (r_{j+1} - r_j) \quad (33)
\end{aligned}$$

$$\gamma_{j+\frac{1}{2}} = \left(\frac{1}{\rho} \frac{\Delta \rho}{\Delta r} \right)_{j+\frac{1}{2}} = 2(\rho_{j+1} - \rho_j) / [(r_{j+1} - r_j)(\rho_j + \rho_{j+1})] \quad (34)$$

$$\beta_{j+\frac{1}{2}} = \frac{1}{2} \Delta r_{j+\frac{1}{2}} \gamma_{j+\frac{1}{2}} = (\rho_{j+1} - \rho_j) / (\rho_j + \rho_{j+1}) \quad (35)$$

$$\begin{aligned}
E_{i,j+\frac{1}{2}} &= \frac{1}{4} r_{j+\frac{1}{2}} \sin \theta_i (K_{r\theta})_{i,j+\frac{1}{2}} \\
&= \frac{1}{16} (r_j + r_{j+1}) \sin \theta_i \left[(K_{r\theta})_{i,j} + (K_{r\theta})_{i,j+1} \right] \quad (36)
\end{aligned}$$

$$\begin{aligned}
 G_{i,j+\frac{1}{2}} &= -\frac{1}{2} r_{j+\frac{1}{2}}^2 (u_r)_{i,j+\frac{1}{2}} \\
 &= -\frac{1}{16} (r_j + r_{j+1})^2 \left[\rho_j (u_r)_{i,j} + \rho_{j+1} (u_r)_{i,j+1} \right] / (\rho_j + \rho_{j+1}) \quad (37)
 \end{aligned}$$

$$\begin{aligned}
 D_{i+\frac{1}{2},j} &= (\sin \theta_{i+\frac{1}{2}})^2 (K_{\theta\theta})_{i+\frac{1}{2},j} / \Delta x_{i+\frac{1}{2}} \\
 &= \frac{1}{8} (\sin \theta_i + \sin \theta_{i+1})^2 \left[(K_{\theta\theta})_{i,j} + (K_{\theta\theta})_{i+1,j} \right] / (\cos \theta_i - \cos \theta_{i+1}) \quad (38)
 \end{aligned}$$

$$\begin{aligned}
 B_{i+\frac{1}{2},j} &= \frac{1}{4} r_j \sin \theta_{i+\frac{1}{2}} (K_{r\theta})_{i+\frac{1}{2},j} \\
 &= \frac{1}{16} r_j (\sin \theta_i + \sin \theta_{i+1}) \left[(K_{r\theta})_{i,j} + (K_{r\theta})_{i+1,j} \right] \quad (39)
 \end{aligned}$$

$$\begin{aligned}
 F_{i+\frac{1}{2},j} &= -\frac{1}{2} r_j \sin \theta_{i+\frac{1}{2}} (u_\theta)_{i+\frac{1}{2},j} \\
 &= -\frac{1}{8} r_j (\sin \theta_i + \sin \theta_{i+1}) \left[(u_\theta)_{i,j} + (u_\theta)_{i+1,j} \right] \quad (40)
 \end{aligned}$$

The coefficients with subscripts $j-\frac{1}{2}$ are obtained by replacing j with $j-1$ and $j+1$ with j in Eqs. (33) to (37). The coefficients with subscripts $i-\frac{1}{2}$ are obtained by replacing i with $i-1$ and $i+1$ with i in Eqs. (38) to (40).

The advection coefficients $\tilde{G}$ and $\tilde{F}$ are obtained from G and F as follows:

$$\tilde{G}_{i,j+\frac{1}{2}} = G_{i,j+\frac{1}{2}} + \alpha |G_{i,j+\frac{1}{2}}| \quad (41)$$

$$\tilde{G}_{i,j-\frac{1}{2}} = G_{i,j-\frac{1}{2}} - \alpha |G_{i,j-\frac{1}{2}}| \quad (42)$$

$$\tilde{F}_{i+\frac{1}{2},j} = F_{i+\frac{1}{2},j} + \alpha |F_{i+\frac{1}{2},j}| \quad (43)$$

$$\tilde{F}_{i-\frac{1}{2},j} = F_{i-\frac{1}{2},j} - \alpha |F_{i-\frac{1}{2},j}| \quad (44)$$

$$0 \leq \alpha \leq 1 \quad (45)$$

The value of α may be specified to obtain first-order, or upstream differencing ($\alpha = 1$), second-order, or central advection differencing ($\alpha = 0$), or any intermediate combination. Upstream differencing causes numerical diffusion, while central differencing causes spurious oscillations when transporting a concentration profile with short wavelength components. An intermediate method can sometimes be used to advantage.

D. The Difference Equations for Boundary Points

At the North and South Poles, because of the geometric symmetry, there can be no flux across the meridional boundary. In addition, because the meridional gradient at the boundary must be zero, there can be no vertical flux due to the $K_{\theta r}$ eddy diffusion term.

1. North Pole, Interior Radii. The difference equation for the North Pole ($i = 1$), interior radii ($j = 2, N_V - 1$), can be obtained from Eq. (32) by eliminating the terms multiplied by $E_{i,j+\frac{1}{2}}$, $E_{i,j-\frac{1}{2}}$, $D_{i-\frac{1}{2},j}$, $B_{i-\frac{1}{2},j}$ and $F_{i-\frac{1}{2},j}$. The final equation is:

$$\begin{aligned} \frac{dC_{1,j}}{dt} = & \frac{1}{r_j^2 \Delta r_j} \left\{ (H_{1,j+\frac{1}{2}} + \tilde{G}_{1,j+\frac{1}{2}}) [C_{1,j+1}(1 - \beta_{j+\frac{1}{2}}) - C_{1,j}(1 + \beta_{j+\frac{1}{2}})] \right. \\ & - (H_{1,j-\frac{1}{2}} - \tilde{G}_{1,j-\frac{1}{2}}) [C_{1,j}(1 - \beta_{j-\frac{1}{2}}) - C_{1,j-1}(1 + \beta_{j-\frac{1}{2}})] \Big\} \\ & + \frac{1}{r_j^2 \Delta x_1} \left\{ (D_{1+\frac{1}{2},j} + \tilde{F}_{1+\frac{1}{2},j})(C_{2,j} - C_{1,j}) \right. \\ & + B_{1+\frac{1}{2},j} \left[\frac{1}{\Delta r_j} (C_{1,j+1} + C_{2,j+1} - C_{1,j-1} - C_{2,j-1}) \right. \\ & \left. \left. - (\gamma_{j-\frac{1}{2}} + \gamma_{j+\frac{1}{2}})(C_{1,j} + C_{2,j}) \right] \right\}, \quad (j = 2, N_V - 1), \quad (46) \end{aligned}$$

2. South Pole, Interior Radii. The difference equation for interior radii ($j = 2, N_V - 1$) of the South Pole ($i = N_h$), can be obtained from Eq. (32) by eliminating the terms multiplied by $E_{i,j+\frac{1}{2}}, E_{i,j-\frac{1}{2}}, D_{i+\frac{1}{2},j}, B_{i+\frac{1}{2},j}$ and $\tilde{F}_{i+\frac{1}{2},j}$. The final equation is:

$$\begin{aligned} \frac{dC_{N_h,j}}{dt} = & \frac{1}{r_j^2 \Delta r_j} \left\{ (H_{i,j+\frac{1}{2}} + \tilde{G}_{i,j+\frac{1}{2}}) [C_{i,j+1}(1 - \beta_{j+\frac{1}{2}}) - C_{i,j}(1 + \beta_{j+\frac{1}{2}})] \right. \\ & - (H_{i,j-\frac{1}{2}} - \tilde{G}_{i,j-\frac{1}{2}}) [C_{i,j}(1 - \beta_{j-\frac{1}{2}}) - C_{i,j-1}(1 + \beta_{j-\frac{1}{2}})] \Big\} \\ & + \frac{1}{r_j^2 \Delta x_i} \left\{ -(D_{i-\frac{1}{2},j} - \tilde{F}_{i-\frac{1}{2},j})(C_{i,j} - C_{i-1,j}) \right. \\ & - B_{i-\frac{1}{2},j} \left[\frac{1}{\Delta r_j} (C_{i-1,j+1} + C_{i,j+1} - C_{i-1,j-1} - C_{i,j-1}) \right. \\ & \left. \left. - (\gamma_{j-\frac{1}{2}} + \gamma_{j+\frac{1}{2}})(C_{i-1,j} + C_{i,j}) \right] \right\}, \quad (i = N_h, j = 2, N_V - 1). \quad (47) \end{aligned}$$

3. Lower Boundary. At present, the lower boundary condition, at the earth's surface ($j = 1$) consists of specifying the initial concentrations at t_0 , after which they remain fixed:

$$\frac{dC_{i,1}}{dt} = 0, \quad (i = 1, N_h), \quad (48)$$

or

$$C_{i,1} = C_{i,1}(t_0), \quad (i = 1, N_h). \quad (49)$$

4. Upper Boundary. Two options are available for the upper boundary condition ($j = N_v$). The first is a fixed boundary condition, as at the lower boundary:

$$\frac{dC_{i,N_v}}{dt} = 0 \quad , \quad (i = 1, N_h) \quad , \quad (50)$$

or

$$C_{i,N_v} = C_{i,N_v}(t_0) \quad , \quad (i = 1, N_h) \quad . \quad (51)$$

This option may also be applied at any specified altitude.

The second option is a modified "zero-flux" boundary condition, designed to avoid any instabilities or negative concentrations. At the upper boundary, it is assumed that the vertical gradient of mixing ratio is zero, so no direct vertical eddy diffusion occurs across the boundary. This eliminates the terms multiplied by $H_{i,j+\frac{1}{2}}$ and $\tilde{G}_{i,j+\frac{1}{2}}$ in Eq. (32). To avoid vertical fluxes caused by steep horizontal gradients, the cross diffusion coefficients $K_{\theta r}$ and $K_{r\theta}$ are assumed to be zero in the upper zones. This eliminates the terms multiplied by E and B in Eq. (32). To keep the advection terms stable when the mean wind is down through the upper boundary, upstream differencing ($\alpha = 1$ in Eqs. (41) to (44)), is used for the vertical mean wind at $j = N_v$ and $j = N_v - \frac{1}{2}$. The resulting difference equation for the upper boundary is as follows:

$$\begin{aligned} \frac{dC_{i,N_v}}{dt} = & \frac{1}{r_j^2 \Delta r_j} \left\{ -(H_{i,j-\frac{1}{2}} - \tilde{G}_{i,j-\frac{1}{2}}) [C_{i,j}(1 - \beta_{j-\frac{1}{2}}) - C_{i,j-1}(1 + \beta_{j-\frac{1}{2}})] \right\} \\ & + \frac{1}{r_j^2 \Delta x_i} \left\{ (D_{i+\frac{1}{2},j} + \tilde{F}_{i+\frac{1}{2},j})(C_{i+1,j} - C_{i,j}) \right. \\ & \left. - (D_{i-\frac{1}{2},j} - \tilde{F}_{i-\frac{1}{2},j})(C_{i,j} - C_{i-1,j}) \right\} \quad , \quad (j = N_v, i = 2, N_h - 1) \quad (52) \end{aligned}$$

where

$$\tilde{G}_{i,N_V-\frac{1}{2}} = G_{i,N_V-\frac{1}{2}} - |G_{i,N_V-\frac{1}{2}}| \quad (53)$$

5. North and South Pole on Upper Boundary. At the North Pole on the upper boundary, there can be no flux across the meridional boundary. The difference equation for the point $(1, N_V)$ can be obtained from Eq. (52) by eliminating the terms multiplied by $D_{i-\frac{1}{2},j}$ and $\tilde{F}_{i-\frac{1}{2},j}$:

$$\begin{aligned} \frac{dC_{1,N_V}}{dt} = & \frac{1}{r_j^2 \Delta r_j} \left\{ -(H_{1,j-\frac{1}{2}} - \tilde{G}_{1,j-\frac{1}{2}}) [C_{1,j}(1 - \beta_{j-\frac{1}{2}}) - C_{1,j-1}(1 + \beta_{j-\frac{1}{2}})] \right\} \\ & + \frac{1}{r_j^2 \Delta x_1} \left\{ (D_{1+\frac{1}{2},j} + \tilde{F}_{1+\frac{1}{2},j})(C_{2,j} - C_{1,j}) \right\}, \quad (j = N_V) \quad (54) \end{aligned}$$

Similarly for the South Pole on the upper boundary:

$$\begin{aligned} \frac{dC_{N_h,N_V}}{dt} = & \frac{1}{r_j^2 \Delta r_j} \left\{ -(H_{i,j-\frac{1}{2}} - \tilde{G}_{i,j-\frac{1}{2}}) [C_{i,j}(1 - \beta_{j-\frac{1}{2}}) - C_{i,j-1}(1 + \beta_{j-\frac{1}{2}})] \right\} \\ & + \frac{1}{r_j^2 \Delta x_i} \left\{ -(D_{i-\frac{1}{2},j} - \tilde{F}_{i-\frac{1}{2},j})(C_{i,j} - C_{i-1,j}) \right\}, \quad (i = N_h, j = N_V). \quad (55) \end{aligned}$$

In Eqs. (54) and (55), $\tilde{G}$ is also given by Eq. (53).

6. Modifications for Points Adjacent to Upper Boundary. In order to make the vertical fluxes across the interfaces between the zones at $j = N_V$ and $j = N_V-1$ equal in each pair of zones, the difference equations for $j = N_V-1$ must also be modified. In Eq. (32), the coefficient $E_{i,N_V-\frac{1}{2}}$ must be made zero. In Eqs. (32), (46), and (47), the coefficient $\tilde{G}_{i,N_V-\frac{1}{2}}$ must be calculated by Eq. (53).

E. The Coefficient Matrix

1. Interior Points. The coefficient matrix a_{mn} of Eq. (31) is obtained for interior points ($i = 2, N_h - 1, j = 2, N_v - 1$), by collecting coefficients in Eq. (32).

$$a_{i-1,j-1} = \frac{1}{r_j^2 \Delta r_j \Delta x_i} (E_{i,j-\frac{1}{2}} + B_{i-\frac{1}{2},j}) \quad (56)$$

$$a_{i-1,j} = \frac{1}{r_j^2 \Delta x_i} \left\{ \frac{1}{\Delta r_j} (E_{i,j-\frac{1}{2}} - E_{i,j+\frac{1}{2}}) + D_{i-\frac{1}{2},j} - \tilde{F}_{i-\frac{1}{2},j} + (\gamma_{j-\frac{1}{2}} + \gamma_{j+\frac{1}{2}}) B_{i-\frac{1}{2},j} \right\} \quad (57)$$

$$a_{i-1,j+1} = \frac{1}{r_j^2 \Delta r_j \Delta x_i} (-E_{i,j+\frac{1}{2}} - B_{i-\frac{1}{2},j}) \quad (58)$$

$$a_{i,j-1} = \frac{1}{r_j^2 \Delta r_j} \left\{ (H_{i,j-\frac{1}{2}} - \tilde{G}_{i,j-\frac{1}{2}})(1 + \beta_{j-\frac{1}{2}}) + \frac{1}{\Delta x_i} (B_{i-\frac{1}{2},j} - B_{i+\frac{1}{2},j}) \right\} \quad (59)$$

$$a_{i,j} = \frac{1}{r_j^2 \Delta r_j} \left\{ -(H_{i,j+\frac{1}{2}} + \tilde{G}_{i,j+\frac{1}{2}})(1 + \beta_{j+\frac{1}{2}}) - (H_{i,j-\frac{1}{2}} - \tilde{G}_{i,j-\frac{1}{2}})(1 - \beta_{j-\frac{1}{2}}) + \frac{1}{r_j^2 \Delta x_i} \left\{ -(D_{i+\frac{1}{2},j} + \tilde{F}_{i+\frac{1}{2},j}) - (D_{i-\frac{1}{2},j} - \tilde{F}_{i-\frac{1}{2},j}) + (\gamma_{j-\frac{1}{2}} + \gamma_{j+\frac{1}{2}})(B_{i-\frac{1}{2},j} - B_{i+\frac{1}{2},j}) \right\} \right\} \quad (60)$$

$$a_{i,j+1} = \frac{1}{r_j^2 \Delta r_j} \left\{ (H_{i,j+\frac{1}{2}} + \tilde{G}_{i,j+\frac{1}{2}})(1 - \beta_{j+\frac{1}{2}}) + \frac{1}{\Delta x_i} (B_{i+\frac{1}{2},j} - B_{i-\frac{1}{2},j}) \right\} \quad (61)$$

$$a_{i+1,j-1} = \frac{1}{r_j^2 \Delta r_j \Delta x_i} (-E_{i,j-\frac{1}{2}} - B_{i+\frac{1}{2},j}) \quad (62)$$

$$a_{i+1,j} = \frac{1}{r_j^2 \Delta x_i} \left\{ \frac{1}{\Delta r_j} (E_{i,j+\frac{1}{2}} - E_{i,j-\frac{1}{2}}) + D_{i+\frac{1}{2},j} + \tilde{F}_{i+\frac{1}{2},j} - (\gamma_{j-\frac{1}{2}} + \gamma_{j+\frac{1}{2}}) B_{i+\frac{1}{2},j} \right\} \quad (63)$$

$$a_{i+1,j+1} = \frac{1}{r_j^2 \Delta r_j \Delta x_i} (E_{i,j+\frac{1}{2}} + B_{i+\frac{1}{2},j}) \quad (64)$$

If $j = N_V - 1$, replace $E_{i,j+\frac{1}{2}}$ with zero, and calculate $\tilde{G}_{i,j+\frac{1}{2}}$ with Eq. (53). This makes the equations consistent with the upper boundary condition.

2. North Pole, Interior Radii. The coefficient matrix a_{mn} of Eq. (31) is obtained for interior radii ($j = 2, N_V - 1$) at the North Pole ($i = 1$), by collecting coefficients in Eq. (46).

$$a_{0,j-1} = a_{0,j} = a_{0,j+1} = 0 \quad (65)$$

$$a_{1,j-1} = \frac{1}{r_j^2 \Delta r_j} \left\{ (H_{1,j-\frac{1}{2}} - \tilde{G}_{1,j-\frac{1}{2}})(1 + \beta_{j-\frac{1}{2}}) - \frac{1}{\Delta x_1} B_{1+\frac{1}{2},j} \right\} \quad (66)$$

$$a_{1,j} = \frac{1}{r_j^2 \Delta r_j} \left\{ -(H_{1,j+\frac{1}{2}} + \tilde{G}_{1,j+\frac{1}{2}})(1 + \beta_{j+\frac{1}{2}}) - (H_{1,j-\frac{1}{2}} - \tilde{G}_{1,j-\frac{1}{2}})(1 - \beta_{j-\frac{1}{2}}) \right\} + \frac{1}{r_j^2 \Delta x_1} \left\{ -(D_{1+\frac{1}{2},j} + \tilde{F}_{1+\frac{1}{2},j}) - (\gamma_{j-\frac{1}{2}} + \gamma_{j+\frac{1}{2}}) B_{1+\frac{1}{2},j} \right\} \quad (67)$$

$$a_{1,j+1} = \frac{1}{r_j^2 \Delta r_j} \left\{ (H_{1,j+\frac{1}{2}} + \tilde{G}_{1,j+\frac{1}{2}})(1 - \beta_{j+\frac{1}{2}}) + \frac{1}{\Delta x_i} B_{1+\frac{1}{2},j} \right\} \quad (68)$$

$$a_{2,j-1} = \frac{1}{r_j^2 \Delta r_j \Delta x_i} \left\{ -B_{1+\frac{1}{2},j} \right\} \quad (69)$$

$$a_{2,j} = \frac{1}{r_j^2 \Delta x_i} \left\{ D_{1+\frac{1}{2},j} + \tilde{F}_{1+\frac{1}{2},j} - (\gamma_{j-\frac{1}{2}} + \gamma_{j+\frac{1}{2}}) B_{1+\frac{1}{2},j} \right\} \quad (70)$$

$$a_{2,j+1} = \frac{1}{r_j^2 \Delta r_j \Delta x_i} \left\{ B_{1+\frac{1}{2},j} \right\} \quad (71)$$

3. South Pole, Interior Radii. The coefficient matrix a_{mn} of Eq. (31) is obtained for interior radii ($j = 2, N_v - 1$) at the South Pole ($i = N_h$), by collecting coefficients in Eq. (47)

$$a_{N_h-1,j-1} = \frac{1}{r_j^2 \Delta r_j \Delta x_{N_h}} \left\{ B_{N_h-\frac{1}{2},j} \right\} \quad (72)$$

$$a_{N_h-1,j} = \frac{1}{r_j^2 \Delta x_{N_h}} \left\{ D_{N_h-\frac{1}{2},j} - \tilde{F}_{N_h-\frac{1}{2},j} + (\gamma_{j-\frac{1}{2}} + \gamma_{j+\frac{1}{2}}) B_{N_h-\frac{1}{2},j} \right\} \quad (73)$$

$$a_{N_h-1,j+1} = \frac{1}{r_j^2 \Delta r_j \Delta x_{N_h}} \left\{ -B_{N_h-\frac{1}{2},j} \right\} \quad (74)$$

$$a_{N_h,j-1} = \frac{1}{r_j^2 \Delta r_j} \left\{ (H_{N_h,j-\frac{1}{2}} - \tilde{G}_{N_h,j-\frac{1}{2}})(1 + \beta_{j-\frac{1}{2}}) + \frac{1}{\Delta x_{N_h}} B_{N_h-\frac{1}{2},j} \right\} \quad (75)$$

$$\begin{aligned} a_{N_h,j} = \frac{1}{r_j^2 \Delta r_j} \left\{ -(H_{N_h,j+\frac{1}{2}} + \tilde{G}_{N_h,j+\frac{1}{2}})(1 + \beta_{j+\frac{1}{2}}) \right. \\ \left. - (H_{N_h,j-\frac{1}{2}} - \tilde{G}_{N_h,j-\frac{1}{2}})(1 - \beta_{j-\frac{1}{2}}) \right\} \\ + \frac{1}{r_j^2 \Delta x_{N_h}} \left\{ -(D_{N_h-\frac{1}{2},j} - \tilde{F}_{N_h-\frac{1}{2},j}) + (\gamma_{j-\frac{1}{2}} + \gamma_{j+\frac{1}{2}}) B_{N_h-\frac{1}{2},j} \right\} \quad (76) \end{aligned}$$

$$a_{N_h,j+1} = \frac{1}{r_j^2 \Delta r_j} \left\{ (H_{N_h,j+\frac{1}{2}} + \tilde{G}_{N_h,j+\frac{1}{2}})(1 - \beta_{j+\frac{1}{2}}) - \frac{1}{\Delta x_{N_h}} B_{N_h-\frac{1}{2},j} \right\} \quad (77)$$

$$a_{N_h+1,j-1} = a_{N_h+1,j} = a_{N_h+1,j+1} = 0 \quad (78)$$

4. Lower Boundary. The coefficient matrix a_{mn} of Eq. (31), is zero for the lower boundary ($j = 1$) for all meridional points ($i = 1, N_h$).

5. Upper Boundary.

a. Constant concentration option: If upper boundary concentrations are specified, and do not change with time, the coefficient matrix a_{mn} of Eq. (31) is zero for the upper boundary ($j = N_v$), for all meridional points ($i = 1, N_h$).

b. Modified zero-flux option: If upper boundary concentrations are determined by the modified zero-flux boundary condition, the coefficient matrix a_{mn} of Eq. (31) is obtained by collecting coefficients in Eq. (52) for interior meridional points ($i = 2, N_h - 1$)

$$a_{i-1, N_v+1} = a_{i, N_v+1} = a_{i+1, N_v+1} = a_{i+1, N_v-1} = a_{i-1, N_v-1} = 0 \quad (79)$$

$$a_{i-1, N_v} = \frac{1}{r_{N_v}^2 \Delta x_i} \left\{ D_{i-\frac{1}{2}, N_v} - \tilde{F}_{i-\frac{1}{2}, N_v} \right\} \quad (80)$$

$$a_{i, N_v-1} = \frac{1}{r_{N_v}^2 \Delta r_{N_v}} \left\{ (H_{i, N_v-\frac{1}{2}} - \tilde{G}_{i, N_v-\frac{1}{2}})(1 + \beta_{N_v-\frac{1}{2}}) \right\} \quad (81)$$

$$a_{i, N_v} = \frac{1}{r_{N_v}^2 \Delta r_{N_v}} \left\{ -(H_{i, N_v-\frac{1}{2}} - \tilde{G}_{i, N_v-\frac{1}{2}})(1 - \beta_{N_v-\frac{1}{2}}) \right\} \\ + \frac{1}{r_{N_v}^2 \Delta x_i} \left\{ -(D_{i+\frac{1}{2}, N_v} + \tilde{F}_{i+\frac{1}{2}, N_v}) - (D_{i-\frac{1}{2}, N_v} - \tilde{F}_{i-\frac{1}{2}, N_v}) \right\} \quad (82)$$

$$a_{i+1, N_v} = \frac{1}{r_{N_v}^2 \Delta x_i} \left\{ D_{i+\frac{1}{2}, N_v} + \tilde{F}_{i+\frac{1}{2}, N_v} \right\} \quad (83)$$

where $\tilde{G}_{i, N_v-\frac{1}{2}}$ is given by Eq. (53).

At the North Pole, ($i = 1$) replace $D_{i-\frac{1}{2},N_V}$ and $\tilde{F}_{i-\frac{1}{2},N_V}$ with zero. At the South Pole ($i = N_h$), replace $D_{i+\frac{1}{2},N_V}$ and $\tilde{F}_{i+\frac{1}{2},N_V}$ with zero.

F. The Mass-Consistency of the Mean Wind

The mass consistency of the mean wind, as interpolated onto the SPHERNEW grid, and as used in the difference equations, may be tested. The difference form of the divergence equation for the total density, Eq. (1), on the SPHERNEW grid is as follows:

$$\frac{d\rho_{i,j}}{dt} = - \frac{2\rho_{i,j}}{r_j^2} \left\{ \frac{1}{\Delta x_i} (F_{i+\frac{1}{2},j} - F_{i-\frac{1}{2},j}) + \frac{1}{\Delta r_j} [G_{i,j+\frac{1}{2}}(1 + \beta_{j+\frac{1}{2}}) - G_{i,j-\frac{1}{2}}(1 - \beta_{j-\frac{1}{2}})] \right\} = \frac{\rho_{i,j}}{\tau_{i,j}} \quad (84)$$

At $i = 1$ or $i = N_h$, $F_{i-\frac{1}{2},j}$ or $F_{i+\frac{1}{2},j}$, respectively, is zero. At $j = 1$, $G_{i,j-\frac{1}{2}}$ is zero. At $j = N_V$, replace the subscript $j+\frac{1}{2}$ with N_V , and $\beta_{j+\frac{1}{2}}$ with zero. Values of $\tau_{i,j}$ have been calculated for a single time, for the mean wind field presently used in the SPHERNEW, and are as small as a few days for some of the zones.

Without the use of a mass-consistent form of the difference equations, significant distortions of the concentrations would result in a few days. This can be tested with the model by modifying the coefficient of $C_{i,j}$ in the coefficient matrix, Eqs. (60), (67), (76), and (82), to convert to the non-mass-consistent form of the difference equations. The modification is to replace $\tilde{F}$ with $-F$, and $\tilde{G}$ with $-G$. This is equivalent to adding $C_{i,j}/\tau_{i,j}$ to all of the difference equations for $\partial C_{i,j}/\partial t$, Eqs. (32), (46), (47), (52), (54), and (55).

V. Nomenclature

The following symbols have used in equations in this report. General definitions, units, and the equation numbers when the symbol is first used or defined are given.

$A_{i,j\pm\frac{1}{2}}$	area normal to radial direction at $\theta_i, r_{i\pm\frac{1}{2}}$, cm^2 . Eq. (22).
$\bar{A}_{i,j\pm\frac{1}{2}}$	approximate value of $A_{i,j\pm\frac{1}{2}}$. Eq. (25).
$A_{i\pm\frac{1}{2},j}$	area normal to meridional direction at $\theta_{i\pm\frac{1}{2}}, r_j$, cm^2 . Eq. (21).
$\bar{A}_{i\pm\frac{1}{2},j}$	approximate value of $A_{i\pm\frac{1}{2},j}$. Eq. (24).
a_{mn}	component of coefficient matrix of difference equations, sec^{-1} . Eqs. (31), (56) to (83).
$B_{i\pm\frac{1}{2},j}$	coefficient of cross diffusion in the meridional direction, cm^3/s . Eq. (39).
C_i	concentration of species i , molecules/ cm^3 . Eq. (2).
$\tilde{C}$	concentration averaged over a time interval, molecules/ cm^3 . Eq. (16).
C'	difference between C and $\tilde{C}$. Eq. (16).
$C_{i,j}$	concentration of a species at θ_i, r_j .
$D_{i\pm\frac{1}{2},j}$	coefficient of meridional diffusion, cm^3/s . Eq. (38).
$E_{i,j\pm\frac{1}{2}}$	coefficient of cross diffusion in the radial direction, cm^3/s . Eq. (36).
$F_{i\pm\frac{1}{2},j}$	coefficient of meridional advection, cm^3/s . Eq. (40).
$\tilde{F}_{i\pm\frac{1}{2},j}$	coefficient of meridional advection, for weighted upstream differencing, cm^3/s . Eqs. (43), (44).

f	general function of time and position on a boundary. Eq. (4).
$G_{i,j\pm\frac{1}{2}}$	coefficient of vertical advection, cm^3/s . Eq. (37).
$\tilde{G}_{i,j\pm\frac{1}{2}}$	coefficient of vertical advection, for weighted upstream differencing, cm^3/s . Eqs. (41), (42).
$H_{i,j\pm\frac{1}{2}}$	coefficient of vertical diffusion, cm^3/s . Eq. (33).
i	subscript indicating species (C_i), or meridional position.
j	subscript indicating radial position.
$\underline{\underline{K}}$	eddy diffusivity tensor (2nd order) with components K_{rr} , $K_{r\theta} = K_{\theta r}$, and $K_{\theta\theta}$, cm^2/s . Eqs. (7), (13).
N_h	number of meridional points in geometric grid for each radius. Eq. (16).
N_s	number of species with concentrations C . Eq. (2).
N_v	number of radial points in geometric grid for each meridian. Eq. (17).
p	general function of time and position or a boundary. Eq. (4).
q	general function of time and position or a boundary. Eq. (4).
r_j	radius from center of earth, cm. Eqs. (17), (19).
S	mixing ratio for a species, C/ρ , dimensionless.
t	time, seconds. Eq.(1).
t_0	time at which initial concentrations are specified, seconds. Eq. (5).
$\underline{u}$	velocity vector, with components u_r and u_θ , cm/s . Eq. (1).
$\tilde{\underline{u}}$	velocity vector averaged over a time interval, with components $\tilde{u}_r$ and $\tilde{u}_\theta$. Eq. (6)..

$\underline{u}'$	difference between u and $\tilde{u}$. Eq. (6).
$V_{i,j}$	volume of a zone associated with a grid point at θ_i, r_j . Eq. (20).
$\bar{V}_{i,j}$	approximate value of $V_{i,j}$. Eq. (23).
x_i	meridional coordinate, equal to $(-\cos \theta_i)$. Eq. (13).
$\cdot$	between two vectors, or a tensor and a vector, indicates dot product. Eq. (3).
∇	vector gradient operator. Eq. (3).
$\nabla \cdot$	vector divergence operator. Eq. (1).
α	weight factor between upstream (1) and central (0) spatial differencing of advection. Eqs. (41)-(45).
$\gamma_{j+\frac{1}{2}}$	fractional density gradient at $r_{j+\frac{1}{2}}$, cm^{-1} . Eqs. (14), (34).
$\Delta r_{j+\frac{1}{2}}$	radial distance between r_j and r_{j+1} , cm. Eq. (28).
$\overline{\Delta r_j}$	radial width of a zone, cm. Eq. (27)
$\overline{\Delta x_i}$	approximate meridional width of a zone, in x coordinate units, dimensionless. Eq. (26).
$\Delta \theta_{i+\frac{1}{2}}$	angular distance between θ_i and θ_{i+1} , radians. Eq. (29).
$\overline{\Delta \theta_{i+\frac{1}{2}}}$	approximate angular distance between θ_i and θ_{i+1} , radians. Eq. (30).
∂	partial differential operation. Eq. (1).
θ_i	meridional angle, between north polar axis and a point, radians. Eqs. (16), (18).
π	the value 3.1415926535... . Eq. (20).
$\rho_{i,j}$	total air density at θ_i, r_j , molecules/ cm^3 . Eq. (1).
$\tau_{i,j}$	time constant for exponential change of total density, seconds. Eq. (84).

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