DEVELOPMENT OF THE RADIATIVE TRANSFER PORTION OF A 1-D PHOTOCHEMICAL DIFFUSIVE STRATOSPHERIC MODEL

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# Development of the Radiative Transfer Portion of a 1-D Photochemical Diffusive Stratospheric Model

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- Hsiao-hua K. Burke
- Nancy Tripp

## Summary
This report summarizes the development and implementation of an advanced state-of-the-art computer code, the Chlorine Model Study Program (CMSP), which models the trace gas composition of the atmosphere from the surface to 80 km employing over sixty relevant chemical reactions and parameterizing vertical transport by a selected eddy diffusion profile.

A significant feature is the computation of solar flux available for photolysis by a multiple scattering atmosphere including the effect of surface reflection.

## Distribution Statement
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20. ABSTRACT (cont)

Program documentation includes a complete listing of the code, a detailed flow chart, and several test case results in addition to a detailed program description and users guide.
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1. Introduction

This report summarizes the implementation and further development of the Chlorine Model Study Program (CMSP) performed by Environmental Research & Technology, Inc. (ERT) under the sponsorship of the Electronic Systems Division, U.S.A.F. Systems Command, Hanscom AFB, Massachusetts.

The CMSP is an advanced state-of-the-art computer code which models the trace gas composition of the atmosphere from the surface to 80 km employing over sixty chemical reactions in addition to allowing for vertical transport parameterized by a selected set of eddy diffusion coefficients. In its original formulation, the model only computed photolysis for the one-way passage of solar radiation through the atmosphere (absorption only). In the present version the effects of multiple scattering and surface reflection have been incorporated into the radiative transfer section of the program thus allowing for more realistic simulation of the effects of injected pollutants into the atmosphere.

The text which follows constitutes a basic program description, documentation, and users guide. Section 2 discusses the theoretical basis of the model including the governing continuity and flux equations for the steady-state version in addition to the chemical system adopted. Section 3 provides a description of the development of the radiative transfer section including the technique employed to perform the multiple scattering calculation and some representative results (Appendix C). Section 4 constitutes a comprehensive program description utilizing a complete program listing (Appendix A) and a flow chart (Appendix B) to aid in the exposition of the detailed calculation. Finally, Section 5 is included as a basic users guide containing instructions for program implementation and execution.
2. Theoretical Basis

2.1 Governing Model Equations

The CMSP program is a 1-dimensional (vertical dependence), steady state (no time dependence) mathematical model of the trace gas chemical composition of the atmosphere from the surface to 80 km. Specifically, the species dealt with include odd oxygen ($\text{O}_3$), odd hydrogen ($\text{H}$, $\text{OH}$, $\text{HO}_2$, $\text{H}_2\text{O}_2$), odd nitrogen ($\text{NO}$, $\text{NO}_2$, $\text{HNO}_3$), and odd chlorine ($\text{Cl}$, $\text{HC}$, $\text{C}_2\text{O}$). Physical processes which determine the local abundances of these and other minor species include chemical kinetics, photochemistry, and turbulent transport. Radiative transfer is indirectly involved since it determines the number of photons available for photodissociation. (See Section 3).

The model is similar to those of Wofsy, McElroy and Sze (1975) and Sze and McElroy (1975) with several modifications. The governing continuity and diffusion equations are:

\[
\frac{\partial \phi_i}{\partial z} = P_i - L_i N f_i \tag{2-1}
\]

and

\[
\frac{\partial f_i}{\partial z} = -\frac{\phi_i}{KN} \tag{2-2}
\]

where $\phi_i$ is the vertical flux ($\text{cm}^{-2} \text{sec}^{-1}$), $N$ the atmospheric total number density ($\text{cm}^{-3}$), $K$ the eddy coefficients ($\text{cm}^2 \text{sec}^{-1}$) and $P_i$ and $L_i$ are respectively the local production ($\text{cm}^{-3} \text{sec}^{-1}$) and loss frequency ($\text{sec}^{-1}$), $i$ denotes the $i^{\text{th}}$ species, and $f_i$ is the mixing ratio (v/v). Distinctions between long lived species (e.g. $\text{N}_2\text{O}$, $\text{CH}_4$, $\text{CF}_2\text{Cl}_2$) and short lived species (e.g. $\text{Cl}$, $\text{OH}$, $\text{NO}$) lead to enormous simplification in calculations.

For instance, the time constants for apportionment of $\text{ClX}$ among various forms of odd chlorine ($\text{Cl}$, $\text{ClO}$, $\text{HC}$, $\text{C}_2\text{O}$) are rapid compared to the time constant for vertical motion. Densities of individual $\text{ClX}$ species
can be calculated with the equations of photochemical equilibrium, i.e.

\[ P_i - L_i N f_i = 0 \quad \text{for each species} \]  

Likewise, photochemical equilibrium can be applied to the short lived hydrogen species (H, OH, HO₂, H₂O₂), to NOₓ (NO, NO₂, HNO₃), to O⁴(P) and to O(¹D). On the contrary, vertical flow is allowed for long-lived species such as CH₄, N₂O, CO, CF₂Cl₂, CFCl₃, and O₃ (below 30 km) and the total family concentrations for HOₓ, NOₓ, and Clₓ. In this case, equations (2-1, 2-2) must be solved simultaneously.

Equations (2-1) and (2-2) are coupled differential equations with two point boundary conditions. They are usually solved by using the conventional finite difference method or the shooting method. However, more efficient schemes have recently been developed to improve computational efficiency. The numerical approach utilized is based on a Riccati scheme developed by Sze (1973) and subsequently applied to investigations relating to the Venus (Sze and McElroy, 1975) and Earth's atmosphere. In essence, the Riccati scheme transforms (2-1) and (2-2) into a non-coupled system with a one point boundary condition. This technique greatly reduces the computational complexity of the problem and facilitates numerical solutions of differential equations of the type described here.

In the one-dimensional model, the crucial transport parameter is the vertical eddy diffusion coefficient \( K_{zz} \). In the current model three options exist to vary the assumed \( K_{zz} \) profile to simulate measured data and perform sensitivity analyses. (See Section 4.3.2). The neutral atmosphere used in the calculation is summarized in Table 2-1 (a particular eddy diffusion profile is demonstrated). Photolysis processes for aeronomically significant molecules are summarized in Table 2-2. Computations of photodissociation rates (or J-values) are accomplished (See Section 3-1).
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<th>Eddy Diffusion Coefficient (cm² sec⁻¹)</th>
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<th>Temperature (°K)</th>
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<td>8.5540E 14</td>
<td>195.36</td>
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<td>4.2000E 06</td>
<td>6.2810E 14</td>
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<td>80</td>
<td>5.3200E 06</td>
<td>4.5560E 14</td>
<td>180.54</td>
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</tbody>
</table>
### TABLE 2-2

**PHOTOLYSIS PROCESSES (sec⁻¹)**

<table>
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<tr>
<th>( J )</th>
<th>Reaction Formula</th>
</tr>
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<tr>
<td>1</td>
<td>( O_2 + h\nu \rightarrow 2 O )</td>
</tr>
<tr>
<td>2</td>
<td>( O_3 + h\nu \rightarrow O(1^D) + O_2 )</td>
</tr>
<tr>
<td>3</td>
<td>( O_3 + h\nu \rightarrow O(3^P) + O_2 )</td>
</tr>
<tr>
<td>4</td>
<td>( H_2O + h\nu \rightarrow H + OH )</td>
</tr>
<tr>
<td>5</td>
<td>( N_2O + h\nu \rightarrow N_2 + O )</td>
</tr>
<tr>
<td>6</td>
<td>( CH_4 + h\nu \rightarrow CH_3 + H )</td>
</tr>
<tr>
<td>7</td>
<td>( CH_3Cl + h\nu \rightarrow CH_3 + Cl )</td>
</tr>
<tr>
<td>8</td>
<td>( CFCl_3 + h\nu \rightarrow CFCl_2 + Cl )</td>
</tr>
<tr>
<td>9</td>
<td>( CF_2Cl_2 + h\nu \rightarrow CFCl + Cl )</td>
</tr>
<tr>
<td>10</td>
<td>( CCl_4 + h\nu \rightarrow CCl_3 + Cl )</td>
</tr>
<tr>
<td>11</td>
<td>( HC1 + h\nu \rightarrow H + Cl )</td>
</tr>
<tr>
<td>12</td>
<td>( NO_2 + h\nu \rightarrow NO + O )</td>
</tr>
<tr>
<td>13</td>
<td>( NO_3 + h\nu \rightarrow NO + O_2 )</td>
</tr>
<tr>
<td>14</td>
<td>( NO_3 + h\nu \rightarrow NO_2 + O )</td>
</tr>
<tr>
<td>15</td>
<td>( N_2O_5 + h\nu \rightarrow NO_3 + NO_2 )</td>
</tr>
<tr>
<td>16</td>
<td>( HNO_3 + h\nu \rightarrow OH + NO_2 )</td>
</tr>
<tr>
<td>17</td>
<td>( NO + h\nu \rightarrow N + O )</td>
</tr>
<tr>
<td>18</td>
<td>( H_2O_2 + h\nu \rightarrow 2OH )</td>
</tr>
<tr>
<td>19</td>
<td>( HO_2 + h\nu \rightarrow H + O_2 )</td>
</tr>
<tr>
<td>20</td>
<td>( C1O + h\nu \rightarrow C1 + O )</td>
</tr>
<tr>
<td>21</td>
<td>( HOC1 + h\nu \rightarrow OH + Cl )</td>
</tr>
<tr>
<td>22</td>
<td>( C10NO_2 + h\nu \rightarrow C10 + NO_3 )</td>
</tr>
<tr>
<td>23</td>
<td>( H_2CO + h\nu \rightarrow H_2 + CO )</td>
</tr>
<tr>
<td>24</td>
<td>( H_2CO + h\nu \rightarrow H + HCO )</td>
</tr>
</tbody>
</table>
using solar flux data obtained from the Handbook of Geophysics and Space Environments (1965). For the spectral region between 1750-3000Å flux measurements were adopted from Detwiler, et. al. (1961). Below 1750Å, the more recent data by Widing, et. al. (1970) are utilized. Computations are made using either a 24-hour averaged value of the solar flux or a single solar zenith angle (specified by ISWIT, Section 4.4). Table 2-3 contains the reactions and adopted rate constants for the relevant odd oxygen, hydrogen, nitrogen, and chlorine species. These rates are referenced to 80 km. Temperature dependence of the rate constants as a function of the temperature profile is given.

2.2 Summary of Relevant Stratospheric Chemistry

This section provides a brief review of the critical atmospheric species handled by the CMSP program.

The chemistry of atmospheric ozone was formulated by Chapman (1930). Chapman's model consists of four reactions involving only oxygen chemistry. He proposed that ozone is initiated by photolysis of $O_2$ in the Herzberg continuum below 2400 Å, as

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

followed by the three body reaction

$$O + O_2 + M \rightarrow O_3 + M$$

(2-5)

Ozone may be recycled by

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

(2-6)

followed by (2-5). Odd oxygen ($O, O_3$) is removed by

$$O + O_3 \rightarrow 2O_2$$

(2-7)

Using reactions (2-4) to (2-7), and assuming photochemical equilibrium conditions, ozone concentration may be expressed in a simple analytic form:

$$[O_3] = \left(\frac{J_1}{J_3}\right)^{1/2} \left(\frac{k_2}{k_4}\right)^{1/2} [O_2][M]^{1/2}$$

(2-8)
TABLE 2-3

REACTION RATE
(AS A FUNCTION OF ALTITUDE, Z) = A
* EXP (B/TEMP (Z))

<table>
<thead>
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<th>REACTION</th>
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<th>B</th>
</tr>
</thead>
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<td>1</td>
<td>OH + CH3Cl = CH2Cl + H2O</td>
<td>1.66E-12</td>
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<td>2</td>
<td>H2O + O('D) = 2OH</td>
<td>2.35E-10</td>
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<tr>
<td>3</td>
<td>CH4 + O('D) = CH3 + OH</td>
<td>1.40E-10</td>
<td>0.</td>
</tr>
<tr>
<td>4</td>
<td>H2 + O('D) = OH + H</td>
<td>1.00E-10</td>
<td>0.</td>
</tr>
<tr>
<td>5</td>
<td>H + O2 + M = H2O + M</td>
<td>1.80E-32</td>
<td>340.</td>
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<td>6</td>
<td>H + O3 = OH + O2</td>
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<td>2.30E-12</td>
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<td>8</td>
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<td>H2O2 + O3 = OH + 2O2</td>
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<td>H2O + O = OH + O2</td>
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<td>-250.</td>
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<td>H2O + ClO = HClO + O2</td>
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<td>-1260.</td>
</tr>
<tr>
<td>31</td>
<td>ClO + O = Cl + O2</td>
<td>1.07E-10</td>
<td>-224.</td>
</tr>
<tr>
<td>32</td>
<td>ClO + NO = Cl + NO2</td>
<td>2.00E-11</td>
<td>0.</td>
</tr>
<tr>
<td>33</td>
<td>O + HCl = OH + Cl</td>
<td>0.0</td>
<td>0.</td>
</tr>
<tr>
<td>34</td>
<td>O + O2 + M = O3 + M</td>
<td>1.05E-34</td>
<td>520.</td>
</tr>
<tr>
<td>35</td>
<td>O + O3 = 2O2</td>
<td>1.30E-11</td>
<td>-2140.</td>
</tr>
<tr>
<td>36</td>
<td>NO2 + NO3 = N2O5*</td>
<td>1.00E-12</td>
<td>0.</td>
</tr>
<tr>
<td>38</td>
<td>N2O5* + M = N2O5 + M</td>
<td>3.70E-11</td>
<td>0.</td>
</tr>
<tr>
<td>39</td>
<td>N2O5 + M = N2O5* + M</td>
<td>9.00E-06</td>
<td>-9700.</td>
</tr>
<tr>
<td>40</td>
<td>NO + O3</td>
<td>NO2 + O2</td>
<td>2.30E-12</td>
</tr>
<tr>
<td>41</td>
<td>NO2 + O3 = NO3 + O2</td>
<td>1.20E-13</td>
<td>-2450.</td>
</tr>
<tr>
<td>42</td>
<td>NO2 + O = NO + O2</td>
<td>9.12E-12</td>
<td>0.</td>
</tr>
<tr>
<td>43</td>
<td>N2O + O('D) = N2 + O2</td>
<td>5.00E-11</td>
<td>0.</td>
</tr>
<tr>
<td>44</td>
<td>N2O + O('D) = 2NO</td>
<td>7.00E-11</td>
<td>0.</td>
</tr>
<tr>
<td>45</td>
<td>N + NO = N2 + O</td>
<td>2.00E-11</td>
<td>0.</td>
</tr>
<tr>
<td>46</td>
<td>N + O2 = NO + O</td>
<td>5.50E-12</td>
<td>-3200.</td>
</tr>
<tr>
<td>47</td>
<td>O('D) + CFCl3 = PRODUCTS</td>
<td>3.00E-10</td>
<td>0.</td>
</tr>
<tr>
<td>48</td>
<td>O('D) + CF2Cl3 = PRODUCTS</td>
<td>3.00E-10</td>
<td>0.</td>
</tr>
<tr>
<td>49</td>
<td>O('D) + CH3Cl = OH + CH2Cl</td>
<td>0.0</td>
<td>0.</td>
</tr>
<tr>
<td>50</td>
<td>O('D) + CCl4 = PRODUCTS</td>
<td>0.0</td>
<td>0.</td>
</tr>
<tr>
<td>51</td>
<td>O('D) + M = O + M</td>
<td>2.00E-11</td>
<td>107.</td>
</tr>
</tbody>
</table>

Reactions Whose Rates Are Calculated By Different Formulæ Are:

<table>
<thead>
<tr>
<th>No.</th>
<th>REACTION</th>
<th>A</th>
<th>B</th>
</tr>
</thead>
<tbody>
<tr>
<td>22</td>
<td>OH + NO2 + M = HNO3 + M</td>
<td>R = 2.5E-13*EXP(880./Temp.(Z))/(2.6E18 * M(Z))</td>
<td></td>
</tr>
<tr>
<td>57</td>
<td>N2O5* = NO2 + NO3</td>
<td>R = 1.0E8<em>M(Z)/(2.6E19</em>G(Z)) + 1.0E7</td>
<td></td>
</tr>
</tbody>
</table>
where \( J_1 \) and \( J_3 \) are the photolysis rates for reaction (2-4) and (2-5) and \( k_2 \) and \( k_4 \) are the rate constants for reactions (2-5) and (2-7), respectively.

Equation (2-8) gives a good first order model of the vertical distribution of atmospheric ozone. It successfully predicts the ozone peak at around 25 km. However, it predicts too much ozone at all altitudes above 22 km, and it overestimates the total ozone abundance by about a factor of 2. Furthermore, Chapman's simple model does not include atmospheric transport processes and cannot account for the observed latitudinal distribution of ozone - low values at low latitudes and high values at high latitudes.

Bates and Nicolet (1950) first attempted to remove the discrepancies between observations and Chapman's theory by introducing catalytic hydrogen chemistry. (the \( \text{HO}_x \) family). Catalysis of odd oxygen recombination by hydrogen species (H, OH, \( \text{HO}_2 \)) may take place either through

\[
H + O_3 \rightarrow \text{OH} + O_2 \tag{2-9}
\]

followed by

\[
\text{OH} + O \rightarrow O_2 + H; \tag{2-10}
\]

or through

\[
H + O_2 + M \rightarrow \text{HO}_2 + M \tag{2-11}
\]

followed by

\[
\text{HO}_2 + O \rightarrow \text{OH} + O_2 \tag{2-12}
\]

These reactions are important above 50 km, and account for a reduction by about a factor of 2 to 3 in the concentration of ozone calculated by Equation (2-8).

Atmospheric odd hydrogen (H, OH, \( \text{HO}_2 \), \( \text{H}_2\text{O}_2 \)) is mainly formed by reactions involving \( \text{H}_2\text{O} \) molecules;

\[
\text{H}_2\text{O} + O(1^D) \rightarrow 2 \text{OH} \tag{2-13}
\]
and

\[ H_2O + hv \rightarrow OH + H \]  
\[ (2-14) \]

They are mainly removed by reactions

\[ OH + HO_2 \rightarrow H_2O + O_2 \]  
\[ (2-15) \]

and

\[ OH + H_2O_2 \rightarrow HO_2 + H_2O \]  
\[ (2-16) \]

For a given \( H_2O \) concentration, the abundance of odd hydrogen is mainly controlled by reactions (2-13) to (2-16). Reaction (2-15) is the dominant loss process for odd hydrogen above 35 km.

The principal stratospheric sink for \( O_3 \) was not identified until 1970 when Crutzen (1970) and Johnston (1971) suggested that nitric oxide (NO) can catalytically recombine \( O \) and \( O_3 \) through the reaction

\[ NO + O_3 \rightarrow NO_2 + O_2 \]  
\[ (2-17) \]

followed by

\[ NO_2 + O \rightarrow NO + O_2 \]  
\[ (2-18) \]

Oxides of nitrogen, \( NO_x \) (NO, NO\(_2\), NO\(_3\), N\(_2\)O\(_5\), HNO\(_3\)) are formed in the stratosphere by photochemical decomposition of N\(_2\)O (McElroy and McConnell, 1971):

\[ N_2O + O(^{1}D) \rightarrow 2NO \]  
\[ (2-19) \]

Nitrous oxide (N\(_2\)O) is mainly produced in soil as a by-product of the denitrification process, with some contribution from high temperature combustion processes.

The possible importance of chlorine chemistry in the stratosphere was noted by Wofsy and McElroy (1974) and by Stolarski and Cicerone (1974). They suggested that free chlorine may play a role similar to \( NO_x \) in the recombination of \( O \) and \( O_3 \) through the reaction

\[ Cl + O_3 \rightarrow ClO + O_2 \]  
\[ (2-20) \]
followed by

\[
\text{ClO} + O \rightarrow \text{Cl} + O_2 \quad (2-21)
\]

A source of stratospheric Cl was not identified until Molina and Rowland (1974) suggested the photolysis of fluoroethers (F-11, F-12) through the reactions

\[
\text{CFCl}_3 + h\nu \rightarrow \text{CFCl}_2 + \text{Cl} \quad (2-22)
\]

and

\[
\text{CF}_2\text{Cl}_2 + h\nu \rightarrow \text{CF}_2\text{Cl} + \text{Cl} \quad (2-23)
\]

These reactions constitute the basis of the C\&X family of the CMSP program.

Theoretical model calculations [Wofsy et. al. (1975), Crutzen (1974)] have shown that continued release of fluoroethers (CFMs) at 1973 production rates might lead to approximately 7 to 12 percent ozone reduction in the year 2200. These results have led to the current concern regarding the effects of CFMs on stratospheric ozone.

Prior to 1976, it was thought that HCl was the only inert form of odd chlorine species. The chemistry of chlorine nitrate, ClONO\(_2\), was ignored until Rowland et. al. (1976) measured the absorption cross section of ClONO\(_2\), which suggested its appreciable lifetime (~1 day) in the mid-stratosphere. Chlorine nitrate is formed by a three body reaction

\[
\text{ClO} + \text{NO}_2 + \text{M} \rightarrow \text{ClONO}_2 + \text{M} \quad (2-24)
\]

with a rate constant

\[
k_{24} = 5.1 \times 10^{-33} \exp(-900/T)
\]

Formation of ClONO\(_2\) would tie up the active Cl and NO\(_x\) -species, and could lower the catalytic efficiency of both the C\&X and NO\(_x\) cycles.
3. Development of the Radiative Transfer Section

3.1 Discussion

In the basic version of the CMSP program only the most elementary radiative transfer process, that of absorption by molecular oxygen and ozone, is incorporated within the calculation of photodissociation rates. However, surface reflection and atmospheric multiple scattering of incident solar radiation by molecules and aerosols can significantly enhance the photolysis rates of certain stratospheric species (Luther and Gelinasa, 1976) and may have an appreciable effect on stratospheric photochemistry (Sze and Tripp, 1977).

The photodissociation rate (sec$^{-1}$) of species i at altitude z is given by:

$$J_i(t,z) = \int \pi F_{\lambda}(t,z) \sigma_{\lambda,i} \Phi_{\lambda,i} \, d\lambda$$

where

$$\sigma_{\lambda,i} = \text{absorption cross section of species } i \text{ at wavelength } \lambda \text{ (cm$^2$)}$$

$$\Phi_{\lambda,i} = \text{quantum yield of species } i \text{ at wavelength } \lambda \text{ (dimensionless)}$$

$$\pi F_{\lambda}(t,z) = \text{flux at level } z \text{ available for photodissociations at a time } t \text{ (photons cm$^{-2}$ sec$^{-1}$ } \mu_0 \text{ A$^{-1}$).}$$

In the pure absorption model, the available photons are calculated based on attenuation of the direct solar beam by $O_2$ and $O_3$ or:

$$\pi F_{\lambda}(t,z) = \pi F_0 \exp \left[-\tau(z)/\mu_0\right]$$

where

$$\pi F_0 = \text{unattenuated solar flux}$$

$$\mu_0 = \text{cosine of the solar zenith angle}$$

$$\tau(z) = \int_0^\infty \sum_i \sigma_{i,a} n_i(z) \, dz$$

$$\sigma_{i,a} = \text{absorption cross section of species } i \text{ (cm$^2$)}$$

$$n_i = \text{local number of density of species } i \text{ (cm$^{-3}$)}$$
The flux depends on time through variation of the solar zenith angle with time of day:

\[ \nu_0 = \cos \theta \cos \delta \cos \left( \frac{t}{240} \right) + \sin \theta \sin \delta \]  

(3-4)

where

\[ \theta = \text{latitude (deg.)} \]
\[ \delta = \text{solar declination angle (deg.)} \]
\[ t = \text{local time (sec)} \]

The single solar zenith angle photolysis rate is given by (3-1).

The 24 hour averaged photolysis rate is given by:

\[ \bar{J}_i(z) = \frac{1}{86400} \int_0^{86400} I_i(t,z) \, dt \]  

(3-5)

In order to account for the effects of multiple scattering, the radiative transfer equation:

\[ \mu \frac{dI(t,\mu)}{d\tau} = I(t,\mu) - S(t,\mu) \]  

(3-6)

must be solved at each level of the atmosphere for each frequency.

The flux available for photodissociation \( \pi F \) is then given by:

\[ F(\tau) = 2 \int_{-1}^{+1} I(\tau,\mu) \, d\mu \]  

(3-7)

In Eqn (3-6), \( S(\tau,\mu) \) is the source function which obeys the integral equation:

\[ S(\tau) = \frac{\omega_0(\tau)}{4} F_0 \cdot \exp \left( -\tau/\mu_0 \right) \]  

\[ + \frac{\omega_0(\tau)}{2} \int_0^{\tau*/2} S(t) E_1(|t-\tau|) \, dt \]

\[ + 2 \cdot \frac{\omega_0(\tau)}{2} \cdot R \cdot E_2(\tau*/\tau) \int_0^{\tau*/2} S(t) E_2(\tau^* - t) \, dt \]  

(3-8)
+ \frac{\omega_0(\tau)}{2} \cdot \mu_0 \cdot F_0 \cdot R \cdot E_2(\tau^* - \tau) \cdot \exp \left( -\tau^*/\mu_0 \right)

where

\[ E_n(x) = \int_0^1 \exp \left( -x/\mu \right) \mu^{(n-1)} \frac{du}{\mu} \]

\( R \) = ground reflectivity

\( \tau^* = \) (total) optical depth = \( \int_0^\infty \Sigma \sigma_i n_i(z) \, dz \)

and

\( \omega_0 = \) single scattering albedo

\[ \omega_0(z) = \frac{\Sigma \sigma_{s,i} n_i(z)}{\Sigma \sigma_{s,i} n_i(z) + \Sigma \sigma_{a,i} n_i(z)} \]

In Eqn (3-8) the optical depth \( \tau \) is computed using the extinction cross section \( (\sigma_i = \sigma_{s,i} + \sigma_{a,i}) \) where \( \sigma_{s,i} \) is the scattering cross section of species \( i \) as compared with the absorption cross section only in Eqn (3-3).

Sources of scattering opacity include both atmospheric gases (Rayleigh scattering) and polydisperse aerosol distributions (Mie scattering).

Evaluation of the Rayleigh scattering cross section at each level is accomplished using (McClatchey, et. al., 1972)

\[ \sigma_{s,\text{Rayleigh}}(z) = \left( 9.807 \times 10^{-25} \nu + 4.0117 \right) \frac{N(z)}{N(z = 0)} \] (3.9)

where:

\( \nu = \) frequency in wave numbers (cm\(^{-1}\))

\( N(z) = \) total number density at level \( z \) (cm\(^{-3}\))

Aerosol models have been adopted from Shettle and Fenn (1976) which provides the wavelength dependence of the absorption and extinction cross sections for four characteristic aerosol models: maritime, urban, rural, and tropospheric. The first three are, strictly speaking, boundary layer models while the tropospheric model is more characteristic of the atmosphere above the boundary.
layer. The altitude variation of the aerosol number densities (Table 3-1) is assumed to be the same for all models and is taken from Elterman (1968).

The surface is assumed to be Lambertian. The reflectivity (R) is defined as the ratio between the incoming and outgoing fluxes at the surface and the reflection is isotropic (i.e. no angle preference for the outgoing radiance). The reflected intensity at surface $I(\tau^*,\mu)$ can be written as

$$I(\tau^*,\mu) = 2 \cdot R \int_0^{\tau^*} S(t) E_2(\tau^*-t) \, dt \quad (3-10)$$

### 3.2 Implementation of the Variational-Iterative (VI) Technique

Once equation (3-8) is solved for the source function, the total flux available for photodissociation $F(\tau)$ in the fully scattering case is given by:

$$F(\tau) = F_0 \exp(-\tau/\mu_0) + 2 \int_0^{\tau^*} S(t) E_1(|t-\tau|) \, dt$$

$$+ 2 \mu_0 F_0 R E_2(\tau^*-t) \exp(-\tau^*/\mu_0)$$

$$+ 4 R \cdot E_2(\tau^*-t) \int_0^{\tau^*} S(t) E_2(\tau^*-t) \, dt \quad (3-11)$$

The physical meaning of each term in Equation (3-11) is as follows:

1) the first term represents the attenuated direct beam. (This is the only term used in a pure absorption model).

2) the second term represents the diffuse radiation in the atmosphere due to scattering of the direct beam;

3) the third term represents the attenuated direct beam reflected from the surface with reflectivity R;

4) the fourth term represents the diffuse radiation due to scattering of the reflected beam.

This may be substituted into (3-1) to evaluate the photodissociation rates.
TABLE 3-1

ALTITUDE VARIATION OF AEROSOL NUMBER DENSITIES

<table>
<thead>
<tr>
<th>Altitude (km)</th>
<th>Aerosol Number Density (cm⁻³)</th>
<th>Altitude (km)</th>
<th>Aerosol Number Density (cm⁻³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>2.8280E+03</td>
<td>42</td>
<td>7.9600E-02</td>
</tr>
<tr>
<td>2</td>
<td>5.3710E+02</td>
<td>44</td>
<td>5.7040E-02</td>
</tr>
<tr>
<td>4</td>
<td>1.1920E+02</td>
<td>46</td>
<td>2.8290E-02</td>
</tr>
<tr>
<td>6</td>
<td>6.3370E+01</td>
<td>48</td>
<td>2.0990E-02</td>
</tr>
<tr>
<td>8</td>
<td>6.7690E+01</td>
<td>50</td>
<td>1.0780E-02</td>
</tr>
<tr>
<td>10</td>
<td>5.6750E+01</td>
<td>52</td>
<td>5.5800E-03</td>
</tr>
<tr>
<td>12</td>
<td>5.5850E+01</td>
<td>54</td>
<td>4.1140E-03</td>
</tr>
<tr>
<td>14</td>
<td>5.1480E+01</td>
<td>56</td>
<td>2.0780E-03</td>
</tr>
<tr>
<td>16</td>
<td>4.5110E+01</td>
<td>58</td>
<td>1.4950E-03</td>
</tr>
<tr>
<td>18</td>
<td>4.3140E+01</td>
<td>60</td>
<td>7.7350E-04</td>
</tr>
<tr>
<td>20</td>
<td>2.6670E+01</td>
<td>62</td>
<td>4.0030E-04</td>
</tr>
<tr>
<td>22</td>
<td>1.4555E+01</td>
<td>64</td>
<td>2.8800E-04</td>
</tr>
<tr>
<td>24</td>
<td>8.1260E+00</td>
<td>66</td>
<td>1.4900E-04</td>
</tr>
<tr>
<td>26</td>
<td>5.7060E+00</td>
<td>68</td>
<td>1.0720E-04</td>
</tr>
<tr>
<td>28</td>
<td>3.5740E+00</td>
<td>70</td>
<td>5.5500E-05</td>
</tr>
<tr>
<td>30</td>
<td>2.2380E+00</td>
<td>72</td>
<td>2.1440E-05</td>
</tr>
<tr>
<td>32</td>
<td>1.1480E+00</td>
<td>74</td>
<td>1.3320E-05</td>
</tr>
<tr>
<td>34</td>
<td>8.2230E-01</td>
<td>76</td>
<td>5.1440E-06</td>
</tr>
<tr>
<td>36</td>
<td>4.2190E-01</td>
<td>78</td>
<td>3.1960E-06</td>
</tr>
<tr>
<td>38</td>
<td>3.0220E-01</td>
<td>80</td>
<td>1.2340E-06</td>
</tr>
<tr>
<td>40</td>
<td>1.5500E-01</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
To solve the integral equation, (3-8), the variational-iterative technique introduced by Sze (1976) was used. This method, in essence, provides a direct way for constructing an approximate source function for equation (3-8) and allows for arbitrary inhomogeneity in the atmosphere. It has been shown by Burke and Sze (1977) that the variational-iterative approach requires relatively little computational time to achieve satisfactory accuracy in comparison to other standard methods.

In the variational-iterative technique, the approximated source function can be expressed as:

\[ S_a(\tau) = U_a(\tau) \sqrt{w_0(\tau)} , \quad (3-12) \]

where

\[ U_a(\tau) = \sum_i C_i V_i(\tau) , \quad (3-13) \]

and \( V_i(\tau) \) is trial function for the \( i \)th layer.

The total optical depth \( \tau^* \) is divided into \( (N-1) \) layers with an average single scattering albedo \( \omega_j \) assigned to each layer \( j \). The simplest piece-wise continuous trial functions are the step functions defined by

\[ V_j(\tau) = \begin{cases} 1 & \tau_j \leq \tau \leq \tau_{j+1} \\ 0 & \tau < \tau_j, \tau > \tau_{j+1} \end{cases} \quad (3-14) \]

It can be shown (Sze, 1976) that the \( C_i \) are solutions to the following set of linear algebraic equations:

\[ \sum_{j=1}^{N} M_{ij} C_j = f_i . \quad (3-15) \]
The $M_{ij}$ are simply given by

$$M_{ij} = \delta_{ij} \Delta \tau_j - \frac{\sqrt{\omega_i \omega_j}}{2} \int_{\tau_i}^{\tau_j+1} B_j(\tau) \, d\tau ,$$

(3-16)

where

$$\delta_{ij} = \begin{cases} 1 & \text{for } i=j \\ 0 & \text{for } i \neq j, \end{cases}$$

$$B_j(\tau) = \int_{\tau_j}^{\tau_j+1} E_i(|\tau-t|) \, dt ,$$

and $f_i$ is

$$f_i = \frac{F_0}{4} \mu_0 \sqrt{\omega_1} \left[ \exp(-\tau_i/\mu_0) - \exp(-\tau_{i+1}/\mu_0) \right]$$

The smoothed approximated source function including the ground reflection can be written as

$$S_1(\tau) = \frac{\omega_0(\tau)}{4} F_0 \exp(-\tau/\mu_0) + \frac{\omega_0(\tau)}{2} \sum_{j=1}^{N-1} C_j \sqrt{\omega_j} B_j(\tau)$$

$$+ \frac{\omega_0(\tau)}{2} \cdot R \cdot E_2(\tau^*-\tau) \left[ \sum_{j=1}^{N-1} C_j \sqrt{\omega_j} D_j + \mu_0 \exp(-\tau^*/\mu_0) \right]$$

(3-17)

where

$$D_j = \int_{\tau_j}^{\tau_j+1} E_2(\tau^*-\tau) \, dt$$
Subsequent iterations

\[ S_{n+1}(\tau) = \frac{\omega_o(\tau)}{4} F_o \exp \left(-\tau/\mu_o\right) + \frac{\omega_o(\tau)}{2} \int_{0}^{\tau^*} E_1(|\tau-t|) S_n(t) \, dt \]

\[ + \frac{\omega_o(\tau)}{2} \cdot R \cdot E_2(\tau^*-\tau) \int_{0}^{\tau^*} E_2(\tau^*-t) S_n(t) \, dt + \mu_o \exp(-\tau^*/\mu_o) \]

would bring the source function to the desired accuracy.

3.3 Results

The results of two relevant calculations using the models described in the previous sections are contained in Appendix C. (A complete description of the output format is given in Section 4.5.) The first set of profiles is for an absorption only model where net fluxes are calculated using Eqn. (3-2). The second set is for a complete multiple scattering calculation [using equation (3-11)] where a surface reflectivity of 0.2 is assumed. Both calculations use a single solar zenith angle given by \( \cos^{-1}(0.707) \).

Several comparisons can be made between the calculations. In particular, the effect of multiple scattering and surface reflection on the photodissociation rate of \( O_3 \) be seen. Figure 3-1 illustrates the percent increase in the value of CJ03 for the two cases cited. A second curve (for a surface reflectivity of 0.8) indicates that highly reflecting surfaces and/or large expanses of cloud deck may have a significant impact on stratospheric photochemistry.
Solar Zenith Angle = \cos^{-1} 0.707
Surface Reflectivity:

- 0.2
- 0.8

Figure 3-1 Percent Increase in Value of CJ03
4. Program Description

4.1 Summary

The Chlorine Model Study Program (CMSP) computer code consists of a main program (MAIN), forty subroutines, function subprograms, and a subprogram Block Data of initialization and model parameters. The primary function of the main program is to select one of two operational modes determined by "keywords" read from the input set (see Section 5). Specification of the keyword PARAMETER calls subroutine INPARM which establishes the initial constants for each case. The keyword "RUN" directs the main program to call subroutine PHOCM which conducts the actual photochemical calculation for each case. A keyword of "ENDJOB" causes the program to terminate.

Since the sequence of program logic is somewhat complex due to the nature of the problem, this section provides a narrative description including considerable detail within many of the relevant subroutines. For clarity, housekeeping subroutines found in the program listing (Appendix A) are neither included in the flow chart (Appendix B) nor discussed further in this section. (These subroutines such as INPUT, PAGE, LINE, DAY, ERRM, etc. perform such functions as page turning and reading, line count, date writing, and error flagging.) The reader is urged to utilize the program listing and flow chart in following through this program description.

Table 4-1 provides a schematic view of the CMSP logic which may be helpful. Here the most important subroutines are listed according to their calling order and priority within the program. Priority is designated by levels: Level 0 is assigned to the MAIN program, while numerically higher levels are more distant from the MAIN program. A level 3 subroutine, for example, will return to a level 2 subroutine and may call a level 4 subroutine. The overall function of each block of coding is designated
<table>
<thead>
<tr>
<th>Level 0</th>
<th>Level 1</th>
<th>Level 2</th>
<th>Level 3</th>
<th>Level 4</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>MAIN</td>
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<td>WEIGHT</td>
<td>QSCATT</td>
<td>Initialize</td>
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<td></td>
<td></td>
<td>RINTER</td>
<td>SETUP 2</td>
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</tr>
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</table>
at the right of the table. For example, PHOCHM (Level 1) calls RJITER
(Level 2) and its higher level subroutines which compute photodissocia-
tion rates (so-called "J" values).

4.2 Initialization: BLOCK DATA

Although not contained explicitly within the flow chart, the BLOCK
DATA section constitutes a significant source of input data and contains
many of the run parameters which are required for model calculations.
These data are introduced by DATA statements which are made accessible
to the user subroutines by means of labeled COMMON statements.
Table 4-2 lists the important model variables contained within BLOCK
DATA including species mixing ratio or number density profiles, rate
constant data, photodissociation cross section and rate values, and
model atmosphere. Additionally, the corresponding labeled COMMON name
is given. Values are compiled into their respective array locations
based on their dependence on altitude or wavelength. Quantities
characterizing the atmospheric model such as temperature (TEMP) and
mixing ratios (H, OH, etc.) are given as level values at 2 km intervals
from the surface to 80 km. Wavelength dependent quantities such as the
solar flux (FL) and photodissociation cross sections (Q02, Q03 etc.) are
digitized at wavelengths given by the array WL such that WL(1) is the
wavelength at which the cross section of O₂ is Q02(1), etc.

In addition to vertical profiles and wavelength dependent spectra,
BLOCK DATA also contains a large number of default values for branching
parameters and other initial conditions specifiable for a particular case
such as the boundary conditions on the fluxes or mixing ratios of certain
species. These BLOCK DATA default values may be changed by utilizing
the NAMELIST $INPUT (see Section 4.3.2) if desired, otherwise the
default values are used. A complete description of these data is given
in Section 5.2.
<table>
<thead>
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<th>Units</th>
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<td>sec⁻¹</td>
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4.3 Initialization Subroutines: ALTGEN, INPARM

4.3.1 Subroutine ALTGEN

Upon entering the MAIN program, subroutine ALTGEN is called. The primary function of this code is to fill the array ALT which is contained in labeled COMMON, MODEL and gives the altitude of each level in 2 km (2.0 x 10^5 cm) increments from 0.0 to 80.0 km. However, ALTGEN also provides revised solar flux data (overiding the values specified in BLOCK DATA) in the 1900 to 2250 km wavelength region and photodissociation cross sections for chlorine nitrate. Additionally, the aerosol model number density distribution with height is specified by the parameter IAERO[ = 0 (23 km) or 1 (5 km)] and the integrated total number density of molecules DMINT, and aerosols DAINT are computed above a given level. These integrated densities are later used in the evaluation of optical depth. After ALTGEN is called control is returned to MAIN.

4.3.2 Subroutine INPARM

The keyword PARAMETERS read from the input set directs the program to call subroutine INPARM. INPARM establishes the basic input parameters required to run the model calculation. This is accomplished both by direct modification of previously stored values in BLOCK DATA and by calling higher level subroutines to perform additional computations on the basic input set. A NAMELIST statement is provided which may be used (see Section 5) to change the values of any of the formatted parameters from the default values.

For example, ISWIT which determines whether a single sun angle (=0) or a 24 hour average (=1) is used in the J-value computation may be changed from the default value (1) to zero by using the NAMELIST $INPUT. The subroutine listing (Appendix A) illustrates which parameters may be changed.
Certain basic calculations are performed by calling subroutines WEIGHT, QSCATT, CPHII, SETUP, and RCONST.

Subroutine WEIGHT computes the length of the day using the parameters LAT and DEL. The day is then divided into twelve equal time intervals (one hour at equinox) and the cosine of the solar zenith angle is computed at the midpoint of these intervals. Six values (those on either side of noon are equal) of the reciprocal of the cosine of the solar zenith angle are stored in array A. These are used to compute the 24 hour average model in subroutine COMTAU (Section 4.4.1).

Subroutine QSCATT computes the Rayleigh scattering coefficient QRAY, aerosol extinction coefficient QAE, and aerosol absorption coefficient QAA at the surface (z=0) as a function of wavelength. A particular aerosol size distribution is specified by the parameter ISIZE which selects one of four given models or a user's own model. (See Section 5.3). These values are later used in subroutine OMEGA to compute optical depth and the single scattering albedo profile when multiple scattering is considered.

Subroutine CPHII allows a quantum yield PHII to be introduced into the evaluation of the photodissociation rate for ClONO2. Furthermore, it may be given one value P11 for wavelengths WL(1) to WL(II), inclusive, and a second value P22 from WL(II+1) to the upper wavelength limit. Default values in BLOCK DATA are 11 = 59, P11 = P22 = 1.0, so that the quantum yield is unity.

Subroutine SETUP establishes the eddy coefficient model to be used and operates on the basic 41 level model atmosphere data. Upon entering the subroutine, Hunten's eddy coefficients are read into array EK by a DATA statement. If NEDDY is zero, these values are used.
I NEDDY is either one or two, subroutine EDC1 or EDC2, respectively, is called which substitutes either Chang's or an analytic form for these values. NEDDY has a default value of zero and may be changed in the NAMELIST $INPUT. A factor FKK (default value = 1.0) may be specified to multiply any of these profiles by a constant value. The basic model atmosphere data (TEMP, DM, and EK) are then interpolated to produce arrays (CTEMP, CDM, and CEK) of 81 levels of 1 km thickness from the data arrays containing 41 levels of 2 km thickness. These results are printed out at 2 km intervals.

Subroutine RCONST calculates the reaction rates of each of the chemical reactions as a function of temperature at the 81 levels of the atmosphere. The required input consists of the model atmosphere temperature profile and the first and second Arrhenius rate constants RA and RB from BLOCK DATA or NAMELIST $INPUT. For each reaction I and atmospheric level J the reaction rate RATE is given by:

\[ RATE(I,J) = RA(I) \times \exp\left(\frac{RB(I)}{CTEMP(J)}\right) \]

Rates are computed explicitly for reactions which do not obey the above relation. A table of reactions and rate constant information is printed. (see listing, Appendix A). After execution of RCONST control reverts to INPARM which returns to MAIN.

4.4 Main Calculation: PHOCHM

As indicated in the flow chart the keyword RUN calls the subroutine PHOCHM. PHOCHM controls the remainder of the calculation for a particular case and may be considered as the main program for most purposes.

As PHOCHM is entered the steady state version is selected by specifying FT = 0., FA = 2., FB = 0. and FM = 0. (these values will be used by subroutine COEF in performing the long-lived species calculations. (see 4.4.3).
The functions performed within PHOC M may be divided into three areas: (a) computation of photodissociation rates; (b) calculations for short-lived species (no diffusion); and (c) calculations for long-lived species (vertical diffusion). Most evaluations are made external to PHOC M by calling appropriate higher level subroutines.

4.4.1 Subroutine RJITER: Computation of Photodissociation Rates

Subroutine RJITER functions as a calling program to facilitate the calculation of photodissociation rates at each atmospheric level. Its two arguments ISWIT and ISCATT are carried in COMMON to PHOC M and specify the nature of the time averaging (single solar zenith angle vs. 24 hour average) and whether multiple scattering is considered, respectively. The upper limit for the wavelength integration IU is set in RJITER. For the absorption only model, the integration stops at 4025A and the contributions to the dissociation of O_3 from the visible are included as a constant factor PJ03. (set in BLOCK DATA). When multiple scattering is considered, however, the integration is extended through the visible region.

RJITER calls subroutine COLDEN which computes the column densities of ozone from a given level to the top of the atmosphere. These values, DO3INT, are used in the computation of optical depth.

Subroutine COMPJ called from RJITER performs the actual wavelength integration. The specific details of the calculation depend on the parameters ISWIT and ISCATT. For the simplest case ISWIT = 0, ISCATT = 0, a fixed solar zenith angle GMU = .707 is used and the number of photons cm^{-2}sec^{-1} available for photodissociation at a particular level is based on simple attenuation of the direct solar beam by O_2 and O_3 above the level. That is, optical depth TAU is computed as:

\[ \text{TAU} = \text{QO3} \times \text{DO3INT} + \text{QO2} \times \text{DMINT} \times \text{P02} \]

and DMINT is the integrated total number density.
J values are then computed in a straightforward manner by taking the product of available flux \((\text{FL} \cdot \exp(-\text{TAU}/\text{GMU}))\), cross section \((\text{Q02, Q03, QHC1, etc.})\), and quantum yield if required \((\text{PHI1})\) at a given wavelength and integrating over the wavelength interval. Flux is reduced by a factor of 0.5 (RDF) for the single angle calculation to account for night and day.

When ISWIT = 1 and a 24 hour average model is required, the transmissivity from the top of the atmosphere to a given level is weighted by calling a subroutine COMTAU which uses the array of coefficients A computed by WEIGHT to simulate the variation of solar zenith angle over a day. The subroutine COMTAU essentially performs the calculation:

\[
\text{TRAN (24 hr average)} = \frac{1}{24} \sum_{i=1}^{12} \exp(-\text{TAU} \cdot A(i))
\]

When a multiple scattering calculation is desired \((\text{ISCATT} = 1)\) two additional subroutines OMEGA and VIM are utilized. (see Section 3 for details of the scattering model). OMEGA computes optical depth from a given level to space as the sum of both attenuation (molecular and aerosol) and scattering (aerosol and Rayleigh). Aerosol absorption and extinction and Rayleigh scattering coefficients QAA, QAE, QRAY are carried in COMMON from subroutine QSCATT. Additionally, a single scattering albedo profile as a function of level is computed. An interpolation scheme creates a single scattering albedo profile as a function of optical depth which is input to subroutine VIM which performs a variational-iterative method multiple scattering calculation and returns the net flux available for photodissociation at a given optical depth normalized to the solar flux. This mean intensity includes contributions from the attenuated direct solar beam (absorption only case) and diffuse contributions reflected from the surface and scattered by molecules and aerosol particles. The surface reflectivity REF is contained in NAMELIST.
Subroutine OMEGA uses its knowledge of the altitude variation of optical depth to reinterpolate the net flux vs. optical depth profile to a net flux at altitude level profile. These values are placed in array F and returned to COMPJ for integration into the J value calculation. Subroutine VIM calls its own family of higher order subroutines which function somewhat independently of the overall CMSP code. A schematic presentation of the VIM subroutine hierarchy is presented in Table 4-3 in relation to the total CMSP sequence.

In order to account for the desired time averaging, OMEGA must be called for each GMU desired. Therefore, if a 24 hour average model is required (ISWIT = 1), OMEGA is called for each GMU using the solar zenith angles computed by WEIGHT (= 1/A) and averaging over 24 hours as was done for the absorption only case.

4.4.2 Subroutines INITIAL, SOLVE: Short-lived Species

After photodissociation rates based on the first guess ozone concentrations are returned to PHOCMH by RJITER, calculations of the species concentration profiles begin. As noted in Table 4.1 the PHOCMH code sequence from this point can be divided into segments handling the short-lived species and the long-lived species. An iteration counter I is incremented by statement 10 in PHOCMH after initialization to zero. This index keeps account of the number of times the program is executed to reach convergence. An upper limit of 50 iterations is assigned. For all iterations after the first the old OH and O₃ profiles (OLDOH,003) are saved for convergence testing before being recomputed. The computed photodissociation rates of O₂, O₃, HNO₃, H₂O₂, and N₂O₅ are substituted for the BLOCK DATA values at each level and the concentration profile of
### TABLE 4-3 SCHEMATIC PRESENTATION OF SUBROUTINE VIM SEQUENCE

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<th>PHOCHM</th>
<th>RJITER</th>
<th>COMPJ</th>
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<th>VIM</th>
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</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>E5</td>
</tr>
</tbody>
</table>
$O(^1D)$, DID, is computed based on equilibrium between the reactions:

$$O_3 + h\nu \rightarrow O_2 + O(^1D) \quad J = CJ031$$
$$O(^1D) + M \rightarrow O + M \quad k = RATE(51)$$

this yields the relationship:

$$DID = CJ031 \times O_3 / RATE(51) \times DM$$

at each level.

The calculation continues with a DO loop from statement 60 to statement 100 in PHOCIM. For each level in the atmosphere concentrations of the short-lived species are computed using the INITIAL and SOLVE subroutines. At a given level, INITIAL sets up a non-linear system of simultaneous equations in four variables: $Y(1) = H$, $Y(2) = OH$, $Y(3) = HO_2$, and $Y(4) = O_3$.

The $Y$ array gives the concentration of these four species at a given level.

(Note: $O_3$ is short-lived above 30 km and long-lived below 30 km.)

Initial concentrations of $CO$, $O_2$, $H_2$, $CH_4$, $CIX$, $NO_x$, $H_2O$, $OH$, and $HO_2$ are first evaluated from input profiles. On subsequent iterations the computed values are used. For example, mixing ratio is converted to number density by multiplying by the total number density. An iteration counter ($J$) is set to monitor convergence and subroutine PCLOX is called.

Subroutine PCLOX computes the level concentrations of $CL$, $CLO$, and $HCL$ by assuming equilibrium of production and loss mechanisms. The following ratios are computed:

$$RRC1 = CLO/CL \quad I$$
$$RRC2 = HCL/CL \quad II$$
$$RRC3A = CLNO3/CLO \quad III$$
$$RRC3B = CLNO3/CL = RRC3A \times RRC1$$

the corresponding reaction schemes assuming steady state at each level are:

$$Cl + O_3 \rightarrow ClO + O_2 \quad k = RATE(29)$$
$$ClO + O \rightarrow Cl + O_2 \quad k = RATE(31)$$
$$ClO + NO \rightarrow Cl + NO_2 \quad k = RATE(32)$$
\[ \text{O} + \text{HCl} \rightarrow \text{OH} + \text{Cl} \quad k = \text{RATE}(33) \]
\[ \text{HCl} + h\nu \rightarrow \text{H} + \text{Cl} \quad J = \text{JHCL} \]
\[ \text{Cl} + \text{CH}_4 \rightarrow \text{HC1} + \text{CH}_3 \quad k = \text{RATE}(30) \]
\[ \text{Cl} + \text{H}_2 \rightarrow \text{HC1} + \text{H} \quad k = \text{RATE}(26) \] II
\[ \text{Cl} + \text{H}_2\text{O}_2 \rightarrow \text{HC1} + \text{H}_2\text{O} \quad k = \text{RATE}(27) \]
\[ \text{HO}_2 + \text{Cl} \rightarrow \text{HC1} + \text{O}_2 \quad k = \text{RATE}(15) \]
\[ \text{OH} + \text{HC1} \rightarrow \text{H}_2\text{O} + \text{Cl} \quad k = \text{RATE}(20) \]
\[ \text{ClONO}_2 + h\nu \rightarrow \text{ClO} + \text{NO}_2 \quad J = \text{JCJ103} \]
\[ \text{ClO} + \text{NO}_2 + \text{M} \rightarrow \text{ClONO}_2 + \text{M} \quad k = \text{RATE}(28) \] III

After PCLOX returns to INITIAL, PNOX is called and an analogous computation of the level values of NO, NO2, HNO3, NO3, N2O5, and ClNO3 is made.

The following ratios are computed:

\[ \text{RR1} = \text{NO}/\text{NO2} \quad \text{I} \]
\[ \text{RR2} = \text{HNO3}/\text{NO2} \quad \text{II} \]
\[ \text{RR3} = \text{NO3}/\text{NO2} \quad \text{III} \]
\[ \text{RR4} = \text{N2O5}/\text{NO2} \quad \text{IV} \]
\[ \text{RR9} = \text{ClNO3}/\text{NO2} \quad \text{V} \]

Reactions determining these ratios assuming steady state at each level of the atmosphere are:

\[ \text{NO}_2 + h\nu \rightarrow \text{NO} + \text{O} \quad J = \text{CJNO2} \]
\[ \text{NO}_2 + \text{O} \rightarrow \text{NO} + \text{O}_2 \quad k = \text{RATE}(42) \] I
\[ \text{ClO} + \text{NO} \rightarrow \text{Cl} + \text{NO}_2 \quad k = \text{RATE}(32) \]
\[ \text{NO} + \text{O}_3 \rightarrow \text{NO}_2 + \text{O}_2 \quad k = \text{RATE}(40) \]
\[ \text{OH} + \text{NO}_2 + \text{M} \rightarrow \text{HNO}_3 + \text{M} \quad k = \text{RATE}(22) \]
\[ \text{HNO}_3 + h\nu \rightarrow \text{OH} + \text{NO}_2 \quad J = \text{JHNO3} \] II
\[ \text{OH} + \text{HNO}_3 \rightarrow \text{H}_2\text{O} + \text{NO}_3 \quad k = \text{RATE}(23) \]
\[ \text{NO}_2 + \text{O}_3 \rightarrow \text{NO}_3 + \text{O}_2 \quad k = \text{RATE}(41) \] III
\[ \text{NO}_3 + h\nu \rightarrow \text{NO} + \text{O}_2 \quad J = \text{JNO3} \]
\[ \text{N}_2\text{O}_5 + \text{M} \rightarrow \text{N}_2\text{O}_5 + \text{M} \quad k = \text{RATE}(38) \]
\[ \text{N}_2\text{O}_5 \rightarrow \text{NO}_2 + \text{NO}_3 \quad k = \text{RATE}(37) \]
\[ \text{N}_2\text{O}_5 + h\nu \rightarrow \text{NO}_2 + \text{NO}_3 \quad J = \text{JN205} \] IV
\[ \text{N}_2\text{O}_5 + \text{M} \rightarrow \text{N}_2\text{O}_5 + \text{M} \quad k = \text{RATE}(39) \]
\[ \text{NO}_2 + \text{NO}_3 \rightarrow \text{N}_2\text{O}_5 \quad k = \text{RATE}(36) \]
\[ \text{CIONO}_2 + h\nu \rightarrow \text{CIO} + \text{NO}_2 \quad J = \text{CICLO3} \]

\[ \text{CIO} + \text{NO}_2 + M \rightarrow \text{CIONO}_2 + M \quad k = \text{RATE}(28) \]

In the course of its calculation PNOX calls subroutine QUAD which solves the quadratic equation. PNOX returns control to INITIAL where a convergence test is made based on comparison of the old and new values of NO, NO2, and HNO3. If convergence occurs (within approximately 0.5%), INITIAL is exited and returns to PHOCHM.

PHOCHM calls subroutine SOLVE which organizes the solution of the chemical system for the short-lived species concentrations at a given level. Basically, the quantities Y (N), N = 1,4 are solved for using the convergent values returned from PNOX and PCLOX for the odd nitrogen and odd chlorine species, respectively. An iteration counter KK is established and the previous values of H, OH, H02, and O3 are saved for convergence testing. Subroutine SOLVE calls subroutine JACOB which organizes the coefficients of the system of chemical equations and calculates certain relevant production and loss terms. Production and loss terms are designated by double alphabetic variable names with a single subscript, while system coefficients to be solved by LINEQNM are stored in the doubly subscripted array, A. Total production terms for a given species are subscripted variables PP while loss (sink) terms are subscripted variables SS. Table 4.4 presents a key to the variables defined in JACOB, identifying each by the corresponding reactions. Note that below 30 km O3 is treated as a long-lived species, while at or above 30 km its equilibrium chemistry is treated explicitly. Subroutine JACOB returns to SOLVE where the net imbalance:

\[ B(J,4) = PP(J) - SS(J) \]

is computed for H, OH, and H02 in addition to the cumulative error:
### TABLE 4-4
CHEMICAL ORIGIN OF VARIABLES DESCRIBED IN SUBROUTINE JACOB

<table>
<thead>
<tr>
<th>Variable</th>
<th>Definition</th>
<th>Reaction</th>
</tr>
</thead>
<tbody>
<tr>
<td>ALP</td>
<td>$O_2/O_3$</td>
<td>$O + O_2 + M \rightarrow O_3 + M$ $k = \text{RATE}(34)$ $O_3 + \text{hv} \rightarrow O_2 + O$ $J = \text{JO3}$</td>
</tr>
<tr>
<td>AA(1)</td>
<td>Production of $H$</td>
<td>$H_2 + O(1D) \rightarrow OH + H$ $k = \text{RATE}(4)$ $H_2O + \text{hv} \rightarrow OH + H$ $J = \text{JH20}$</td>
</tr>
<tr>
<td>AA(2)</td>
<td>Loss of $H$</td>
<td>$H + O_2 + M \rightarrow HO_2 + M$ $k = \text{RATE}(5)$ $H + O_3 \rightarrow OH + O_2$ $k = \text{RATE}(6)$</td>
</tr>
<tr>
<td>AA(3)</td>
<td>Loss of $H$</td>
<td>$H + HO_2 \rightarrow H_2 + O_2$ $k = \text{RATE}(16)$ $+ 2OH$ $k = \text{RATE}(17)$</td>
</tr>
<tr>
<td>PP(1)</td>
<td>$= AA(1) + AA(2) + AA(3) + AA(4) + AA(5)$</td>
<td></td>
</tr>
<tr>
<td>BB(1)</td>
<td>Loss of $H$</td>
<td>$H + O_2 + M \rightarrow HO_2 + M$ $k = \text{RATE}(5)$</td>
</tr>
<tr>
<td>BB(2)</td>
<td>Loss of $H$</td>
<td>$H + O_3 \rightarrow OH + O_2$ $k = \text{RATE}(6)$</td>
</tr>
<tr>
<td>BB(3)</td>
<td>Loss of $H$</td>
<td>$H + HO_2 \rightarrow H_2 + O_2$ $k = \text{RATE}(16)$ $+ 2OH$ $k = \text{RATE}(17)$</td>
</tr>
<tr>
<td>CC(1)</td>
<td>Production of $OH$</td>
<td>$H_2O + O(1D) \rightarrow 2OH$ $k = \text{RATE}(2)$</td>
</tr>
<tr>
<td>CC(2)</td>
<td>Production of $OH$</td>
<td>$Cl_4 + O(1D) \rightarrow CH_3 + OH$ $k = \text{RATE}(3)$</td>
</tr>
<tr>
<td>CC(3)</td>
<td>$O + HO_2 \rightarrow OH + O_2$ $k = \text{RATE}(10)$</td>
<td></td>
</tr>
<tr>
<td>CC(4)</td>
<td>$HO_2 + O_3 \rightarrow OH + 2O_2$ $k = \text{RATE}(9)$</td>
<td></td>
</tr>
<tr>
<td>CC(5)</td>
<td>$NO + HO_2 \rightarrow NO_2 + OH$ $k = \text{RATE}(11)$</td>
<td></td>
</tr>
<tr>
<td>CC(6)</td>
<td>$H_2O_2 + \text{hv} \rightarrow 2OH$ $J = \text{JH202}$</td>
<td></td>
</tr>
<tr>
<td>CC(7)</td>
<td>$H + O_3 \rightarrow O_2 + OH$ $k = \text{RATE}(6)$</td>
<td></td>
</tr>
<tr>
<td>CC(8)</td>
<td>$HNO_3 + \text{hv} \rightarrow NO_2 + OH$ $J = \text{JHNO3}$</td>
<td></td>
</tr>
<tr>
<td>CC(9)</td>
<td>$H + HO_2 \rightarrow 2OH$ $k = \text{RATE}(17)$</td>
<td></td>
</tr>
<tr>
<td>CC(10)</td>
<td>$= AA(1)$</td>
<td></td>
</tr>
<tr>
<td>PP(2)</td>
<td>$= CC(1) + CC(2) + CC(3) + CC(4) + CC(5) + CC(6) + CC(7) + CC(8) + CC(9) + CC(10)$</td>
<td></td>
</tr>
<tr>
<td>DD(1)</td>
<td>Loss of $OH$</td>
<td>$OH + O_3 \rightarrow O_2 + HO_2$ $k = \text{RATE}(7)$</td>
</tr>
<tr>
<td>DD(2)</td>
<td>Loss of $OH$</td>
<td>$H_2O_2 + OH \rightarrow H_2O + HO_2$ $k = \text{RATE}(8)$</td>
</tr>
<tr>
<td>DD(3)</td>
<td>Loss of $OH$</td>
<td>$HO_2 + OH \rightarrow H_2O + O_2$ $k = \text{RATE}(14)$</td>
</tr>
<tr>
<td>DD(4)</td>
<td>$= AA(3)$</td>
<td></td>
</tr>
<tr>
<td>DD(5)</td>
<td>$= AA(2)$</td>
<td></td>
</tr>
</tbody>
</table>

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### TABLE 4-4 (Continued)

**CHEMICAL ORIGIN OF VARIABLES DESCRIBED IN SUBROUTINE JACOB**

<table>
<thead>
<tr>
<th>Variable</th>
<th>Definition</th>
<th>Reaction</th>
</tr>
</thead>
<tbody>
<tr>
<td>DD(6)</td>
<td>(\text{DD}(6) = 011 + HC1 + H2O + Cl)</td>
<td>(k = \text{RATE}(20))</td>
</tr>
<tr>
<td>DD(7)</td>
<td>(\text{DD}(7) = 011 + CH4 + CH3 + H2O)</td>
<td>(k = \text{RATE}(21))</td>
</tr>
<tr>
<td>DD(8)</td>
<td>(\text{DD}(8) = 011 + NO2 + M + HNO3 + M)</td>
<td>(k = \text{RATE}(22))</td>
</tr>
<tr>
<td>DD(9)</td>
<td>(\text{DD}(9) = \text{HNO3} + \text{OH} + \text{H2O} + \text{NO3})</td>
<td>(k = \text{RATE}(23))</td>
</tr>
<tr>
<td>DD(10)</td>
<td>(\text{DD}(10) = 011 + \text{OH} + \text{H2O} + \text{H})</td>
<td>(k = \text{RATE}(24))</td>
</tr>
<tr>
<td>DD(11)</td>
<td>(\text{DD}(11) = 011 + \text{112} + \text{1120} + \text{H})</td>
<td>(k = \text{RATE}(25))</td>
</tr>
<tr>
<td>SS(2)</td>
<td>(\text{SS}(2) = \text{DD}(1) + \text{DD}(2) + \text{DD}(3) + \text{DD}(4) + \text{DD}(5) + \text{DD}(6) + \text{DD}(7) + \text{DD}(8) + \text{DD}(9) + \text{DD}(10) + \text{DD}(11))</td>
<td></td>
</tr>
<tr>
<td>EE(1)</td>
<td>Production of (\text{HO2})</td>
<td>(\text{H} + \text{O2} + \text{M} + \text{HO2} + \text{M})</td>
</tr>
<tr>
<td>EE(2)</td>
<td>(\text{EE}(2) = \text{OH} + \text{O3} + \text{HO2} + \text{O2})</td>
<td>(k = \text{RATE}(7))</td>
</tr>
<tr>
<td>EE(3)</td>
<td>(\text{EE}(3) = \text{Cl} + \text{H2O2} + \text{ClO} + \text{H2O})</td>
<td>(k = \text{RATE}(27))</td>
</tr>
<tr>
<td>EE(4)</td>
<td>(\text{EE}(4) = \text{DD}(2))</td>
<td></td>
</tr>
<tr>
<td>PP(3)</td>
<td>(\text{PP}(3) = \text{EE}(1) + \text{EE}(2) + \text{EE}(3) + \text{EE}(4))</td>
<td></td>
</tr>
<tr>
<td>GG(1)</td>
<td>Loss of (\text{HO2})</td>
<td>(\text{HO2} + \text{O3} + \text{OH} + 2\text{O2})</td>
</tr>
<tr>
<td>GG(2)</td>
<td>(\text{GG}(2) = \text{CC}(3))</td>
<td></td>
</tr>
<tr>
<td>GG(3)</td>
<td>(\text{GG}(3) = \text{CC}(5))</td>
<td></td>
</tr>
<tr>
<td>GG(4)</td>
<td>(\text{GG}(4) = \text{ClO} + \text{HO2} + \text{HC10} + \text{O2})</td>
<td>(k = \text{RATE}(12))</td>
</tr>
<tr>
<td>GG(5)</td>
<td>(\text{GG}(5) = \text{HO2} + \text{HO2} + \text{H2O2} + \text{O2})</td>
<td>(k = \text{RATE}(13))</td>
</tr>
<tr>
<td>GG(6)</td>
<td>(\text{GG}(6) = \text{DD}(3))</td>
<td></td>
</tr>
<tr>
<td>GG(7)</td>
<td>(\text{GG}(7) = \text{Cl} + \text{HO2} + \text{HC1} + \text{O2})</td>
<td>(k = \text{RATE}(15))</td>
</tr>
<tr>
<td>GG(8)</td>
<td>(\text{GG}(8) = \text{BB}(3))</td>
<td></td>
</tr>
<tr>
<td>SS(3)</td>
<td>(\text{SS}(3) = \text{GG}(1) + \text{GG}(2) + \text{GG}(3) + \text{GG}(4) + \text{GG}(5) + \text{GG}(6) + \text{GG}(7) + \text{GG}(8))</td>
<td></td>
</tr>
<tr>
<td>PP(4)</td>
<td>Production of (02)</td>
<td>(02 + \text{hv} \rightarrow 20)</td>
</tr>
<tr>
<td>HH(1)</td>
<td>(\text{HH}(1) = \text{BB}(2))</td>
<td>Loss of Odd (0)</td>
</tr>
<tr>
<td>HH(2)</td>
<td>(\text{HH}(2) = \text{DD}(1))</td>
<td></td>
</tr>
<tr>
<td>HH(3)</td>
<td>(\text{HH}(3) = \text{CC}(4))</td>
<td></td>
</tr>
<tr>
<td>HH(4)</td>
<td>(\text{HH}(4) = \text{CC}(3))</td>
<td></td>
</tr>
<tr>
<td>HH(5)</td>
<td>(\text{HH}(5) = \text{AA}(2))</td>
<td></td>
</tr>
<tr>
<td>HH(6)</td>
<td>(\text{HH}(6) = \text{NO2} + 0 \rightarrow \text{NO} + \text{O2})</td>
<td>(k = \text{RATE}(42))</td>
</tr>
<tr>
<td>HH(7)</td>
<td>(\text{HH}(7) = \text{ClO} + 0 \rightarrow \text{Cl} + \text{O2})</td>
<td>(k = \text{RATE}(31))</td>
</tr>
<tr>
<td>HH(8)</td>
<td>(\text{HH}(8) = 0 + \text{O3} \rightarrow 2\text{O2})</td>
<td>(k = \text{RATE}(35))</td>
</tr>
</tbody>
</table>
### TABLE 4-4 (Continued)

CHEMICAL ORIGIN OF VARIABLES DESCRIBED IN SUBROUTINE JACOB

<table>
<thead>
<tr>
<th>Variable</th>
<th>Definition</th>
<th>Reaction</th>
</tr>
</thead>
<tbody>
<tr>
<td>SS(4)</td>
<td>HB(1) + HB(2) + HB(3) + HB(4) + HB(5) + HB(6) + HB(7) + HB(8)</td>
<td></td>
</tr>
</tbody>
</table>

**COEFFICIENTS OF SYSTEM OF EQUATIONS**

\[
A(1,1) = -\frac{SS(1)}{y(1)}
\]

\[
A(1,2) = \frac{(AA(2) + AA(3) + AA(4) + AA(5))}{y(2)}
\]

\[
A(1,3) = -\frac{BB(3)}{y(3)}
\]

\[
A(2,1) = \frac{(CC(7) + CC(9))}{y(1)}
\]

\[
A(2,2) = -(SS(2) + DD(10))/y(2)
\]

\[
A(2,3) = \frac{(CC(3) + CC(4) + CC(5) + CC(9) -DD(3))}{y(3)}
\]

\[
A(3,1) = \frac{(EE(1) -GG(8))}{y(1)}
\]

\[
A(3,2) = \frac{(EE(2) + EE(4) -GG(6))}{y(2)}
\]

\[
A(3,3) = -(SS(3) + GG(5))/y(3)
\]

At levels < 30 km  \( y(4) = O_3(k) \)

At levels > 30 km:

\[
T1 \quad \text{Loss of } O \quad NO_2 + O + NO + O_2 \quad k = \text{RATE}(42)
\]

\[
T2 \quad \text{OH} + O + O_2 + H \quad k = \text{RATE}(19)
\]

\[
T3 \quad \text{HO}_2 + O + OH + O_2 \quad k = \text{RATE}(10)
\]

\[
T4 \quad O + ClO \rightarrow Cl + O_2 \quad k = \text{RATE}(31)
\]

\[
TT1 = (T1 + T2 + T3 + T4) \quad \text{ALP}
\]

\[
T5 \quad \text{Loss of } O_3 \quad H + O_3 + OH + O_2 \quad k = \text{RATE}(6)
\]

\[
T6 \quad \text{OH} + O_3 + HO_2 + O_2 \quad k = \text{RATE}(7)
\]

\[
T7 \quad \text{HO}_2 + O_3 + OH + 2O_2 \quad k = \text{RATE}(9)
\]

\[
T8 \quad \text{NO}_2 + O_3 + NO_3 + O_2 \quad k = \text{RATE}(41)
\]

\[
TT2 = T5 + T6 + T7 + T8
\]

\[
B1 = TT1 + TT2
\]
Logical function LINEQN is called to solve the system of equations B where B(J,I) for J,I = 1,3 are the A(I,J) computed in JACOB using Gaussian elimination. If the matrix of coefficients is singular, values of H, OH, and HO₂ are scaled by a factor of 0.9 to remove the singularity and the calculation is repeated from the call to subroutine JACOB in statement 1 (This is permitted up to three times). If the parameter ERR is not less than 10⁻⁵ the concentrations are corrected by the magnitude of the net imbalance and the calculation is repeated from statement 1. (A maximum of 20 iterations are permitted.) If neither of the above error conditions occurs, the equilibrium concentrations of H, OH, HO₂ and O₃ have been found. The O concentration is computed using the parameter ALP from JACOB and the HO₂ concentration follows from the set of reactions:

\[
\begin{align*}
\text{HO}_2 + \text{HO}_2 & \rightarrow \text{H}_2\text{O}_2 + \text{O}_2 \\
\text{OH} + \text{H}_2\text{O}_2 & \rightarrow \text{H}_2\text{O} + \text{HO}_2 \\
\text{H}_2\text{O}_2 & \rightarrow \text{2OH} \\
\text{H}_2\text{O}_2 & \rightarrow \text{RATE}(13) \cdot \text{HO}_2 \cdot \text{HO}_2 / (\text{RATE}(8) \cdot \text{OH} + \text{JH}_2\text{O}_2)
\end{align*}
\]

Subroutines PNOX and PCLOX are called to compute the apportionment of nitrogen and chlorine species. Finally, the old and new values of H, OH, HO₂, and O₃ are compared. If the solutions do not compare within 1/2%, the calculation is repeated. If the solution is found, however, subroutine JACOB is called again to recompute the production and loss terms given by its coefficients (for printing purposes at final solution). Subroutine SOLVE then returns the PHOCHM. This sequence is repeated for each 2 km level in the atmosphere.
4.4.3 Subroutine CFLOW: Long-lived Species

At this stage in the calculation, concentration profiles have been computed for the short-lived species, that is the individual members of the HO_x, NO_x and ClX families, which are consistent with calculated J-values and input profiles for the long-lived species. Upon returning to PHOCHM, the values of O_3 are saved for comparison and subroutine CFLOW is called to accomplish the evaluation of profiles for the long-lived species: N_2O, HO_x, NO_x, ClX, CH_4, and O_3 below 30 km. In these cases (as discussed in Section 2) it is not adequate to equate production and loss processes at each level. These species, on the contrary, have longer chemical lifetimes and their profiles must be consistent both with chemical sources and sinks at each level and the gradient of vertical flux parameterized in terms of the eddy diffusion coefficient profile. The resultant equation which must be solved for the mixing ratio \( f_i \) as a function of \( z \) is of second order with coefficients given by the vertical profiles of both production and loss and the eddy coefficients. Therefore, boundary conditions at the top (designated U) and at the bottom (designated L) of the atmosphere must be specified. Certain basic coefficients are evaluated in entry SETUP 2 of subroutine SETUP (Section 4.3.2) which is called at the beginning of PHOCHM. These arrays are essentially the product NK which appears in the definition of vertical flux (equation 2.2) or in coding: CEK(I) * CDM(I).

Also, at the beginning of PHOCHM are definitions for the factors PPL, PPU, and QQU which are used to specify lower and upper boundary conditions. The program offers the versatility of specifying either flux (proportional to \( \frac{df_i}{dz} \)) or mixing ratio (i.e. \( f_i \) boundary conditions, the basic relationship being in the form:

\[
P_{L,U} \frac{df_i}{dz} + Q_{L,U} f_i = R_{L,U}
\]  

42
where $f_i$ is the mixing ratio of the $i$th species at the lower (L) or upper (U) boundary. For example, if a fixed mixing ratio is to be specified at both boundaries, then $P_L,U = 0$, $Q_L,U = 1$, and $f_i = R_{L,U}$ where $R_{L,U}$ is the mixing ratio of the $i$th species at the lower and upper boundaries, respectively.

All of the cases in the program (subroutine CFLOW) use: $P_U = 1$, $Q_U = \text{QU} \times \text{XL}(N)$, $R_U = 0$, where $\text{QU} = 6.0E + 05/\text{KE}(N) \times \text{CDM}(N)$, $\text{XL}(N)$ is the loss frequency of level $N$, and $N = 81$ is the uppermost level or:

$$\frac{df_i}{dz} = Q_U f_i$$

for the upper boundary condition. The corresponding lower boundary condition is given by specifying $R_L$ as either mixing ratio or flux:

(a) $R_L$ (flux): $Q_L = 0$, $P_L = PPL = -\text{CE}(1) \times \text{CDM}(1)$:

$$P_L \frac{df_i}{dz} = R_L$$

(b) $R_L$ (mixing ratio): $Q_L = 1$, $P_L = 0$:

$$f_i = R_L$$

After CFLOW is called by PHOCHM, a series of layer interpolations is accomplished using subroutine RINTER for the species: DID, OH, HO2, NO2, NO, 03, CLO, CL, H, and H20 and photodissociation rates: CJN20, CJCF3, CJCF2, CJCH3C, CJ02, CJ03, and CJCCL4. RINTER increases the vertical resolution from 2 km to 1 km using square root interpolation. The next sequence in CFLOW is a series of subroutine calls to CSPEC, each of which provides the calculation of the flow dependent (but time independent) vertical profile of a particular species. A test on the magnitude of the specified lower boundary condition (given in BLOCK DATA or namelist; see Section 4.2, TABLE 4.2 LABELLED COMMON: RLOW) determines whether flux or mixing ratio has been specified (i.e. a value greater than 1.0 is a flux while one less than 1.0 is a mixing ratio.) The appropriate boundary condition parameter is then set ($Q = 0$. for flux; $Q = 1$. for mixing ratio) for the CSPEC calculation.
The order in which the individual long-lived species are handled is as follows: \( \text{N}_2\text{O}, \text{NO}_x, \text{CH}_4, \text{F}11, \text{F}12, \text{CH}_3\text{Cl}, \text{CCl}_4, \text{CICl}, \) and \( \text{H}_2 \). The arguments of subroutine \text{CSPEC} (see program listing, Appendix A) relate to the previous boundary conditions discussion and are in order: \( (P_U, R_U, P_L, Q_L, \text{RLOW}, \text{DFP}, XL, \text{CXL}) \).

As noted above, the upper boundary conditions require \( P_U = 1 \) and \( R_U = 0 \).

As can be seen from the listing, the first two arguments are 1. and 0., respectively. The quantity \( P_L \) is set equal to PPL (defined in (a) above) and \text{CSPEC} changes this to zero if \( Q_L \) is equal to one (for fixed lower boundary mixing ratio). The next argument is the lower boundary condition value (either flux or mixing ratio as given by \( Q_L \)). The term \( \text{DFP} \) is the time dependent term which is set equal to zero for the steady state case (in each \text{CXL} subroutine). \( XL \) is the loss frequency returned and \text{CXL} is a family of subroutines (\text{CXL1, CXL2, etc.}) which computes the level-by-level production \( \text{PR} \) and loss frequency and returns these values to \text{CSPEC}. As a reference, Table 4.5 identifies the particular species dependent reaction schemes relevant to each \text{CXL} subroutine. Next, \text{CSPEC} calls subroutine \text{COEF} which utilizes the level production and loss frequency data and the particular type of boundary conditions specified to compute the necessary coefficients to solve the system of equations resulting for a given species. The arrays \( \text{AA(I)} \) and \( \text{T(I)} \) used here can be found in \text{SETUP2}. Once, the relevant coefficients are evaluated, the system is solved by subroutine \text{TRIDIA} which computes the mixing ratio \( (X_i) \) profile for each species \( i \). Finally, \text{CSPEC} calculates the net production and loss and returns this value \( (XL) \) to \text{CFLOW}:

\[
XL = \text{PR} - XL * X
\]

This procedure is carried out for each long-lived species with two exceptions. There is a convergence test for the solution of the \( \text{NO}_x \) profile.
# Table 4-5

## Subroutine Family CXL

<table>
<thead>
<tr>
<th>Subroutine</th>
<th>Species</th>
<th>Production</th>
<th>Loss</th>
</tr>
</thead>
<tbody>
<tr>
<td>CXL1</td>
<td>(N_2O)</td>
<td>From Surface</td>
<td>(N_2O + O(1^D) \rightarrow N_2 + O_2 + 2\text{NO})</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(N_2O + h\nu \rightarrow N_2 + O)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(NO + h\nu \rightarrow N + O)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(N + NO \rightarrow N_2 + O)</td>
</tr>
<tr>
<td>CXL2</td>
<td>(NO_x)</td>
<td>(N_2O + O(1^D) \rightarrow 2\text{NO})</td>
<td></td>
</tr>
<tr>
<td>CXL3</td>
<td>(CH_4)</td>
<td>From Surface</td>
<td>(CH_4 + O(1^D) \rightarrow CH_3 + OH)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(CH_4 + OH \rightarrow CH_3 + CH_3 + H_2O)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(CH_4 + Cl \rightarrow CH_3 + HCl)</td>
</tr>
<tr>
<td>CXL4</td>
<td>CFC(_{13})</td>
<td>From Surface</td>
<td>CFC(<em>{13}) + h\nu \rightarrow CFC(</em>{12}) Cl</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>CFC(_{13}) + O(1^D) \rightarrow \text{PRODUCTS}</td>
</tr>
<tr>
<td>CXL5</td>
<td>CF(_2Cl_2)</td>
<td>From Surface</td>
<td>CF(_2Cl_2) + h\nu \rightarrow CF(_2Cl + Cl)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>CF(_2Cl_2) + O(1^D) \rightarrow \text{PRODUCTS}</td>
</tr>
<tr>
<td>CXL6</td>
<td>CH(_3Cl)</td>
<td>From Surface</td>
<td>CH(_3Cl + h\nu \rightarrow CH_3 + Cl)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>CH(_3Cl + OH \rightarrow CH_2Cl + H_2O)</td>
</tr>
<tr>
<td>CXL7</td>
<td>ClX</td>
<td>CFC(<em>{13}) + h\nu \rightarrow CFC(</em>{12}) Cl</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>CF(_2Cl_2) + h\nu \rightarrow CF(_2Cl + Cl)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>CH(_3Cl + h\nu \rightarrow CH_3 + Cl)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>CCl(_4) + h\nu \rightarrow CCl(_3) + Cl</td>
<td></td>
</tr>
<tr>
<td>CXL8</td>
<td>O(_3)</td>
<td>O(_2 + h\nu \rightarrow 2O)</td>
<td>HO(_2 + O_3 \rightarrow OH + 2O_2)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>HO(_2 + NO \rightarrow OH + NO_2)</td>
<td></td>
</tr>
<tr>
<td>CXL9</td>
<td>CCl(_4)</td>
<td>From Surface</td>
<td>Cl + H(_2 \rightarrow HC1 + H)</td>
</tr>
<tr>
<td>CXL11</td>
<td>H(_2)</td>
<td>(H_2O + O(1^D) \rightarrow 2O)</td>
<td>OH + H(_2 \rightarrow H_2O + H)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>H + HO(_2 \rightarrow H_2 + O_2)</td>
<td>H(_2 + O(1^D) \rightarrow OH + H)</td>
</tr>
</tbody>
</table>
above level 40 (39 km) where the mixing ratio profile for $NO_x$ is given by X2. Additionally, the calculations for O3 are limited to the region from the surface to 30 km above which it is considered short-lived. There is also a convergence test for O3 whose mixing ratio profile is given by X8. If convergence is reached, subroutine REPCN is called which repeats the calculation of $NO_x$ and ClX apportionment using the new O3 values below 30 km by calling PNOX and PC10X. The values of ClO and NO2 are compared and if they have not converged, the O3 computations are repeated using the new ClX, NOX values. If convergence is reached, the values of the concentration profiles are computed from the resultant mixing ratios for NOX, CH4, CLX, H2, and O3 ($z < 30$ km), and control is returned to PHOCHM.

4.4.4 Final Convergence Testing

After return from CFLOW, the calculation is complete except for final verification of convergence. First, the previous O3 values from the short-lived calculation and those resulting from the long-lived calculation are averaged for a new profile. This is to help quicker convergence. Second, previous J values are saved since new ones (consistent with the new species profiles) will be computed for comparison. RJITER is called to accomplish this.

The final comparison is made level by level between previous and new J03 and OH values. An accuracy of 1/10% is accepted in the latter. If not achieved, the program is directed back to statement 10 in PHOCHM which increments the iteration index by one and restarts the calculation. After successful accomplishment of the desired accuracy, the program computes the integrated O3 density (O3INT) and the integrated odd O loss from levels 9-36 (by calling O3LINT). Finally, the major output subroutine PRINTX is called before the program is terminated.
4.5 Subroutine PRINTX: Output Profiles

Before terminating a particular run PHOCHM calls subroutine PRINTX. For each case run, thirteen pages of results are generated. (There are also a few pages of input parameters to identify the case printed out. See sample test cases Appendix C.) The beginning of the output is identifiable by the keyword RUN printed on a separate page.

Pages 1 and 2 of the output print J-values used in the final iteration of PHOCHM. They are headed with the note: "LAST ITERATION = I" where I is the final iteration index from PHOCHM. Page 1 gives the vertical profiles of the J values: CJ02, CJ03, CJCF2, CJCF3, CJ031 and in addition gives the O₃ number density, integrated O₃i, integrated total number density, and the OH number density for the previous iteration. Page 2 gives the profiles of the J values: CJIC03, CJN20, CJHNO3, CJH202, CJN205, CHCCL4, and CJCH3CL.

Pages 3-4 labelled "LAST ITERATION + 1" refer to results for the computation of J values using the final program results. Page 5 contains number densities of H, OH, HO2, H2O2, O, O², and O(^1D) in addition to the integrated O₃ density (HOX and odd oxygen families). Page 6 contains number densities of NO, NO2, HNO3, NO3, N2O5, and NOX (NOX family). Page 7 contains number densities and mixing ratios for CL, CLO, HCL, CLNO3, and CLX (CLX family).

Beginning on page 8 are level profiles of production and loss rates for particular reactions defined in PHOCHM and subroutine JACOB. (ref. Table 4-4). Page 8 in particular describes processes concerned with production and loss of odd oxygen. At the bottom of the page the integrated values of these rates are presented (they were calculated by 03LINT in PHOCHM). Page 9 gives the rates for reagents producing odd hydrogen in addition to the reaction Cl + CH₄. Page 10 gives the complementary losses of odd hydrogen.
Page 11 contains a listing of mixing ratio profiles for N20, NOX, CH₄, FC11, FC12, CH3C, CLX and CCL₄ and H₂. At the bottom of this page integrated fluxes for these long-lived species are provided by integrating the net production and loss terms from subroutines CXL using by a trapezoidal rule (subroutine TRAP). These should not differ substantially from the initial flux lower boundary conditions. Page 12 gives the mixing ratio of oxygen and the number densities of FC11, FC12, CH3CL, CCL4, and CLX.

Page 13 continues with N20, NOX, and CH₄.

If the keyword PARAMETERS appears next in the input stream to initialize constants for the next case to continue, the program is entered and the calculation repeated for the new case. However, the keyword ENDJOB will cause the program to print "NORMAL JOB END" and it will then terminate.
5. Users Guide

5.1 Program Initiation

The input deck required to initiate a model calculation using the CMSP program is relatively simple due to its modular, self-contained nature. As discussed in Section 4.2, the basic vertical profiles, wavelength dependent spectra, and rate constants required for the calculation are incorporated within BLOCK DATA and, consequently, need not be specified for each case (unless a change is desired.) Table 5-1 illustrates the configuration of the input deck which consists for the most part of keywords specification and a title to identify the output for the case run. For added versatility, however, the user can take advantage of the NAMELIST provision of subroutine INPARM in order to modify any of the listed (Table 5.2) variables for a particular case. For a single model run including one card of NAMELIST changes, a total of eight input cards are necessary. Note that multiple cases may be run by stacking cards 3-6 for each new case before the ENDDJOB card.

5.2 Default Parameter Values

In addition to listing the parameters which may be changed during input by the NAMELIST provision, Table 5-2 provides the current BLOCK DATA provided default values and subroutine location of primary utilization for each variable. Generally, these parameters may be divided into two subgroups: (1) branching parameters which control the type of calculation being made, and (2) run variables which are input data to the calculation.

The primary branching parameters are: INSWIT, ISCATT, NEDDY, and ISIZE. These have been discussed in Section 4 under the headings of their respective subroutines.
The various run variables include rate constants (RA, RB), profile multiplicative constants (FCL, FH2O, etc.), boundary condition data (RN2O, RF11, etc.), and multiple scattering factors (=1.0, they are not used).

5.3 Aerosol Model Specification

As discussed in Section 3.1, the user may select one of four internal aerosol models by specifying the parameter ISIZE which chooses a set of optical constants (extinction and absorption coefficients) in subroutine QSCATT (Section 4.3.2). An additional provision allows the user to substitute another size distribution by using ISIZE = 5 and adding the necessary extinction QE(5,J) and absorption QA(5,J) coefficients as a function of wavelength ALAM(J) within the subroutine. The height distribution specified by IAERO (Table 3-1) will be utilized for either IAERO = 0 (23 km visibility) or IAERO = 1 (5 km visibility). This parameter is set in subroutine ALTGEN (Section 4.3.1). The height distribution may be changed by amending the BLOCK DATA array DA23.
### TABLE 5-1
CMSM INPUT DECK CONFIGURATION

<table>
<thead>
<tr>
<th>Card Number</th>
<th>Description</th>
<th>Columns Used</th>
</tr>
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<tbody>
<tr>
<td>1</td>
<td>the word TITLE</td>
<td>1-5</td>
</tr>
<tr>
<td>2</td>
<td>any title desired</td>
<td>1-80</td>
</tr>
<tr>
<td>3</td>
<td>the word PARAMETERS</td>
<td>1-10</td>
</tr>
<tr>
<td>4</td>
<td>$ INPUT</td>
<td>beginning in column 2</td>
</tr>
<tr>
<td>4a</td>
<td>as many cards as</td>
<td></td>
</tr>
<tr>
<td>4b</td>
<td>necessary to input,</td>
<td></td>
</tr>
<tr>
<td></td>
<td>in NAMELIST format</td>
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</tr>
<tr>
<td></td>
<td>any constants which</td>
<td></td>
</tr>
<tr>
<td></td>
<td>differ from the default values set in</td>
<td></td>
</tr>
<tr>
<td></td>
<td>BLOCK DATA</td>
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</tr>
<tr>
<td>5</td>
<td>$ END</td>
<td>beginning in column 2</td>
</tr>
<tr>
<td>6</td>
<td>the work RUN</td>
<td>1-3</td>
</tr>
<tr>
<td></td>
<td>(cards 3-6 may be repeated for any</td>
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</tr>
<tr>
<td></td>
<td>number of runs with changed</td>
<td></td>
</tr>
<tr>
<td></td>
<td>constants)</td>
<td></td>
</tr>
<tr>
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<td>1-6</td>
</tr>
<tr>
<td>Name</td>
<td>BLOCK DATA Default Value</td>
<td>Subroutine Used</td>
</tr>
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<td>-----------------</td>
</tr>
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</tr>
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REFERENCES


APPENDIX A

PROGRAM LISTING
```
COMMON /IN0DEW/ DOINT (141), DMINT (141), DMINT (141)
COMMON /MODEL/ ALT (141), TEMP (141), DM (141), DMINT (141), DA23 (141)
COMMON /SOLCOV/ ML (100), FL (100), QO2 (100), QO3 (100)
COMMON /SOL2CN/ QCF2 (100), QCF3 (100), QOCL4 (100), QCH3C (100),
X QCN03 (100), QN20 (100), QMN03 (100), QM20 (100), QN205 (100),
Y QCN2L (100), QCN4L (100), QMN02 (100), QM20 (100)
REAL DA05 (3)
DATA DA05 = 1.378E04, 1.844E03, 2.453E02/

*          *          *

ALTI = 0.0
10  ALTI = ALTI -1 + 2.0E5

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<td>FL (31) = 3.75E+12</td>
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<p>| | |</p>
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</tr>
<tr>
<td>QCNO3 (57) = 5.00E-21</td>
<td>QCNO3 (58) = 3.10E-21</td>
</tr>
<tr>
<td>QCNO3 (59) = 4.80E-21</td>
<td>QCNO3 (60) = 3.80E-21</td>
</tr>
<tr>
<td>QCNO3 (61) = 3.20E-21</td>
<td>QCNO3 (62) = 2.90E-21</td>
</tr>
<tr>
<td>QCNO3 (63) = 2.50E-21</td>
<td>QCNO3 (64) = 2.30E-21</td>
</tr>
<tr>
<td>QCNO3 (65) = 2.10E-21</td>
<td>QCNO3 (66) = 1.90E-21</td>
</tr>
<tr>
<td>QCNO3 (67) = 1.70E-21</td>
<td>QCNO3 (68) = 1.50E-21</td>
</tr>
<tr>
<td>QCNO3 (69) = 1.30E-21</td>
<td>QCNO3 (70) = 1.10E-21</td>
</tr>
<tr>
<td>QCNO3 (71) = 9.70E-22</td>
<td>QCNO3 (72) = 4.80E-21</td>
</tr>
</tbody>
</table>

AEROSOL HEIGHT MODEL: T AER0 = 0 (23KM), = 1 (5KM)
COMPUTE INTEGRATED AEROSOL DENSITY
```

IÆRO=0
IF(IÆRO.FJ.0)G0 10 16
DO 15 J=1,3
15 OA23(J)=OA05(J)
16 NT = 41
DAINT(NT)=DA23(NT)*3.78E05
NTM1 = NT - 1
DELZ = 2.0E05
DMINT (NT) = DMINT (NT) * 5.0E05
DO 20 J = 1,NTM1
I = NT - J
IPL = I + 1
DAINT(I)=DAINT(IPL)+(DA23(IPL)+DA23(I))*DE1Z*5
20 DMINT(I) = DMINT(IPL) + (DM(IPL) + DM(I)) * DELZ*5
C A.L. PAGE
3 WRITE (6,601)
WRITE (6,602) (J,ML(J),FL(J),Q02(J),Q03(J),ICF2(J),ICF3(J),QCCL4(J),QCHR3(J),J=1,39)
C A.L. PAGE
WRITE (6,603)
WRITE (6,604) (J,ML(J),FL(J),QCLN03(J),QH2O(J),QN03(J),QH2O(J),QH2O(J),QH2O(J),J=1,39)
3 601 FORMAT (1H0,12X,*ML*,11X,*FL*,10X,*Q02*,10X,*Q03*,10X,*QCF2*,9X,*QCF3*,8X,*QCCL4*,6X,*QCHR3*)
3 602 FORMAT (1H0,15,IPBELJ,3.4)
3 603 FORMAT (1H0,12X,*ML*,11X,*FL*,9X,*QCLN03*,8X,*QH2O*,8X,*QN03*,8X,*QH2O*)
3 604 FORMAT (1H0,15,IP7ELJ,3.4)
RETURN
END
SUBROUTINE INPARM

+-------------------------------------------------
+ CMS04 - CHLORINE MODEL STUDY PROGRAM
+ SUBROUTINE INPARM - READS AND WRITES RUN VARIABLES
+ VERSION 4.0 LEVEL 770214
+ E.R.T., INC. N.Tripp
+-------------------------------------------------
COMMON /EDDY/ FKK,II,P11,P22,NE0DY
COMMON /MSCAT/ SCNO2,SCCL03,SCH2O2,SCN05
COMMON /NL./ JO/ XM(81),XH2O(81),PM20,PM21,XII(81)
COMMON /PARM/ ISMUT,ISTEP1,ISTOP,ITHPN,ISIZE,ISCAI
REAL JNO3
COMMON /RATES/ RATE(65,81),RA(65),RB(65),JNO3,PJ03
COMMON /SFACT/ FCL,FH20,FCLN03,NO
COMMON /RLMJ/ RN2O,RNOX,RCH4,RF11,RF12,RCH3,RCLX,RCL3,RCL4,R03
COMMON /SPE20V/ FJ,FIJC,FJCL,TL
REAL LAT
COMMON /MT/ A(6),DL,LAT,DEL
COMMON /PARA/ U0,M1,M2,NN,NN1,NN2,REF
3 NAMELIST /INPUT/ FCL,FCLN03,FH20,FNO,FKK,II,P11,P22,PJ03,ISMUT
1 FJ,FIJC,FJCL,T1,RNOX,RCH4,RF11,RF12,RCH3,RCLX,RCL4,
2 NE0DY,R03,SCNO2,SCCL03,SCH2O2,SCN05,PM20,PM21,LAT,DEL,JNO3,RA,RE
3 ISIZE,ISCAI,REF
READ (5,INPUT)
CALL PAGE

58
IF (ISWIT.EQ.0) WRITE(6,510) ISWIT
510 FORMAT (1H0,3X,*FIXED SUN ANGLE* MODEL - ISWITCH=*,I2)
IF (ISWIT.EQ.1) WRITE(6,511) ISWIT
511 FORMAT (1H0,3X,*24 HOUR AVERAGE* MODEL - ISWITCH=*,I2)

CALL WEIGHT
WRITE (6,514) LAT,DEL,A,O1
61'. FORMAT (1H0,3*X,CONTOUR FACTORS FOR THIS RUN*//X,5X,F3.9 LATITUDE*)
1,F5.1,* & SOLAR DECLEATION=*,F6.1,3X,*ASS=S=*,6(F3.4,**)/
2 5X,*DL =*,F9.4,* SECS=* IF ISCATT.EQ.0 GO TO 10
WRITE (6,520) ISCATT
520 FORMAT (1H0,4X,*MULTIPLE SCATTERING CALCULATION, ISCATT=*,I2)
CALL QSCATT
10 CONTINUE

WRITE (6,504)
504 FORMAT (1H0,4X,*FLUXES AND MIXING RATIOS FOR THIS RUN*)
WRITE (6,505) RN02,RN0X,RCH4,RF11,RF12,RCH32,RCLX,RCLL4,RO3,RH2
505 FORMAT (1H0,4X,*S-FACTORS FOR THIS RUN*)
WRITE (6,506) FCl,FCLNO3,FH2O,FNO
506 FORMAT (1H0,3X,*FCL=*,F5.2,2X,*FCLNO3=*,F5.2,2X,*FH2O=*,F5.2)
1 2X,*FNO=*,F5.2
WRITE (6,512)
512 FORMAT (1H0,4X,*MULTIPLE SCATTERING FACTORS FOR THIS RUN*)
WRITE (6,513) SCN02,SCCLO3,SCM22,SCN205
513 FORMAT (1H0,3X,*SCNO2=*,F5.2,2X,*SCCLO3=*,F5.2,2X,*SCM22=*,F5.2,2X,*SCN205=*,F5.2)

CALL CPU11 (PL1,PL2,PL11)
CALL SETUP (STEP,11)
CALL SETUP (STEP,11)
RETURN
END

SUBROUTINE SETUP (STEP,N)

CM03 - CHLORINE MODEL STUDY PROGRAM
SUBROUTINE SETUP TO TRANSFER RAW DATA WITH 41 LEVELS TO A SET OF NEW DATA WITH 81 LEVELS
ENTRY SETUP2 TO COMPUTE CERTAIN BASIC COEFFICIENTS

VERSION 3.2 LEVEL 761222
F.R.T.* INC. N.O. SIZE, N.TRIP

COMMON /COEFF/AA(81),BB(81),CC(81),DL(81),UU(81),U1(81)
COMMON /EDDY/ FKK,I1,I11,P11,P22,NE3DY
COMMON /MODE2/ ALT(41),TEMP(41),OM(41),DOD(41),DA23(41)
COMMON /NDATA/ CERK(81),CDM(81),CTEMP(81),CDA(81)
COMMON /FTFIR/ FT,FA,FB,FM
REAL EK(41),E(81)

59
C HUNTLEY'S EDDY DIFFUSION COEFFICIENTS (MODIFIED) - UP TO 50 KMS.

DATA EK/10.00,10.00,10.00,10.00,10.00,10.00,10.00,3.00,3.00,3.00,0.26,0.33,
10.42,0.53,0.65,0.65,1.01,1.3,0.6,2.05,2.59,3.2,2.0,5.00,6.4,0.32,0.4,0.002730
25.00,10.0,12.00,16.00,20.00,25.00,31.00,36.00,50.00,62.00,75.00,0.32,0.002740
396.00,12.00,150.00,190.00,240.00,300.00,360.00/0.002750

IF (MENDDY.EQ.1) CALL EDC1 (EK)
IF (MENDDY.EQ.2) CALL EDC2 (EK)
D0 10 I=1,41
J=2*N-1
CEK(J) = EK(I)*1.0E4*FKK
CDM(J) = DM(I)
COD(J) = DA23(I)
D0 10 CTEMP(J) = TEMP(I)
D0 15 I=1,41
J=2*I+n
ICE(J) = SQRT (ECK(I)*ECK(IP(I)))*1.0E4*FKK
CODP(I) = SQRT (ECK(I)*ECK(IP(I)))

DO 31 J=1,2*N-1
CC(J) = SQRT (E(J)*E(J))
C02(J) = CC(J)
CTEMP(J) = CTMP(J)
CALL PAGE
IF (MENDDY.EQ.0) WRITE (6,60) FK(
IF (MENDDY.EQ.1) WRITE (6,61) FK(
IF (MENDDY.EQ.2) WRITE (6,62) FK(
WRITE (6,65) (J,ALT(I),CEK(2*I-1),DM(2*I-1),CENTP(2*I-1),
60 FORMAT (1H0,9X,*FKK =*,F5.2,* FACTOR MULTIPLYING HJNTY'S EDDY DIFFUSION COEFFICIENTS)
61 FORMAT (1H0,9X,*FKK =*,F5.2,* FACTOR MULTIPLYING 44 YTC EDDY DIFFUSION)
62 FORMAT (1H0,9X,*FKK =*,F5.2,* FACTOR MULTIPLYING C144G'S EDDY DIFFUSION COEFFICIENTS)
63 FORMAT (1H0,12X,*ALT*,10X,*ECK*,13X,*DM*,11X,*TEMP*,13X,*OU*/)
64 FORMAT (2X,12,0PF11.0,1P2E15.4,0PF11.2,1PE15.4)
RETURN

ENTRY SETUP2
N1=M-1
N2=M-2
JT=3.19576E7*STEP
37 I=1,M
E(I) = CEK(I)*DM(I)
32 J=1,2*M-1
U(J) = 0.5E-10*OT/DM(I)
30 I=1,M
33 CC(I) = SQRT (E(I)*E(I))
30 I=1,M
34 BB(I) = CC(I)
35 I=1,M
BB(I) = SQRT (E(I)*E(I))
33 I=1,M
AA(I) = CEK(I)+0.03(I)
34 I=1,M
DL(I) = U(I)*BB(I)*FA
34 I=1,M
DU(I) = U(I)*CC(I)*FA
RETURN

END

SUBROUTINE WEIGHT

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

.....CM03 - CHLORINE MODEL STUDY PROGRAM

VERSION 3.3  LEVEL 770201


%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
REAL LAT
COMMON /MT/ A(6),DL,LAT,DEL
DIMENSION T(6)
DATA DTOR,RTD0/-.01745329,57.29579/

LAT * LAT * DTOR
DEL = DEL * DTOR
X1 = COS(LAT) * COS(DEL)
X2 = SIN(LAT) * SIN(DEL)
DDL = ACOS(-TAN(LAT)*TAN(DEL))
DT = DDL/6.
DO 10 I = 1,6
   T(I) = DT/2. + (I-1)*DT
   T(I) = (T(I)/240.) * DTOR
COSANG = X1*COS(T(I)) + X2
10 A(I) = T(I)/COSANG
DL = 2.*DDL
LAT = LAT * RTD0
DEL = DEL * RTD0
RETURN
END
SUBROUTINE CP11 (P11,P22,I1)
COMMON /PHIN/ PHIN(100)

DO 10 J = 1,I1
   PHI1(J) = P11
10 PHI1(J) = P22
RETURN
END
SUBROUTINE EDC1 (EK)

ANALYTIC EDDY DIFFUSION COEFFICIENTS (* 1.E-4)
DIMENSION EK(441)
DO 10 I=1,5
   EK(I) = 0.
10 EK(I) = 3.
   EK(I) = 3.
   EK(I) = 3.
   EK(I) = 3.
   EK(I) = 3.
   EK(I) = 3.
   EK(I) = 3.
20 EK(I) = 35*EXP((2*(I-1)-14)/9.55)
RETURN
END
SUBROUTINE EDC2 (EK)

CHANGE'S EDDY DIFFUSION COEFFICIENTS - UP TO 50 KMS. (* 1.E-4)
DIMENSION EK(441),CK(441)
DATA CK/630.,
1.1,1.2,1.2,1.7,1.4,60.,50.,42.,39.,37.,39.,42.,50.,66.,80.,
2.1,1.1,1.1,1.5,1.3,1.4,1.5,1.6,1.7,1.9,2.2,49.,49.,155.,192.
30 EK(I) = 1.41
10 EK(I) = CK(I)
RETURN
END
SUBROUTINE RCONST

******************************************************************************
******CHMS04 - CHLORINE MODEL STUDY PROGRAM
******SUBROUTINE RCONST - CALCULATES REACTION RATES FOR PROGRAM
<table>
<thead>
<tr>
<th>DATA REACT1/4OH + 4H CH3,HCl,2H,2H2O,2H2</th>
<th>004200</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 4HO2 + 4H CH2O,4H + 2H,2H2O,2H2</td>
<td>004210</td>
</tr>
<tr>
<td>3 4HCO + 4H CH2O,4H + 2H,2H2O,2H2</td>
<td>004200</td>
</tr>
<tr>
<td>4 4H2 + 4H CH2O,4H + 2H,2H2O,2H2</td>
<td>004230</td>
</tr>
<tr>
<td>5 4OH + 4H2 O,4H + 2H,2H2O,2H2</td>
<td>004240</td>
</tr>
<tr>
<td>6 4H2O + 4H NO,4H + 2H,2H2O,2H2</td>
<td>004270</td>
</tr>
<tr>
<td>7 4H2O + 4H CH2O,4H + 2H,2H2O,2H2</td>
<td>004290</td>
</tr>
<tr>
<td>8 4H2O + 4H H2O,4H + 2H,2H2O,2H2</td>
<td>004300</td>
</tr>
<tr>
<td>9 4H2O + 4H ClH4O,4H + 2H,2H2O,2H2</td>
<td>004310</td>
</tr>
</tbody>
</table>

**DATA REACT2/4HCO2 + 4H CH2O,4H + 2H,2H2O,2H2**

**DATA REACT3/4HCO + 4H CH2O,4H + 2H,2H2O,2H2**

**DATA REACT4/4ClO + 4H NO,4H + 2H,2H2O,2H2**

**DATA REACT5/4M2O5,4H + 4H + 2H,2H2O,2H2**

**DATA REACT6/4H + 4NO2,4H + 2H,2H2O,2H2**

**DATA REACT7/4HO1,4H + 4HCF3,4H + 2H,2H2O,2H2**

**DATA REACT8/4HO1,4H + 4HCH3,4H + 2H,2H2O,2H2**

---

**COMMON/RTA1*/ RTA(81),RTB(81),RTM(81),RTN(81)**

**COMMON/RTB1*/ RTB(81),RTD(81),RTF(81)**

**COMMON/RTA1*/ RTA(81),RTA(81),RTA(81),RTA(81)**

**DIMENSION REACT1(7,9),REACT2(7,9),REACT3(7,9)**

**EQUIVALENCE (REACT1(1,1),REACT1(1,1),REACT1(1,1),REACT1(1,1))**

**DATA REACT1/4OH + 4H CH3,HCl,2H,2H2O,2H2**
SET UP RATES ARRAY FOR 65 REACTIONS
DO 10 I = 1, 65
10 RATE(I,J) = RA(I) * EXP(RB(I)/TEMP(J))

RE-CALCULATE RATE CONSTANTS THAT DO NOT FIT ABOVE FORMULA
DO 20 J = 1, 81
RATE(22,J) = 2.3E-13*EXP(880./TEMP(J))/(2.61E16*CDM(J))
RATE(37,J) = 1.0E-08*CDM(J)/(2.61E19*CDM(J)) + 1.0E7
20 CONTINUE

PRINT OUT ALL REACTIONS AND RATE CONSTANTS A & B
CALL PAGE
WRITE (6, 600)
600 FORMAT (1HO, 3X, "REACTION RATE (IS A FUNCTION OF ALTITUDE, Z) = A * "

DO 30 I = 1, 21
30 WRITE (6, 601) (REACT(I,J), N = 1, 7, RA(I), R3(I))
601 FORMAT (1H) +15X, "REACTION", 17X, "A", 11X, "B"

DO 90 J = 23, 36
90 WRITE (6, 601) (REACT(I,J), N = 1, 7, RA(I), R3(I))

PRINT EXCEPTIONAL CASES
WRITE (6, 602) (REACT(I,22), N = 1, 7)
1.
WRITE (6, 603) (REACT(I,37), N = 1, 7)
1.

IF FORMULAE ARE DIFFERENT
2.
4X, "22", 4X, "7A", 5X, "R = 2.3E-13", "1H", 
3.
"* EXP(880./TEMP(Z))/(2.61E16 * M(Z))/*
4.
4X, "37", 4X, "7A", 5X, "R = 1.0E-08", "1H", 
5.
"* (Z)/(2.61E19+M(Z)) + 1.0E7*
RETURN
END

SUBROUTINE CHLORINE MODE
DIMENSION Y(10)
COMMON /JVAR/ CJO2(50), CJ03(50), CJCF2(50), CJCF3(50), JCCL4(50),
1.
1 CJCHSC(50), CJCL03(50), CJN02(50), CJN03(50),
2.
2 CJN20(50), CJ30(50), CJNO2(50), CJNO3(50),
COMMON /DATA/ CEK(81), COM(81), TEMP(81), CDA(81),
COMMON /NETPRO/ PP(4), SS(6)
COMMON /OLD/ OJ02(41), OJ03(41), JCF2(41), OJCF3(41), JCCG4(41),
1.
1 OJCHSC(41), OJCL03(41), OJN02(41), OJN03(41), OJN20(41), OJN03(41),
2 OJNO2(41), OJNO3(41), OJNO3(41), OJNO3(41),
COMMON /PARA/ STEP, QUP, PLL, PPC, N,M
COMMON /RM/ ISW1, JSTEP, JSTOP, JLOOP, JTRI, ISEQ, ICOUNT
REAL J02, J33, JN02, JN03, JN03, JCH4, JCFC
COMMON /PHRATE/ J02(41), J03(41), JH20(41), JN32(41), JN20(41),
COMMON /JDFL(41), JCM4(41), JCF2(41), JCF3(41), JMLC(41), JH202(41), COMMON /JX3CL(41),
COMMON /JRATC/ AA(10), BB(10), CC(10), DE(10), EE(10), FF(10), HH(10),
COMMON /JIMC/ JN03(41), JNO2(41), JNO3(41), JNO(41), JN02(41), JN01(41),
COMMON /JX0M(41), JX03(41), JX05(41), JX07(41), JX09(41), JX01(41),
COMMON /JX0M(41), JX03(41), JX05(41), JX07(41), JX09(41), JX01(41),
COMMON /JX0M(41), JX03(41), JX05(41), JX07(41), JX09(41), JX01(41),
COMMON /SOLA4V/ FL(100), JQ03(100), JQ04(100), JQ05(100), JQ06(100),
REAL JN03, JNO2, JN01, JN03, JN05, JN07, JN09, JN11, JN13, JN15, JN17,
REAL JN03, JNO2, JN01, JN03, JN05, JN07, JN09, JN11, JN13, JN15, JN17,
REAL JN03, JNO2, JN01, JN03, JN05, JN07, JN09, JN11, JN13, JN15, JN17,
REAL JN03, JNO2, JN01, JN03, JN05, JN07, JN09, JN11, JN13, JN15, JN17,
REAL JN03, JNO2, JN01, JN03, JN05, JN07, JN09, JN11, JN13, JN15, JN17,
REAL JN03, JNO2, JN01, JN03, JN05, JN07, JN09, JN11, JN13, JN15, JN17,
DO3DM(2,K) = CC(1)  
DO3DH(3,K) = CC(2)  
DO3DM(4,K) = CC(3)  
DO3DM(5,K) = AA(3)  
DO3DM(6,K) = CC(5)  
DO3DH(7,K) = CC(6)  

CLM44(K) = RATE(30,L) * CL(K) * CH4(K)  
SODH(1,K) = OD(2) * 2.  
SODH(2,K) = OD(3) * 2.  
DO 105 J = 3, 7  
305 SODH(J,K) = OD(J+3)  
SODH(8,K) = 2.0 * RATE(16,L) * H(K) * HO2(L)  
SODH(9,K) = GG(7)  
100 CONTINUE  

DO 108 K = LLL,LLU  
108 OD3J(K) = O3(K)  
CALL CFLOW(M1,I)  
DO 110 K = LLL,LLU  
110 ODJ(K) = (O3I(K) + OD3J(K)) / 2.  

DO 20 J = LLL,LLU  
OJ2J(J) = CJ02(J)  
OJ3J(J) = CJ03(J)  
OJCF2(J) = CJCF2(J)  
OJCF3(J) = CJCF3(J)  
OJCL4(J) = CJCL4(J)  
OJCH3(J) = CJCH3(J)  
OJCL03(J) = CJCL03(J)  
OJN20(J) = CJN20(J)  
OJHNO3(J) = CJHNO3(J)  
OJH2O2(J) = CJH2O2(J)  
OJJO3(J) = CJO3(J)  
OJN2O5(J) = CJN2O5(J)  
O03INT(J) = O03INT(J)  
20 CONTINUE  

CALL RJITER(ISWIT,ISCATT)  
IF (I.EQ.1) GO TO 10  

DO 50 J = LLL,LLU  
E = ABS((CJ03(J) - OJ03(J))/CJ03(J))  
IF (E.GE.EPS) GO TO 10  

E1 = ABS((OH(J) - OLOH(J))/OH(J))  
IF (E1.GE.EPS1) GO TO 10  

50 CONTINUE  

502 CONTINUE  
CALL Q3INT (HHH,YY9,36)  
Q3INT(LLLU) = Q3(LLLU) * 5.0E5  
LLML = LLJ - LLL  
DO 310 K = 1,LLML  
J = LLU - K  
JPI = J + 1  
310 Q3INT(J) = Q3INT(JPI) + (Q3(JPI) + Q3(J)) * 1.0E5  
CALL PRINTX(I,LLL,LLU)  
NEXT = .TRUE.  
RETURN  

501 I = I - 1  
WRITE (6,601) I  
601 FORMAT (1H8/10X,'DID NOT CONVERGE IN*:I4," IERATIONS")  
GO TO 502  

EN}
COMMON /RATES/RATE(65,81),RA(65),RB(65),JNO3,PJO3  
NT = 41  
HAV = 5.0E05  
IL = 1  
IU = 72  
IF(ISCATT,EQ.1)IU=99  
IF(ISCATT,EQ.1)PJO3=0.0  
RDF = 1.0  
IF(ISWIT,EQ.0)RDF = 0.5  
GMJ = .707  
CALL COLODEN(NT,HAV)  
CALL COMPJ(IL,IL,GMJ,ROF,NT,IS41,ISCAT)  
RETURN  
END  
SUBROUTINE COLODEN(NT,HAV)  
NT IS THE INDEX NUMBER OF THE TOP LAYER  
HAV IS THE AVERAGE SCALE HEIGHT OF TOP LAYER  
REAL NO,NO2,NOX,N205  
COMMON /SPECIE/ H(41),OH(41),H2(41),H2O(41),O2(41),O3(41),NO(41)  
1 NO2(41),HNO3(41),NOX(41),CO(41),O2(41),CH4(41),H2(41),H2O(41),  
2 Cl(41),ClO(41),HCl(41),Cl2(41),OCl(41),ClO2(41),  
3 CLNO3(41)  
COMMON /MODEL/ALT(41),TEMP(41),OM(41),DID(41),DA2(41)  
COMMON /INJEN/D2O3INT(41),DMINT(41),D4INT(41)  
NTM1 = NT - 1  
DE.Z = 2.0E05  
DO3INT(N) = O3(N) * HAV  
DO 10 J = 1,NTM1  
I = NT - J  
IP1 = I + 1  
10 DO3INT(I) = D3O3INT(IP1) + (O3(IP1) + O3(I)) * DE.Z*5  
RETURN  
END  
SUBROUTINE COMPJ(IL,IL,GMJ,ROF,NT,IS41,ISCAT)  
THIS ROUTINE COMPUTES COLUMN DESEITYS OF OZONE  
GMJ = SOLAR ZENITH ANGLE  
ROF = FLUX REDUCTION FACTOR  
NT = INDEX NUMBER OF TOP LAYER  
IS41 = SWITCH USED IN COMPUTING TRAN FROM FAU  
ISCAT = SWITCH FOR ABSORBING OR SCATTERING MODEL  
COMMON /MODEL/ALT(41),TEMP(41),OM(41),DID(41),DA2(41)  
COMMON /INJEN/D2O3INT(41),DMINT(41),D4INT(41)  
COMMON /JVAL/ CJH2O2(50),CJNO3(50),CJCFC3(50),CJCFC2(50),CJCFC1(50),CJCCL4(50),  
1 CJH3SC(50),CJCLO3(50),CJMN2O5(50)  
2 CJH2O2(50),CJNO3(50),CJMN2O5(50)  
70720
COMMON /MSCAT/ SCMO2,SCCLO3,SCH2O2,SCN05
COMMON /PHII1/ PHII(100)
REAL JO2,JO3,JM02,JM02,JM20,JM25,JMN03,JCH4,JCF2,
X JCF3,JHCL,JH2O2,JH0CL
COMMON /PHRATE/ JO2(41),JO3(41),JM02(41),JMN02(41),JMN20(41),
X JMN25(41),JMN03(41),JCH4(41),JCF2(41),JCF3(41),JH2(41),
COMMON /OL22/ WLI(100),FL(100),QO2(100),QO3(100),
COMMON /OL34/ QCF2(100),QCF3(100),QCL4(100),QCHS(100),
COMMON /ISOLCOM/ WCL(100),FL(100),QO2(100),QO3(100),
COMMON /PK RATE/ JOZ(41),JO3(41),QH2O(100),QH2O3(41),
COMMON /ISOLCOM/ WCL(100),FL(100),QO2(100),QO3(100),
COMMON /PK RATE/ JOZ(41),JO3(41),QH2O(100),QH2O3(41),
REAL LAT
COMMON /LAT,DEL
REAL LAT
COMMON /OL22/ WLI(100),FL(100),QO2(100),QO3(100),
COMMON /OL34/ QCF2(100),QCF3(100),QCL4(100),QCHS(100),
COMMON /ISOLCOM/ WCL(100),FL(100),QO2(100),QO3(100),
COMMON /PK RATE/ JOZ(41),JO3(41),QH2O(100),QH2O3(41),

COMPUTE COLUMN DENSITIES, STORE IN DOSINT,DMINT,
COMPUTED IN SUBROUTINE COLDEM
IF ISWIT THEN FIX GMU FOR INTEGRAL ELSE CALL COMPTAU
IF ISCATT DO MULTIPLE SCATTERING CALCULATION AND
WEIGHT FLUX FACTORS IF ISWIT
PO2 = 0.21
IFIISCATT.EQ.0 GO TO 50
IFIISMWT.EQ.0 GO TO 60
DO 55 I = 1 ,NT
DO 66 J = IL, IU
FAV(I,J) = 0.0
F(I,J) = 0.0
CONTINUE
CONTINUE
DO 70 KK = 1,5
SMU = 1.0/AA(KK)
CALL OMEGA(N,T,IL, IU, GMU)
DO 80 I = 1,NT
DO 90 J = IL, IU
FAV(I,J) = FAV(I,J)*F(I,J)
CONTINUE
CONTINUE
DO 75 I = 1, NT
DO 76 J = IL, IU
F(I,J) = FAV(I,J)*D*L*Z/1036800.
CONTINUE
CONTINUE
GO TO 50
CONTINUE
50 CALL OMEGA(N,T,IL, IU, GMU)
CONTINUE
DO 10 I = 1, NT
TEMP2 = 0.0
TEMP3 = 0.0
TEMP4 = 0.0
TEMP5 = 0.0
TEMP6 = 0.0
TEMP7 = 0.0
TEMP8 = 0.0
TEMP9 = 0.0
TEMP10 = 0.0
TEMP11 = 0.0
TEMP12 = 0.0
TEMP13 = 0.0
TEMP14 = 0.0
TEMP15 = 0.0
TEMP16 = 0.0
DO 20 J = IL, IU
IFIISCATT.EQ.1) GO TO 7
TAJ = QO3(J)*QDINT(I) + QO2(J)*QDINT(I)*PO2
IF (ISWIT.GT.0) GO TO 100
TAU = -TAU/SMU
IF (TAU.GE.-150.) GO TO 5
TRAN = 0.
GO TO 6
5 TRAN = EXP(TAU)
GO TO 6
100 CALL CONTAU (TAU,TRAN)
TRAN = TRAMP(OL/1036800.)
GO TO 6
7 TRAN=F(I,J)
6 TEP2 = TEMP1*FL(J)*Q02(J)*TRAN
TEP3 = TEP3 + FL(J)*Q03(J)*TRAN
TEP4 = TEP4 + FL(J)*QCF2(J)*TRAN
TEP5 = TEP5 + FL(J)*QCF3(J)*TRAN
TEP6 = TEP6 + FL(J)*QCL3(J)*TRAN
TEP7 = TEP7 + FL(J)*QCH3C(J)*TRAN
TEP8 = TEP8 + FL(J)*QCLNO3(J)*TRAN
TEP9 = TEP9 + FL(J)*Q2O2J(J)*TRAN
TEP10 = TEP10 + FL(J)*QHNO3(J)*TRAN
TEP11 = TEP11 + FL(J)*Q2H202(J)*TRAN
TEP12 = TEP12 + FL(J)*QH2O5(J)*TRAN
TEP13 = TEP13 + FL(J)*QHC(J)*TRAN
TEP14 = TEP14 + FL(J)*QHCL3(J)*TRAN
TEP15 = TEP15 + FL(J)*Q2H2O2(J)*TRAN
TEP16 = TEP16 + FL(J)*QH2O2(J)*TRAN
CONTINUE
20 CJO2(I) = TEMP2*RDF
CJO3(I) = TEMP3*RDF
CJO31(I) = TEMP4*RDF
CJCF3(I) = TEMP5*RDF
CJCL4(I) = TEMP6*RDF
CJCH4(I) = TEMP7*RDF
CJCL5(I) = TEMP8*RDF
CJ20(I) = TEMP9*RDF
CJHNO3(I) = TEMP10*RDF
CJH202(I) = TEP11*RDF*SC2H202
CJ205(I) = TEMP12*RDF*SC2H205
JHC1(I) = TEMP13*RDF
JH2CL(J) = TEMP14*RDF
JNC2(I) = TEMP15*RDF
JNC20(I) = TEMP16*RDF
CONTINUE
10 PHI(J) = .7
PHI(54) = .05
DO 30 I = 1,NT
TEMP31 = 0.
DO 40 J = 1,IL54
IF (ISCAT. EQ.1) GO TO 110
TAJ = QO3(J)*DO3INT(I) + Q02(J)*OMINT(I)*PO2
IF IISWIT .GE. 01 GO TO 25
TAU = TAU/GM
IF (TAU.GE.-150.) GO TO 24
TRAN=0.
GO TO 27
24 TRAN=EXP(TAU)
GO TO 27
25 CALL CONTAU (TAU,TRAN)
TRAN = TRAMP(OL/1036800.)
GO TO 27
110 TRAN=F(I,J)
27 IF (J.GT.52) GO TO 40
PHI(J) = 1.0
40 TEP31 = TEP31 + FL(J)*PHI(J)*Q03(J)*TRAN
J031(J) = TEP31*RDF
LLL = 1
SUBROUTINE CONTAU (TAU,TRAN)

REAL LAT
COMMON /W T/ 4(6). DL,LAT,DEL
IF (TAU.GT.1.E—3) D TO 10
RETURN
10 TRAN = 0.0
IF (TAU.GT.50.0) RETURN
T = -TAU * A(1)
TEST FOR UNDERFLOW
IF (T.LT.100.0) RETURN
TRAN = EXP(T) * 2.0
T = -TAU * A(2)
IF (T.LT.100.0) RETURN
TRAN = TRAN + 2.0 * EXP(T)
T = -TAU * A(3)
IF (T.LT.100.0) RETURN
TRAN = TRAN + 2.0 * EXP(T)
T = -TAU * A(4)
IF (T.LT.100.0) RETURN
TRAN = TRAN + 2.0 * EXP(T)
T = -TAU * A(5)
IF (T.LT.100.0) RETURN
TRAN = TRAN + 2.0 * EXP(T)
T = -TAU * A(6)
IF (T.LT.100.0) RETURN
TRAN = TRAN + 2.0 * EXP(T)
RETURN
END
SUBROUTINE INI(TL,X,Y,II,NEXT)
LOGICAL NEXT

IF(NEXT) GO TO 10
IF (T1.GT.1) GO TO 10
FC0 = 1.0

GO(K) = GO(K) * OM(K) * FC0
O2(K) = 0.2 * DM(K)
H2(K) = 0.5 * DM(K)
CH4(K) = CH4(K) * DM(K)
DCLX(K) = CLX(K) * FCL
CLX(K) = CLX(K) * DM(K) * FCL
H2O(K) = H2O(K) * DM(K) * FM20

N0X(K) = N0X(K) * DM(K)
OH(K) = OH(K) * 1.1
H02(K) = H02(K) * 1.1

10 V(1) = H(K)
Y(2) = DM(K)
Y(3) = H02(K)
V(4) = 0.3(K)
J=0

20 J=J+1
IF(J.GT.10) GO TO 50

TNO = N0(K)
N02 = NO2(K)

THNO3 = HNO3(K)
CALL PCLOX(K)
CALL PNOX(K)
RR(1) = TNO/N02(K)
RR(2) = TNO2/NO2(K)
RR(3) = THNO3/HNO3(K)

DO 25 M=1,3
IF(RR(M).GT.1.005.OR.RR(M).LT.0.995) GO TO 20
25 CONTINUE
RETURN

50 J=J-1
WRITE(6,650) J

650 FORMAT(1H0,5X,*DID NOT CONVERGE IN INITIAL IV,*,13,* TIMES*)
STOP
END

SUBROUTINE PCLOX(K)

COMMON /JVA/ CJO2(50),CJO3(50),CJCWF2(50),CJCWF3(50),JJCCL4(50),
1 CJCH3C(50),CJCL03(50),CJNO2(50),CJNO3(50)
2 CJHO2(50),CJNO3(50),CJCH4(50),CJCF2(50),CJCF3(50),JJCCL4(50),
3 CJCH3C(50),CJCL03(50),CJNO2(50),CJNO3(50)
4 COMMON /MODEL/ ALT(41),TEMP(41),DM(41),DIO(41),DA23(41)
REAL JO2,JO3,JH2O,JN2O5,JHNO3,JCH4,JCF2,
X JCF3,JHCL,JH22,JHOC1
COMMON /PFRA/ JO2(41),JO3(41),JH2O(41),JN2O5(41),JCH4(41),JCF2(41),
X JCF3, JHCL, JH22, JHOC1
REAL JNO3

COMMON /RES/ RATE(65,41),RA(65),RB(65),JN03,PJO3
COMMON /FACT/ FCL,FH20,FCLN03,FNO
REAL NO,N02,N0X,N03,N205

COMMON /SPECIE/ H(41),OH(41),HO2(41),O3(41),O(41),NO(41),
1 ND2(41),N02(41),N03(41),NO(41),CO(41),O2(41),CH4(41),H2O(41),H2(41),
2 CL(41),CLO(41),HCL(41),CLX(41),DCLX(41),N03(41),N205(41),
3 CN03(41)

L = 2*K - 1

RRC1 = (CL/CL)
RRC2 = (HCL/CL)
RRC3 = (RATE(30, L)*CH4(K)+RATE(26, L)*H2(K)+RATE(15, L)*NO2(K)+
1 RATE(27, L)*H2O2(K)+RATE(26, L)*HM(K)+RATE(33, L)*3(K)+JHCL(K))}

000500
RETURN

END

SUBROUTINE SOLVE (K,ALP,Y,N1)

CALL JACOB (K,ALP,Y,N1)

ERR = 0.
DO 20 J = 1,N

B(J,NPI) = PP(J) - SS(J)

ERR = ERR + (B(J,NPI)/SS(J))**2
20 CONTINUE

IF (LINEQN(N)) GO TO 50

DO 55 J = 1,N

Y(J) = Y(J) - B(J,NPI)

55 CONTINUE

100 CONTINUE

XX = 1

XX = XX + N

DO 20 J = 1,N

B(J,NPI) = PP(J) - SS(J)

ERR = ERR + (B(J,NPI)/SS(J))**2
20 CONTINUE

IF (LINEQN(N)) GO TO 50

DO 55 J = 1,N

Y(J) = Y(J) - B(J,NPI)

55 CONTINUE

100 CONTINUE

XX = XX + N

RETURN

END

SUBROUTINE SOLVE (K,ALP,Y,N1)

CALL JACOB (K,ALP,Y,N1)

ERR = 0.
DO 20 J = 1,N

B(J,NPI) = PP(J) - SS(J)

ERR = ERR + (B(J,NPI)/SS(J))**2
20 CONTINUE

IF (LINEQN(N)) GO TO 50

DO 55 J = 1,N

Y(J) = Y(J) - B(J,NPI)

55 CONTINUE

100 CONTINUE

XX = XX + N

RETURN

END

SUBROUTINE SOLVE (K,ALP,Y,N1)

CALL JACOB (K,ALP,Y,N1)

ERR = 0.
DO 20 J = 1,N

B(J,NPI) = PP(J) - SS(J)

ERR = ERR + (B(J,NPI)/SS(J))**2
20 CONTINUE

IF (LINEQN(N)) GO TO 50

DO 55 J = 1,N

Y(J) = Y(J) - B(J,NPI)

55 CONTINUE

100 CONTINUE

XX = XX + N

RETURN

END
CALL PCLOX (K)
CALL PNOX(K)
IF (KK.GE.50) GO TO 145
DO 75 II = 1,50
IF ((YII(YII).LT.0.995) GO TO 5
IF ((YII(YII).GT.1.005) GO TO 5
75 CONTINUE
CALL JACOB (K,ALP,Y,N1)
RETURN
C
145 WRITE (6,151)
151 FORMAT (/N* * KK EQUAL TO 50 - SUBROUTINE SOLVE*/)
RETURN
C
50 WRITE (6,155) K
155 FORMAT (/N* * MATRIX SINGULAR LEVEL = *,I3/,)
KKK = KKK + 1
IF (KKK.GE.3) RETURN
DO 501 J = 1,Y
501 Y(J) = 0.99*Y(J)
GO TO 1
C
101 WRITE (6,157)
157 FORMAT (/N* * DOES NOT CONVERGE - SUBROUTINE SOLVE*/)
RETURN
C
END
C
SUBROUTINE JACOB (K,ALP,Y,N1)
C
CM504 - CHLORINE MODEL STUDY PROGRAM
C
SUBROUTINE JACOB - FORMS JACOBIAN OF CHEMICAL SYSTEM
C
VERSION 4.0 LEVEL 770214
C
E.RX.INC. N. O. SZE; N. TRIPP
C
DIMENSION Y(10)
REAL A
COMMON /MATRIX/ A(20,21)
COMMON /MODEL/ALT(41),TEMP(41),HM(41),DID(41),DA23(41)
COMMON /NETPRO/ PP(4),SS(4)
REAL J02, J03, J120, JN2O, JN2O5, JN2O3, JCH4,
X JCF3, JHCL, JH20, JN02, JN2O, JMN03, JC4H, JCF2,
COMMON /PHRATE/ J02(41),J03(41),JH20(41),JMN03(41),JC4H(41),JCF2(41),JCF3(41),JH20(41)
COMMON /PRATE/ AA(10),BB(10),CC(10),DD(10),EF(10),SG(10),NH(10)
REAL JNO3
 COMMON /RATES/ RATE(65,81),RA(65),RB(65),JN03,PJ03
 REAL NO2,NOX,NO3,N205
 COMMON /SPEC/ H(41),OH(41),O2(41),O2(41),O3(41),O(41),NO(41)
 1 NO2(41),NOX(41),NOX(41),NC0(41),NC0(41),NM02(41),N20(41),H20(41),H2(41),
 2 CL(41),C1O(41),HC(41),CLX(41),CLXX(41),NO3(41),N235(41),
 3 C,NO3(41)
C
L = 2*K - 1
ALP = (J03(1) + PJ03)/RATE(34,1)*O2(K)*OM(41)
REAL (1) = RATE(41)*DID(41)*H2(K) + JM02(K)*H2(K)
REAL (2) = RATE(19,1)*ALP*V(4,4)*V(2)
REAL (3) = RATE(18,1)*V(2)*D(C0(K)
REAL (4) = RATE(21,1)*CH4(K)*Y(2)
REAL (5) = RATE(25,1)*Y(2)*H2(K)
PP(1) = AA(1) + AA(2) + AA(3) + AA(4) + AA(5)
PB(1) = RATE(5,1)*O2(K)*D(PM,K)*V(1)
PB(2) = RATE(5,1)*Y(4)*V(1)
PB(3) = RATE(16,1) + RATE(17,1)*Y(3)*V(1)
9 \( SS_1 = BB_1 + BB_2 + BB_3 \)
10 \( A(1,1) = SS_1/Y(1) \)
11 \( A(1,2) = (AA_2 + AA_3 + AA_4) + AA(5)/Y(2) \)
12 \( A(1,3) = BB_3/Y(3) \)

\[
CC_1 = 2.0*RATE_{2,1}*DID_{K}*H_2O_2(K)
\]

\[
CC_2 = 2.0*RATE_{3,1}*DID_{K}*CH_4(K)
\]

\[
CC_3 = RATE_{10,1}*Y_4*ALP*Y_3
\]

\[
CC_4 = RATE_{11,1}*Y_4*Y_3
\]

\[
CC_5 = RATE_{11,1}*NO_{2}(K)*Y_3
\]

\[
CC_6 = 2.0*JOIN2(K)*H_2O_2(K)
\]

\[
CC_7 = RATE_{5,1}*Y_1*Y_4
\]

\[
CC_8 = JHNO_3(K) * HNO_3(K)
\]

\[
CC_9 = 2.0*JOIN_{17,1}*Y_1*Y_3
\]

\[
CC_{10} = AA(1)
\]

\[
PP_2 = CC_1 + CC_2 + CC_3 + CC_4 + CC_5 + CC_6 + CC_7 + CC_8 + CC_9
\]

\[
1 + CC_{10}
\]

\[
DD_1 = RATE_{7,1}*Y_4*(Y_2)
\]

\[
DD_2 = RATE_{8,1}*H_2O_2(K)*Y_2
\]

\[
DD_3 = RATE_{9,1}*Y_3*Y_2
\]

\[
DD_4 = AA(1)
\]

\[
DD_5 = AA(2)
\]

\[
DD_6 = RATE_{20,1}*HCL(K)*Y_2
\]

\[
DD_7 = RATE_{21,1}*CH_4(K)*Y_2
\]

\[
DD_8 = RATE_{22,1}*NO_{2}(K)*Y_2
\]

\[
DD_9 = RATE_{23,1}*HNO_3(K)*Y_2
\]

\[
DD_10 = 2.0*RATE_{24,1}*Y_2*Y_2
\]

\[
DD_{11} = AA(5)
\]

\[
SS_2 = DD_1 + DD_2 + DD_3 + DD_4 + DD_5 + DD_6 + DD_7 + DD_8 + DD_9 + DD_{10}
\]

\[
1 + DD_{11}
\]

\[
A(2,1) = (CC_1 + CC_2)/Y(1)
\]

\[
A(2,2) = -(SS_2 + DD_{11})/Y(2)
\]

\[
A(2,3) = (CC_3 + CC_4 + CC_5 - DD_{13})/Y(3)
\]

\[
EE_1 = BB_1
\]

\[
EE_2 = DD_1
\]

\[
EE_3 = RATE_{27,1}*CL(K)*H_2O_2(K)
\]

\[
EE_4 = DD_2
\]

\[
PP_3 = EE_1 + EE_2 + EE_3 + EE_4
\]

\[
GG_1 = CC_4
\]

\[
GG_2 = CC_5
\]

\[
GG_3 = CC_6
\]

\[
GG_4 = RATE_{12,1}*CLO(K)*Y_3
\]

\[
GG_5 = RATE_{13,1}*Y_3*Y_3
\]

\[
GG_6 = DD_{13}
\]

\[
GG_7 = RATE_{15,1}*CL(K)*Y_3
\]

\[
GG_8 = BB_3
\]

\[
SS_3 = GG_1 + GG_2 + GG_3 + GG_4 + GG_5 + GG_6 + GG_7 + GG_8
\]

\[
A(3,1) = EE_1 - GG_8(Y_1)
\]

\[
A(3,2) = EE_2 + EE_3 - GG_6(Y_2)
\]

\[
A(3,3) = -(SS_3 + GG_5)/Y(3)
\]

\[
PP_4 = 2.0*JOIN_2(K)*O_2(K)
\]

\[
HH_1 = BB_2
\]

\[
HH_2 = DD_3
\]

\[
HH_3 = CC_4
\]

\[
HH_4 = CC_3
\]

\[
HH_5 = AA(2)
\]

\[
HH_6 = 2.0*RATE_{42,1}*NO_{2}(K)*ALP
\]

\[
HH_7 = 2.0*RATE_{31,1}*CLO(K)*ALP*Y_4
\]

\[
HH_8 = 2.0*AA_{P-RATE_{35,1}*Y_4*Y_4}
\]

\[
SS_4 = HH_1 + HH_2 + HH_3 + HH_4 + HH_5 + HH_6 + HH_7 + HH_8
\]

\[
M_1 = (N_S-L)/2
\]

IF (K_LE_M_1) GO TO 80

\[
T_1 = 2.0*RATE_{42,1}*NO_2(K)
\]

\[
T_2 = RATE_{13,1}*Y_2
\]

\[
T_3 = RATE_{10,1}*Y_3
\]

\[
T_4 = 2.0*RATE_{31,1}*CLO(K)
\]

\[
T_1 = (T_1+T_2+T_3+T_4)*ALP
\]
T5 = RATE(6,L) \times Y(1) 012610
T6 = RATE(7,L) \times Y(2) 012620
T7 = RATE(9,L) \times Y(3) 012630
T8 = 2.0 \times RATE(4,L) \times Y(1) 012640
T9 = T5 + T6 + T7 + T8 012650
81 = T9 + T10 012660
A1 = 2.0 \times RATE(35,L) \times ALP 012670
C1 = P(4) 012680
CALL QUAD(A1,81,C1,XX) 012690
Y(4) = XX 012700
O(C) = ALP \times XX 012710
70 RETURN 012720
80 Y(4) = 03(K) 012730
RETURN 012740
END 012750
SUBROUTINE :FLOW(NI,NTER)

FLOW PROGRAM FOR VARIOUS SPECIES:

SP1 = N2O, SP2 = NOX, SP3 = CH4
SP4 = FC11, SP5 = FC12
SP6 = CCL4, SP7 = CLX, SP8 = J3, SP9 = CCL4, SP10 = CO
TIME-DEPENDENT TERM FOR EACH SPECIES IS DFP
(SHOULD ALL BE SET = 0 FOR STEADY-STATE CASE)
CALL RINTER (NO,XNO)
CALL RINTER (O3,XO3)
CALL RINTER (JCJCL4,XJCCL4)
CALL RINTER (CL,XCL)
CALL RINTER (H2O,XH2O)
IF (RN2O,GT,1.0) QL1 = 0.
IF (RN2O,LE,1.0) QL1 = 1.
CALL CSPEC1(I,0,PPL,QL1,RN2O,PR1,DFP1,XL1;XL1)
DO 1 I = 1,4
1 X1(I) = X(I)
CONV = .FALSE.
IF (RNNO,GT,1.0) QL2 = 0.
IF (RNNO,LE,1.0) QL2 = 1.
K1 = 1
IF (NITER,GT,1) K1 = 2
DO 205 I = 1,4
205 X2(I) = (X2(I) + X(I))/2.
GO TO 206
206 CONTINUE
GO TO 500
2 CONTINUE
IF (RCH4,GT,1.0) QL3 = 0.
IF (RCH4,LE,1.0) QL3 = 1.
CALL CSPEC1(I,0,PPL,QL3,RCH4,PR3,DFP3,XL3;XL3)
DO 3 I = 1,4
3 X3(I) = X(I)
IF (RF12,GT,1.0) QL4 = 0.
IF (RF12,LE,1.0) QL4 = 1.
CALL CSPEC1(I,0,PPL,QL4,RF12,PR4,DFP4,XL4;XL4)
DO 4 I = 1,4
4 X4(I) = X(I)
IF (RCH3C,GT,1.0) QL5 = 0.
IF (RCH3C,LE,1.0) QL5 = 1.
CALL CSPEC1(I,0,PPL,QL5,RCH3C,PR5,DFP5,XL5;XL5)
DO 5 I = 1,4
5 X5(I) = X(I)
IF (RCH3C,GT,1.0) QL6 = 0.
IF (RCH3C,LE,1.0) QL6 = 1.
CALL CSPEC1(I,0,PPL,QL6,RCH3C,PR6,DFP6,XL6;XL6)
DO 6 I = 1,4
6 X6(I) = X(I)
IF (RCH3C,GT,1.0) QL7 = 0.
IF (RCH3C,LE,1.0) QL7 = 1.
CALL CSPEC1(I,0,PPL,QL7,RCH3C,PR7,DFP7,XL7;XL7)
DO 7 I = 1,4
7 X7(I) = X(I)

76
IF (RH2 GT 1.0) QL11 = 0.
IF (RH2 LE 1.0) QL11 = 1.
CALL CSPEC11, 0., PPL, QL11, RH2, PR11, DFP11, XL11, GKL11
DO 11 I = 1, N
11 XI(I) = X(I)
M = N
DO 801 I = 1, N
801 X8(I) = XO3(I)/CDM(I)
CONV = .FALSE.
RUO3 = XO3(M)/CDM(M)
IF (RUO3 GT 1.0) QL6 = 0.
IF (RUO3 LE 1.0) QL6 = 1.
DO 806 KX = 1, 25
CALL CSPEC (O., RUO3, PPL, QL6, RO3, PR8, FP8, XL8, GKL8)
EMAX = 0.
DO 802 I = 1, N
EI = ABS ((X8(I) - X(I))/X(I))
IF (EI GT EMAX) EMAX = EI
802 CONTINUE
IF (EMAX LT 0.01) CONV = .TRUE.
804 DO 805 I = 1, N
805 X8(I) = X(I)
IF (CONV) GO TO 6
805 CONTINUE
GO TO 501
8 CONTINUE
OKPO3 = .FALSE.
CALL REPAM (NI, OKPO3)
IF (OKPO3) GO TO 50
CALL RINTER (CLD, XCLD)
CALL RINTER (NO2, XNO2)
GO TO 600
50 W = W1
CALL SETUP2 (STEPS, M)
M12 = (M1 + 1)/2
DO 100 J = 1, M12
10 XX J = XX(J) + 1
I = 2*J - 1
NOX(J) = X2(I) * CDMM(I)
CH2(J) = X3(I) * CDMM(I)
CLX(J) = X7(I) * CDMM(I)
H2(J) = XI(I) * CDMM(I)
IF (J GT M12) GO TO 100
33(J) = X8(I) * CDMM(I)
100 CONTINUE
RETURN
500 WRITE (6, 600)
600 FORMAT (1H0, * X2 DOES NOT CONVERGE IN 25 ITERATIONS - CFL3WM*)
STJP
501 WRITE (6, 601)
601 FORMAT (1H0, * X8 DOES NOT CONVERGE IN 25 ITERATIONS - CFL3WM*)
STJP
END
SUBROUTINE RINTER (XX, XXX)
DIMENSION XX(50), XXX(81)
DO 10 I = 1, M1
J = 2*I - 1
10 XXX(J) = XX(I)
DO 20 I = 1, M12
J = 2*I
IP1 = I + 1
20 XXX(J) = SORT (XX(I) * XX(IP1))
RETURN
END
IF (KKK.EQ.1) GO TO 10

XJDO = 4.0E-6*EXP((I-61)/7.0)

XL2(I) = 12.0*RATE(46,I)*XJMO/(RATE(46,I) + 21)*COM(I)*X2(I)*XL2T(I)

10 CONTINUE

RETURN

END

SUBROUTINE CXL3 (PR3,DFP3,XL3,N)

COMMON /CHLORX/ XCL(81),

/INTI/ XOM(81),XDID(81),XJN2O(81),XJC3(81),XJCF2(81),

1 XJCH3(81),XJ02(81),XJ03(81),XH02(81),XNO2(81),X03(81)

2, XJCCCL(81),XCL0(81),XNO(81)

COMMON /NDATA/ CKE(81),COM(81),CTEMP(81),CDA(81)

REAL JMO3

COMMON /RATES/ RATE(65,81),RA(65),RB(65),JMO3,PS03

COMMON /SPECOM/ FJ,FJFC,T1

DIMENSION PR3(81),DFP3(81),XL3(81)

DO 10 I = 1,N

PR3(I) = 0.

DFP3(I) = 0.

XL3(I) = (RATE(3,I)*XOM(I)) + RATE(21,I)*XOM(I)) * COM(I)

XL3(I) = XL3(I) + RATE(30,I)*XCL(I)*COM(I)

10 CONTINUE

RETURN

END

SUBROUTINE CXL4 (PR4,DFP4,XL4,N)

COMMON /CHLORX/ XCL(81),

/INTI/ XOM(81),XDID(81),XJN2O(81),XJC3(81),XJCF2(81),

1 XJCH3(81),XJ02(81),XJ03(81),XH02(81),XNO2(81),X03(81)

2, XJCCCL(81),XCL0(81),XNO(81)

COMMON /NDATA/ CKE(81),COM(81),CTEMP(81),CDA(81)

REAL JMO3

COMMON /RATES/ RATE(65,81),RA(65),RB(65),JMO3,PS03

COMMON /SPECOM/ FJ,FJFC,T1

DIMENSION PR4(81),DFP4(81),XL4(81)

DO 10 I = 1,N

PR4(I) = 0.

DFP4(I) = 0.

XL4(I) = (FJ*KJCF2(I) + 1./TL + RATE(47,I)*XOM(I)) * COM(I)

SP4(I) = XL4(I)

10 CONTINUE

RETURN

END

SUBROUTINE CXL5 (PR5,DFP5,XL5,N)

COMMON /CHLORX/ XCL(81),

/INTI/ XOM(81),XDID(81),XJN2O(81),XJC3(81),XJCF2(81),

1 XJCH3(81),XJ02(81),XJ03(81),XH02(81),XNO2(81),X03(81)

2, XJCCCL(81),XCL0(81),XNO(81)

COMMON /NDATA/ CKE(81),COM(81),CTEMP(81),CDA(81)

REAL JMO3

COMMON /RATES/ RATE(65,81),RA(65),RB(65),JMO3,PS03

COMMON /SPECOM/ FJ,FJFC,T1

DIMENSION PR5(81),DFP5(81),XL5(81)

DO 10 I = 1,N

PR5(I) = 0.

DFP5(I) = 0.

XL5(I) = (FJ*KJCF2(I) + 1./TL + RATE(48,I)*XOM(I)) * COM(I)

SP5(I) = XL5(I)

10 CONTINUE

RETURN

END

SUBROUTINE CXL6 (PR6,DFP6,XL6,N)

COMMON /CHLORX/ XCL(81),

/INTI/ XOM(81),XDID(81),XJN2O(81),XJC3(81),XJCF2(81),

1 XJCH3(81),XJ02(81),XJ03(81),XH02(81),XNO2(81),X03(81)

2, XJCCCL(81),XCL0(81),XNO(81)

COMMON /NDATA/ CKE(81),COM(81),CTEMP(81),CDA(81)

REAL JMO3

RETURN

END
COMMON /RATES/ RATE(65, 81),RA(65),RB(65),JN03, PJ03
COMMON /SPECOV/ FJ, FJFC, TL
COMMON /SPLOSS/ SPL(81),SPL4(81),SPL5(81),SPL6(81),SPL9(81)
DIMENSION P6(81),DF6(81),XL6(81)
DO 10 I = 1,N
PR6(I) = 0.
DF6(I) = 0.
XL0(I) = (FJ*XCH3(I) + RATE(I,1)*XCH2(I)) + CD0(I)
SPL6(I) = XL6(I)
10 CONTINUE
RETURN
END

SUBROUTINE CXL7(PR7,DFP7,XL7,N)
COMMON /INT81/ XOH(81),XHID(81),XHINO(81),XJCF(81),XJCFZ(81),
1 XCH3C(81),XJ02(81),XJ03(81),XOH2(81),XNO2(81),XO3(81)
2,XJCL4(81),XCL0(81),XNO(81)
COMMON /NDA1/ CEK(81),CD0(81),CTM8P(81),CDA(81)
COMMON /SPECOV/ FJ,FJFC, TL
COMMON /SPLOSS/ SPL(81),SPL4(81),SPL5(81),SPL6(81),SPL9(81)
COMMON /XESX/ X1(81),X2(81),X3(81),X4(81),X5(81),X6(81),X7(81),
1 X8(81),X9(81),X10(81)
DIMENSION PR7(81),DFP7(81),XL7(81)
DO 10 I = 1,7
XL7(I) = CD0(I)/(7.*8.64E4)
10 CONTINUE
DO 20 I = 8,11
XL7(I) = (CD0(I)/10.*8.64E4)
20 CONTINUE
DO 30 I = 12,81
XL7(I) = 0.0
30 CONTINUE
RETURN
END

COMMON /RATES/ RATE(65, 81),RA(65),RB(65),JN03, PJ03
COMMON /SFACT/ FCL,FM20,FCLNOS,NO
COMMON /XESX/ X1(81),X2(81),X3(81),X4(81),X5(81),X6(81),X7(81),
1 X8(81),X9(81),X10(81)
DIMENSION PR3(81),DFF6(81),XL0(81),XX(81)
DO 10 I = 1,N
ALP = (XJ03(I) + PJ03)/((RATE(34,1)*2.1*CD0(I))**2)
XX(I) = XCL0(I) + ALP
XR = RATE(6,1)*XNO2(I)
XL = RATE(7,1)*XCM(I)
KL = 2.0*RATE(42,1)*XNO2(I) + ALP
KO = RATE(10,1)*XNO3(I)*ALP
KL = RATE(11,1)*XNO4(I)*ALP
KL = RATE(12,1)*XNO5(I)*ALP
KL = RATE(13,1)*XNO6(I)*ALP
10 CONTINUE
RETURN
END
COMMON /INT5/ XOM(81),XID(61),XJM20(81),XJC3(81),XJC3(81),XK02(91),XNO2(81),XO3(81)
1 XJ3C(81),XJ02(81),XJO3(81),XK02(91),XNO2(81),XO3(81)
2,XJ3C(81),XCLD(81),XNO(81)
COMMON /NODATA/ CEK(81),COM(81),CTEMP(81),CODA(81)
COMMON /SPECW/ FJ,FJFC,TL
COMMON /SPLOSS/ SPL1(81),SPL4(81),SPL5(81),SPL6(81),SPL9(81)
DIMENSION P29(81),DFP9(81),XL9(81)
DO 10 I = 1,N
10 PR9(I) = 0.
DFP9(I) = 0.
XL9(I) = FJ*XJ3C(I)*COM(I)
SPL9(I) = XL9(I)
10 CONTINUE
RETURN
END

SUBROUTINE CX.II (PR1,DFPI,XXLI,N)
COMMON /CHLOR/ XLCL(81)
COMMON /INT5/ XOM(81),XID(61),XJM20(81),XJC3(81),XJC3(81),XK02(91),XNO2(81),XO3(81)
1 XJ3C(81),XJ02(81),XJO3(81),XK02(91),XNO2(81),XO3(81)
2,XJ3C(81),XCLD(81),XNO(81)
COMMON /MOL4/ XM(81),XH20(81),PH2O,RH2,XXLI(81)
COMMON /NODATA/ CEK(81),COM(81),CTEMP(81),CODA(81)
REAL JNO3
COMMON /RATES/ RATE(65,81),RA(65),RB(81),JNO3,JPO3
COMMON /SPECW/ FJ,FJFC,TL
DIMENSION P21(81),DFP11(81),XXLI(81)
DO 10 I = 1,N
XXLI(I) = RATE(I)*XM(I)*XH20(I)*RATE(2)*XK02(I)*PM20
XL1(I) = (RATE(26,I)*XXLI(I) + RATE(25,I)*XM(I))
10 CONTINUE
RETURN
END

SUBROUTINE COEF (PR,XXL,DFP)
COMMON /COEF/ AA(81),UB(81),CC(81),DL(81),DJ(81),U8(81)
COMMON /COEF2/ A(81),B(81),C(81),F(81),X(81)
COMMON /NODATA/ CEK(81),COM(81),CTEMP(81),CODA(81)
COMMON /PARAV/ STEP,QOU,PL,PPU,PPN,N
COMMON /TFCTR/ FH,FB,FM
REAL PR(81),X(81),DFP81(81),T(81),DD(81),DDK(81),D8(81)
TF (FH, EQ. 1.) GO TO 5
DO 21 I = 1,4
21 DFP(I) = 0.
5 D21.0E05
DT=3.5576*STEP
AA(1) = 2.0*CFK1(I)*COM(I)
TT = AA(1)/J1(I)
NML=N-1
DO 10 I = 1,N
10 Y(I) = 0.5*XXL(I)*DT/COM(I)
DO 50 I = 2,NM1
S(I) = PR(I)*DT/COM(I)
50 DD(I) = -(FT + TT*U1(I)*AA(I(I)))/S(I)
DO(I) = -(FT/TT + T/TT + 1.0)*FA
DO(I) = -(FT/TT + T/TT + 1.0)*FA
DO(I) = -(FT/TT + T/TT + 1.0)*FA
END


C FLUX AT TOP, SPECIFIED MIXING RATIO AT BOTTOM

60 S(1) = RL(1)

DD(1) = 5*FA
DU(1) = 0*FA


F(j) = DDR(j)*DPP(j) + DU(j)*DPP(j) + S(j)

GO TO 70

C FLUX SPECIFIED AT TOP

70 IF (ABS(QU) .LE. 1.E-60) GO TO 71

IF (ABS(PU) .LE. 1.E-60) GO TO 72

S(N) = 0

DD(N) = (1+QU)*DFA
DL(N) = -1*FA

DD(N) = -DD(N)*FB

GO TO 73

C MIXING RATIO SPECIFIED AT TOP

72 S(N) = 2*S2*RU*DZ/P

DD(N) = 0.5*FA

DL(N) = 0

DD(1) = 5*FA

73 DD(N) = 0.5*FA

GO TO 73

C SUBROUTINE TRIDIA (N)

COMMON /C0E2/A(81),B(81),C(81),F(51),X(81)

REAL ALPNA(81),GAMMA(61),G(81)

IF (A(N) .EQ. 0.0) GO TO 100

ALPHA(1) = C(1)

GAMMA(1) = D(1)*DFP(1)

DO 10 I = 1, N

10 X(N) = G(N)

RETURN

END

C SUBROUTINE TRIDIA TO COMPUTE MIXING RATIO

COMMON /COEF/A(81),B(81),C(81),F(51),X(81)

REAL ALPNA(81),GAMMA(81),G(81)

IF (A(1) .EQ. 0.0) GO TO 100

ALPHA(1) = A(1)

GAMMA(1) = C(1)/ALPHA(1)

N1 = N-1

DO 10 I = 1, N1

IF (ALPHA(I) .EQ. 0.0) GO TO 100

GAMMA(I) = C(I)/ALPHA(I)

XI(I) = 1

10 ALPHA(IP1) = A(IP1) - B(IP1)*GAMMA(I)

G(I) = F(I)/ALPHA(I)

DO 30 I = 2, N

30 G(I) = (F(I) - B(I)*G(I-1))/ALPHA(I)

X(N) = G(N)

DO 40 I = 1, N1

J = I + 1

40 X(J) = G(J) - GAMMA(J)*X(J-1)

GO TO 101

100 WRITE (6,105) I
1 0 5 FORMAT (/, 2 *, 'SINGULAR MATRIX - I = ', I 3 /) 017860
101 RETURN 017870
END
SUBROUTINE RCPN (N1, OKPO3) 017890
LOGICAL OKPO3 017890
COMMON /JVAL/ CJ02(50), CJ03(50), CJCF2(50), CJCF3(50), CJCL4(50), 017920
1 CJCh3C(50), CJCL03(50), CJNO2(50), CJNO3(50) 017940
2 CJM202(50), CJ031(50), CJSN05(50) 017950
COMMON /MODEL/ ALT(41), TEMP(41), DN(41), D10(41), DA23(41) 017970
REAL JMO3 017980
COMMON /RATES/ RATE(65, 81), RA(65), RB(65), JN03, PJO3 018000
REAL NO, NO2, NO3, N205 018020
COMMON /SPECIF/ H(41), OH(41), HO'(41), 112O2(41), O3(41), 3(41), 018040
2 CL(41), CL02(41), N03(41) 018060
CLNO3(41) 018070
COMMON /XXES/ X1(81), X2(81), X3(81), X6(81), X7(81), X8(81), 018090
1 X9(81) 018100
REAL CL01(41), N021(41) 018110
411 = (N1 - 1)/2 018120
E1MAX = 0. 018130
E2MAX = 0. 018140
DO 10 I = 1, N11 018150
L = 2*I - 1 018160
CLO1(I) = CLO1(I) 018170
NO21(I) = NO21(I) 018180
ALP = (CJO3(I) + PJO3)/ (RATE(34, L) * 21 * DM(I))**2 018190
D31(I) = X6(2*I - 1) * DM(I) 018200
031(I) = ALP * 031(I) 018210
CLX(I) = X7(I)*DM(I) 018220
NOX(I) = X2(I)*DM(I) 018230
CALL PNOX(I) 018240
CALL PCL0X(I) 018250
E1 = ABS((CLO1(I) - CLO1(I))/CLO1(I)) 018260
IF (E1 .GT. E1MAX) E1MAX = E1 018270
E2 = ABS((NO21(I) - NO21(I))/NO21(I)) 018280
IF (E2 .GT. E2MAX) E2MAX = E2 018290
CLO1(I) = (CLO1(I) + CLO1(I))/2. 018300
NO21(I) = (NO21(I) + NO21(I))/2. 018310
10 CONTINUE 018320
IF (E1MAX .LT. 0.01 AND E2MAX .LT. 0.10) OKPO3 = .TRUE. 018330
RETURN 018340
END 018350
SUBROUTINE O3LINT (X, Y, IL, IU) 018370
DIMENSION X(9, 41), Y(9) 018380
IF (IU .LE. LE(4)) GO TO 5 018390
WRITE (6, 800) IU 018400
600 FORMAT (11H0, * IN SUBROUTINE O3LINT, IU = **, IU** - TOO HIGH FOR INTE18350
183600
183700
183800
183900
184000
83 STOP 018410
5 DO 10 I = 1, 3 018420
Y(I) = 0. 018430
DO 10 J = IL, IU 018440
10 Y(I) = Y(I) + (X(I, J) + X(I, J+1))*1.E5 018450
RETURN 018460
END 018470
SUBROUTINE PRMTX (I, LLL, LLU) 018490
COMMON /INDEX/ D80SINT(41), DMINT(41), DAINt(41) 018500
COMMON /JVAL/ CJ02(50), CJ03(50), CJCF2(50), CJCF3(50), CJCL4(50), 018510
1 CJCh3C(50), CJCL03(50), CJNO2(50), CJNO3(50) 018530
2 CJM202(50), CJ031(50), CJSN05(50) 018540
COMMON /MODEL/ ALT(41), TEMP(41), DN(41), D10(41), DA23(41) 018550
N1 = (N1 - 1)/2 018560
E1MAX = 0. 018570
E2MAX = 0. 018580
DO 10 I = 1, N11 018590
L = 2*I - 1 018600
CLO1(I) = CLO1(I) 018610
NO21(I) = NO21(I) 018620
ALP = (CJO3(I) + PJO3)/ (RATE(34, L) * 21 * DM(I))**2 018630
D31(I) = X6(2*I - 1) * DM(I) 018640
031(I) = ALP * 031(I) 018650
CLX(I) = X7(I)*DM(I) 018660
NOX(I) = X2(I)*DM(I) 018670
CALL PNOX(I) 018680
CALL PCL0X(I) 018690
E1 = ABS((CLO1(I) - CLO1(I))/CLO1(I)) 018700
IF (E1 .GT. E1MAX) E1MAX = E1 018710
E2 = ABS((NO21(I) - NO21(I))/NO21(I)) 018720
IF (E2 .GT. E2MAX) E2MAX = E2 018730
CLO1(I) = (CLO1(I) + CLO1(I))/2. 018740
NO21(I) = (NO21(I) + NO21(I))/2. 018750
10 CONTINUE 018760
IF (E1MAX .LT. 0.01 AND E2MAX .LT. 0.10) OKPO3 = .TRUE. 018770
RETURN 018780
END 018790
SUBROUTINE O3LINT (X, Y, IL, IU) 018800
DIMENSION X(9, 41), Y(9) 018810
IF (IU .LE. LE(4)) GO TO 5 018820
WRITE (6, 800) IU 018830
600 FORMAT (11H0, * IN SUBROUTINE O3LINT, IU = **, IU** - TOO HIGH FOR INTE18840
188500
188600
188700
188800
188900
83 STOP 018900
5 DO 10 I = 1, 3 018910
Y(I) = 0. 018920
DO 10 J = IL, IU 018930
10 Y(I) = Y(I) + (X(I, J) + X(I, J+1))*1.E5 018940
RETURN 018950
END 018960
SUBROUTINE PRMTX (I, LLL, LLU) 018970
COMMON /INDEX/ D80SINT(41), DMINT(41), DAINt(41) 018980
COMMON /JVAL/ CJ02(50), CJ03(50), CJCF2(50), CJCF3(50), CJCL4(50), 018990
1 CJCh3C(50), CJCL03(50), CJNO2(50), CJNO3(50) 019010
2 CJM202(50), CJ031(50), CJSN05(50) 019020
COMMON /MODEL/ ALT(41), TEMP(41), DN(41), D10(41), DA23(41) 019030

CALL PRINT9 (*1,X?,X3,X 5.,X5,X6,*7,X9,Xj1,NN2O ,5.N143*,4IIC45. ,FLX,HCCL5.,5.P4 H? )
CALL TRAP (ELI, FN ?O ,1,e1)
CALL TRAP (XL2, FP 1OX, 1,81)
CALL TRAP (XL3,FCHI ,1,81)
CALL TRAP (XL5,FCH3C,1,81)
CALL TRAP (XL7,FCLX,1,81)
CALL TRAP (XL9,FCL4,1,81)
CALL TRAP (XLS ,FCHI ,1,81)
CALL TRAP (XLS, FCH 3C,1,ej)
CALL TRAP (XL T,FCLX,1,61)
CALL TRAP (XL9,FCL4.,I,5j)
CALL TRAP (XLII,F112,1,6I)
WRITE (6,70) FN2O,FNOX ,FCH 4,FFII,FFI2,FCH 3C, FCLX, FC L1.,F92
J = 2*J - 1
C4(J) = X4(K) * CD M(K)
C5(J) = X5(K) * CD M(K)
C6(J) = X6(K) * CD M(K)
C9(J) = X9(K) * CD M(K)
C1(J) = X1(K) * CD M(K)
M8(J) = Q3(J)/DM(J)
100 CONTINUE
CALL PAGE
WRITE (6,611) (K,ALT(K),M8(K),C4(K),C5(K),C6(K),C9(K),
1 CLX(K),K=LLL,LLL)
CALL PAGE
WRITE (6,611?) (K,ALT(K), C1(K),40 X(K),CM 4(K),
1 RETURN
70 FORMAT (1H0,3X,*FN2O =",1PE13.5,4X,*FNOX =",E13.5,4X,
1 *FC4K =",E13.5,4X,*FFII =",E13.5,4X,*FFI2 =",E13.5,4X,
1 *FCLX =",E13.5,4X,*FCL4 =",E13.5,4X,
1 3 X*FM2 =",E13.5)
601 FORMAT (1H0,5X,*LAST ITERATION =",I3 // SX,*ALT",6X,"CJ32", 7X,
1 C J03*, 6X,*CJGF2*, 6X,*CJCF3*, 6X,*CJ031*, 5X,*PREVJ3", 5X,
1 2 *DO3INT*,5X,*DMINT*,6X,*PREV0*//)
602 FORMAT (1H0,5X,*LAST ITERATION =",I3 // SX, *ALT",6X,"CJ32", 7X,
1 C J03*, 6X,*CJGF2*, 6X,*CJCF3*, 6X,*CJ031*, 5X,*PREVJ3", 5X,
1 2 *DO3INT*,5X,*DMINT*,6X,*PREV0*//)
603 FORMAT (1H0,5X,*LAST ITERATION =",I3 // SX, *ALT",6X,"CJ32", 7X,
1 C J03*, 6X,*CJGF2*, 6X,*CJCF3*, 6X,*CJ031*, 5X,*PREVJ3", 5X,
1 2 *DO3INT*,5X,*DMINT*,6X,*PREV0*//)
604 FORMAT (1H0,5X,*LAST ITERATION =",I3 // SX, *ALT",6X,"CJ32", 7X,
1 C J03*, 6X,*CJGF2*, 6X,*CJCF3*, 6X,*CJ031*, 5X,*PREVJ3", 5X,
1 2 *DO3INT*,5X,*DMINT*,6X,*PREV0*//)
605 FORMAT (1H0,5X,*LAST ITERATION =",I3 // SX, *ALT",6X,"CJ32", 7X,
1 C J03*, 6X,*CJGF2*, 6X,*CJCF3*, 6X,*CJ031*, 5X,*PREVJ3", 5X,
1 2 *DO3INT*,5X,*DMINT*,6X,*PREV0*//)
615 FORMAT (1H0,12,0PF11.0,1P9E13.4)  019970
616 FORMAT (1H0,2X,3K7,4X,2ALT,5X,H2O + HO,6X,H2O + OH,7X,5K9)  019950
1 C=H + O2,5X,HNO3 + HO,8X,H2O + CO + OH,9X,KOH + NO + H2O,10X,5K9  019930
2 JH02 = H2O2,5X,2CL + CH4/*)  019900
617 FORMAT (1H0,13,0PF11.0,1P9E13,4)  019970
618 FORMAT (1H0,2X,3K7,4X,2ALT,5X,H2O2 + OH2,6X,H2O2 + OH,7X,5K9)  019950
1 C=O + OH,5X,C=H + OH,5X,KOH + OH2,6X,KOH + HO,7X,5K9  019930
2 JH02 = H2O2,5X,2CL + CH4/*)  019900
714 FORMAT (1H0,* INTEGRATED LOSS FOR OZONE*)  019950
715 FORMAT (1H0,13,0PF11.0,1P9E13,4)  019970
1601 FORMAT (1H0,5X,*LAST ITERATION + 1* // 5X,*ALT,6X,*CJ02*, 7X)  019970
1 C=O3*, 5X,*CJC3F2*, 6X,*CJCF3*, 5X,*CJ03*, 5X,*PREV03*, 5X  019950
2 *DO3INT*, 5X,*DOINT*, 6X,*PREV0H/*)  019930
1603 FORMAT (1H0,5X,*LAST ITERATION + 1* // 5X,*ALT,6X,*CJ02*, 7X)  020000
1 C=O3*, 5X,*CJC3*, 5X,*CJ02*, 5X,*CJCF3*, 5X,*CJC3L*/))  020020
END

SUBROUTINE TRAP (XX,XXX,N1,N2)  020040
DIMENSION XX(31)  020050
XXX = (XX(N1) + XX(N2)) * .5  020060
N1P2 = N1 + 1  020070
N2M2 = N2 - 1  020080
DO 10 I = N1P2,N2M2  020090
10 XXX = XXX + XX(I)  021000
XXX = XXX*1.0E5  021010
RETURN  021020
END

SUBROUTINE PRINT9 (X1,X2,X3,X4,X5,X6,X7,X8,X9,H01,H02,H03,H04,H05)  021030
DIMENSION X1(91),X2(91),X3(91),X4(91),X5(91),X6(91),X7(91),X8(91),X9(91)  021040
COMMON /MODEL/ALT(41),TEMP(41),JMK(41),IDC(41),DA2A(41)  021050
600 FORMAT (1H0,6X,'ALT',2X,9(6X,A4,3X)/)  021060
601 FORMAT (1H0,6X,*NIXING RATIOS*) /*)  021070
603 FORMAT (1H0,5X,*MIXING RATIOS*/))  021080
CALL PAGE  021090
WRITE (6,603)KEY,IC,IFORM,TITLE,JF  021100
50 (0 FORMAT (3A4,13,2X,1A24))  021110
IF (EOF(5))800,I5  021120
1 IC'—IC  021130
READ IC  021140
CALL LINES (1.),RETURNS(25)  021150
WRITE (6,6035)IC,TITLE(021160
IF (JF.NE.BLANK) CALL LINE(IC,.TRUE.)  021170
RE W IC  021180
IF (EOF(IC))800,50  021190
49 IC'S  022100
REAL NAME  022110
INTEGER KEYS(4),TITLE(13),KEYW(3),KEY(3),BLANK  022120
DATA KEY/*HPARA,4HGOM4,HHCMP4,HENDJ4,H9993*/BLANK/14/*  022130
X NAME/*HINPUT/*  022140
10 READ(5,5010)KEY,IC,IFORM,TITLE,JF  022150
5010 FORMAT(3A4,13,9,2X,1A24,2A2)  022160
IF(EOF(5))800,15  022170
15 IF(10)20,49,22  022180
20 IC=IC  022190
RE MIND IC  022200
22 CALL PAGE  022210
C ALL LINES(1.),RETURNS(25)  022220
25 WRITE(6,6025)IC,TITLE  022230
6025 FORMAT(1T21,*TAPE*12,T31,*LABEL*12A4,2A2//)  022240
IF(JF.WE.BLANK) CALL LINE(IC,.TRUE.)  022250
READ IC,5010)KEY,IC,IFORM,TITLE,JF  022260
IF(EOF(IC))800,50  022270
86
50 DO 60 K=1.5
  IF(KEY(I).EQ.KEY(K)) GO TO (100,200,10,400,10),K
60 CONTINUE
  DO 80 K=1,4
  IF(KEY(I).EQ.KEYS(K)) GO TO 90
80 CONTINUE
  CALL ERRX(80,NAME)
90 IF(I(EC).EQ.5) CALL PAGE
  WRITE(6,6090) KEY,TITLE,IC
6090 FORMAT(*2,J3,4A,21,12A,A2,TB1,*UNIT *,12,)*/)
  CALL LINES(I3),RETURNS(95)
95 RETURN
100 CALL IMPARM
  GO TO 10
200 CALL LINES(IC,TRUE.)
  GO TO 10
800 CALL ERRM(800,NAME),RETURNS(400)
100 RETURN

END

SUBROUTINE PAGE
C
C VERSION 1.0 LEVEL 71112

REAL TITLE(6)
COMON /H(AD/ TITLE,ICODE,VERS,LEVEL,DAT,IRUN,NPAGE,NLOG)
COMMON/LXNM/LINE
C
LINE=4
NPA=NPAGE+1
WRITE (6,2030) ICODE,IRUN,TITLE,VERS,LEVEL,DAT, NPAGE;
2030 FORMAT(*1*,I3,16,5X,6A8,* VERSION *,F5.1,* (*16*)*,11X,
X A10,10X,*PAGE *,I3/1X,127(*-*)
  RETURN

END

SUBROUTINE LINES(N),RETURNS(A)
C
C VERSION 1.0 LEVEL 760921

REAL TITLE(6)
INTEGER ICODE,IRUN,NPAGE
COMON /HEAD/ TITLE,ICODE,VERS,LEVEL,DAT,IRUN,NPAGE,NLOG
COMMON/LXNM/LINE
C
LINE=LINE+N
IF(LINE.LT.~C1) RETURN
  LINE=LINE+1
  NPA=NPAGE+1
  WRITE (6,2030) ICODE,IRUN,TITLE,VERS,LEVEL,DAT, NPAGE;
2030 FORMAT(*1*,I3,16,5X,6A8,* VERSION *,F5.1,* (*16*)*,11X,
X A10,10X,*PAGE *,I3/1X,127(*-*)
  RETURN

END

SUBROUTINE IMPARM
C
C VERSION 1.0 LEVEL 720602

READS AND PRINTS COMMENTS CARDS
C
REAL NAME
LOGICAL PRINT
INTEGER IFORM,IF(I),COM(I),BLANK
DATA IF/1H,1,1H/,NAME,COM,1H/
10 READ(IC,5010) IFORM,COM,IF

87
5010 FORMAT(14X,A15X,12A4,A2,A2)
IF(.NOT.PRINT) GO TO 50
DO 20 I=1,3
IF(I.EQ.IF(I)) GO TO (30,30,40),I
20 CONTINUE
CALL ERRX(20, NAME)
CALL LINES(I),RETURNS(32)
WRITE(6,6032) IF(I),CON
GO TO 50
40 CALL PAGE
I=2
GO TO 30
50 IF(JF.NE.BLANK) GO TO 10
RETURN
END
SUBROUTINE JAY
**************************************************************************
VERSION 1.0 LEVEL 760921
**************************************************************************
REAL TITLE(S) COMMON /HEAD/ TITLE,ICODE,VERS,EVEL,DAT,NPAGE,LOG
**************************************************************************
DAT = DATE(3)
**************************************************************************
RETURN
END
SUBROUTINE ERRX(N,NAME)
INTEGER N REAL NAME
WRITE(6,6000) N,NAME
FORMAT('EXECUTION TERMINATED DUE TO ERROR NO. *16* IN *48')
END
SUBROUTINE ERRM(N,NAME)
INTEGER N REAL NAME
WRITE(6,6100) N,NAME
FORMAT('ERROR NO. *16* IN *48')
END
SUBROUTINE JSCATT
**************************************************************************
CHLORINE MODEL STUDY PROGRAM
**************************************************************************
SUBROUTINE JSCATT COMPUTES AEROSOL AND MOLECULAR EXTINCTION
COEFFICIENTS
2RAY(J) = RAYLEIGH SCATTERING COEFFICIENT
QAE(J) = AEROSOL EXTINCTION COEFFICIENT
QAA(J) = AEROSOL ABSORPTION COEFFICIENT
SIZE DISTRIBUTION PARAMETER ISIZE= 1 (RURAL) FROM SELBY ET AL
2 (MARITIME) 1976
3 (URBAN)
4 (TROPOSPHERE)
5 (SPECIAL)
TO INPUT SPECIAL MODEL DIMENSION ALAM(A) AND QE(S),QA(S)
**************************************************************************
C 4= 0 OF WAVELENGTH INTERVALS AEROSOL DATA DIGITIZE) 021550
C ALAM= ARRAY OF WAVELENGTH VALUES CORRESPONDING TO DIGITIZATION 021550
COMMON /SOLV/AR/GRAY(100),QAE(100),QAA(100) 021550
COMMON /SOLCON/ML(100),FL(100),202(100),Q03(100) 021590
COMMON /PARM/ ISWIT,TSTEP,TSTOP,TLOOP,TPRNT,ISTIZE,ISCAT 021590
DIMENSION ALA4(4),QE(5,6),QA(5,3) 021630
DATA ALA4/200.,250.,300.,400.,480.,550.,694.,860./ 021630
DATA IL,IL,N/1,99,77 021630
C SPECIFY AEROSOL MODEL 021650
GO TO (1,2,3,4,5)ISIZE 021650
C RURAL 021670
1 QE(1,1)= .38223 021690
QE(1,2)= .32979 021690
QE(1,3)= .28540 021690
QE(1,4)= .20266 021690
QE(1,5)= .17998 021690
QE(1,6)= .14880 021690
QE(1,7)= .12064 021690
QE(1,8)= .09151 021690
QA(1,1)= .07345 021690
QA(1,2)= .0661 021690
QA(1,3)= .06210 021690
QA(1,4)= .01317 021690
QA(1,5)= .01114 021690
QA(1,6)= .01095 021690
QA(1,7)= .01066 021690
QA(1,8)= .01066 021690
GO TO 20 021690
C MARITIME 021710
2 QE(2,1)= .20332 021730
QE(2,2)= .19518 021730
QE(2,3)= .18179 021730
QE(2,4)= .17032 021730
QE(2,5)= .16213 021730
QE(2,6)= .15412 021730
QE(2,7)= .1456 021730
QE(2,8)= .1365 021730
QA(2,1)= .09456 021730
QA(2,2)= .00864 021730
QA(2,3)= .00442 021730
QA(2,4)= .00243 021730
QA(2,5)= .00193 021730
QA(2,6)= .00186 021730
QA(2,7)= .00155 021730
QA(2,8)= .00171 021730
GO TO 20 021730
C JRBAN 021750
3 QE(3,1)= .31030 021770
QE(3,2)= .29416 021770
QE(3,3)= .28005 021770
QE(3,4)= .26604 021770
QE(3,5)= .25211 021770
QE(3,6)= .23828 021770
QE(3,7)= .22535 021770
QE(3,8)= .21242 021770
QA(3,1)= .1092 021770
QA(3,2)= .08649 021770
QA(3,3)= .07571 021770
QA(3,4)= .06376 021770
QA(3,5)= .05474 021770
QA(3,6)= .04882 021770
QA(3,7)= .04386 021770
QA(3,8)= .04022 021770
GO TO 20 021770

**TROPOSPHERE**

```
1. OE(5, 0) = 10272
1. OE(4, 2) = 85505
1. OE(4, 3) = 29674
1. OE(4, 0) = 25565
1. OE(4, 1) = 18187
1. OE(4, 6) = 15600
1. OE(4, 7) = 11722
1. OE(4, 8) = 98537
1. QA(4, 1) = 98042
1. QA(4, 2) = 131761
1. QA(4, 3) = 91767
1. QA(4, 4) = 90371
1. QA(4, 5) = 90772
1. QA(4, 6) = 88745
1. QA(4, 7) = 88519
1. QA(4, 8) = 88683
GO TO 20
```

5 CONTINUE

```
3. INPUT SPECIAL MODEL

20 DO 40 J = 1, IU
WL ( J ) = WL ( J ) / 1.0E4
QRAY ( J ) = (9.307E-20)*(1.0E4/WLMIC)**4.0117
QRAY ( J ) = QRAY ( J )*1.0E-5
IF(WLMIC<LT.0.2)GO TO 35
DO 30 K = 1, N
KPI = K + 1
IF(WLMIC<GE.2.0)GO TO 31
30 CONTINUE
```

```
31 XD = WLMIC-ALAM ( K )
QAE(J) = (QE(ISIZE,KPI)-QE(ISIZE,K))**K/(ALAM(KPI)-ALAM(K)) +
1*OE(ISIZE,K)
QAE(J) = QAE(J)*1.0E-5
QA(J) = (QA(ISIZE,KPI)-QA(ISIZE,K))**K/(ALAM(KPI)-ALAM(K)) +
1*OE(ISIZE,K)
QA(J) = QA(J)*1.0E-5
GO TO 40
35 QAE(J) = 0.0
QA(J) = 0.0
40 CONTINUE
```

```
WRITE(6,101)ISIZE
101 FORMAT(5, AEROSOL MODEL = "", I4)
WRITE(6,105)
105 FORMAT(3X,*,P,11X,*8X,QRAY(J),*9X*,QAE(J),*9X*,QA(J))
DO 50 J = 1, IU
WRITE(6,102)J, WL ( J ), QRAY ( J ), QAE ( J ), QA ( J )
50 CONTINUE
```

```
RETURN
```

```
END
```

```
SUBROUTINE OMEGA(NX, IL, IU, GMU)

**SUBROUTINE OMEGA COMPUTES SINGLE SCATTERING ALBEDO PROFILE AND OPTICAL DEPTH AS A FUNCTION OF ALTITUDE FOR INPUT TO VM.**

MEAN INTENSITY RETURNED AS A FUNCTION OF TAJ REINTERPOLATED FOR ALTITUDE LEVELS.
```

```
COMMON /SCAPAR/ QRAY(100), QAE(100), QA(100)
COMMON /SOLCOV/WL(100), FL(100), J02(100), Q03(100)
COMMON /INTDEN/DO3INT(41), DMIN(41), D1INT(41)
COMMON /MODEL/ALT(41), TEMP(41), DM(41), D2O(41), DA23(41)
```

```
```

90
COMMON/SPCIE/H(41),OH(41),HO2(41),H2O2(41),O3(41),I(41),N(41), 023170
1 NO2(41),NO3(41),NOX(41),CO(41),O2(41),CH4(41),H2O(41),H2(41), 023180
2 Cl(41),ClO(41),NCl(41),ClX(41),OClX(41),NO3(41),N25(41), 023190
3 ClNO3(41), 023200

COMMON/VRP/TAUZ(41,100),OMEGAZ(41,100),TAU(41),OMEGAT(41) 023210
COMMON/SCA/TAUINT(100),E(41,100),FAV(41,100),FLUX(41) 023220
COMMON/PARAMU,N,II,NN,NNP,REF 023230
DIMENSION IN(100),INN(100),II(41) 023240

COI

COMPUTE OPTICAL DEPTH AND ALBEDO AS A FUNCTION OF
WAVELENGTH FOR EACH LEVEL
POZ=0.21 023250
J0=GMEU 023260
DO 20 I=1,NT 023270
  DO 10 J=1,II,IIU 023280
  TAUZ(I,J)=QQ(J)*DOINT(I)+QQ(J)*P02*OMINT(I)+GRAY(J)*OMINT(I) 023290
  1 /OM1(I)+QAE(J)*OMINT(I)/DA23(I) 023300
  GAMSCA=GRAY(J)*OM1(I)/OM1(I)+QAE(J)-QAA(J)*DA23(I)/DA23(I) 023310
  GAMEXT=QAE(J)*DA23(I)/DA23(I)+GRAY(J)*OM1(I)/OM1(I)+QQ(J)* 023320
  1 O3(I)+QQ(J)*P02*OM1(I)
  OMEGAZ(I,J)=GAMSCA/GAMEXT 023330
  IF(I.NE.NT)1O=3 023340
  TAU=TAUZ(I,J) 023350
  N=NT=5+1.5 023360
  IF(N.GT.3)N=3 023370
  IF(N.GT.21)N=21 023380
  IN(J)=N 023390
  NN=(N-1)*2 023400
  IF(TZ.LE.1.)NN=10 023410
  IF(TZ.GT.1. AND TZ.LE.3.)NN=(N-1)*5 023420
  IF(TZ.GT.3. AND TZ.LE.5.)NN=(N-1)*3 023430
  INN(J)=NN 023440
  TAUINT(J)=TZ/NN 023450
10 CONTINUE 023460
20 CONTINUE 023470
C COMPUTE SINGLE SCATTERING ALBEDO VS TAU AT EQUAL TAU INTERVALS 023480
DO 50 J=1,IIU 023490
  NN=INN(J) 023500
  NNP=NN+1 023510
  IM(I)=1 023520
  II(NNP)=NN 023530
  TAU(1)=TAUZ(1,J) 023540
  TAU(NNP)=0.0 023550
  OMEGAT(1)=OMEGAZ(1,J) 023560
  OMEGAT(NNP)=OMEGAZ(NN,J) 023570
  DO 40 K=2,NN 023580
  KK=NNP-K 023590
  TAU(K)=TAUINT(J)*KK 023600
  DO 30 I=1,NT 023610
  IM(I)=1 023620
  DELTAU=TAU(K)-TAUZ(I,J) 023630
  IF(DELTAU).GE.0.0 GO TO 75 023640
  30 CONTINUE 023650
  DO 50 J=1,IIU 023660
  50 CONTINUE 023670
  IF(TZ.GT.32. AND TZ.LE.55)GO TO 85 023680
  85 CONTINUE 023690
DO 86 I=1,Nr
FR=0.
IFI(-TAU(Z(I,J))/GMU,I,J,-70.)GO TO 87
FR=GMU*EXP(-TAU(Z(I,J)))*EXP(-TAU(I,J))/FR
IFI(I,J)=FR
IFI(-TAU(Z(I,J))/GMU,I,J,-70.)GO TO 86
87 CONTINUE
GO TO 50
88 CALL VIM
C CONVERT FLUX FROM TAU TO 2 LEVELS FOR COMPJ
F(I,J)=FLUX(I,J)
DO 70 K=2,N
IK=II(K)
IKU=II(K+1)
IFI(IKU,EQ.IK)GO TO 70
IFI(IKU,EQ.IKU)GO TO 70
DO 60 I=IKL,IKU
KPI=K+1
TAUEXP=TAU(K)-TAU(I,J)
TAUEXP=TAUEXP/TAUINT(J)
F(I,J)=(FLUX(KPI)**TAUEXP*(FLUX(K)**(1.0-TAUEXP)))
60 CONTINUE
70 CONTINUE
50 CONTINUE
RETURN
END

SUBROUTINE VIM
VARIATIONAL ITERATIVE METHOD CALCULATES ATMOSPHERIC MULTIPLE SCATTERING AND SURFACE REFLECTION EFFECTS WHICH AFFECT PHOTODESOCIATION RATES
INPUT INFORMATION INCLUDES SURFACE REFLECTION COEFFICIENT, SINGLE SCATTERING ALBEDO AND OPTICAL DEPTH PROFILES
RESULTANT FLUX ADJUSTMENT PROFILE RETURNS TO OMEGA
ADAPTED FROM I. K. BURKE, E.R.T., TNC. 1977

LOGICAL LINEQV
REAL MMIN
COMMON/PARA/VO,N,M1,N2,NN,NNP1,REF
COMMON/SCA/TAUJN(100),OMEGAZ(41,100),TAU(41),OMEGAT(41)
COMMON/VRP/TAUZ(41,100),OMEGA(41,100),TAU(41),OMEGAT(41)
COMMON/MATRIX/(20,21)
COMMON/MES4/T(21),G(101),W(21)
COMMON/FUN/E3T(21),E2T(101),E1T(101),E1T(101)
COMMON/COEFF/A(20),AA(20)
DIMENSION S1(101),T1(101),S0(101)
DIMENSION S52(101),F(101),F1(101),F2(101)
DIMENSION GG(101),FF(21),W(101)
DIMENSION U(50),INT(50),GA(101)
DIMENSION F3(101),EQ(101)

4 FORMAT(*1*,5X,*MATRIX ELEMENTS, ML*",X4)
5 FORMAT(4X,1P11E11.3)
6 FORMAT(*5X,*TAU",8X,*A(J)*,10X,*AA(J)*)
7 FORMAT(6X,1E9.3,2E16.6)
8 FORMAT(* SINGULAR MATRIX*)
9 FORMAT(* SINGULAR MATRIX*)
10 FORMAT(* SINGULAR MATRIX*)
11 FORMAT(* SINGULAR MATRIX*)
12 FORMAT(* SINGULAR MATRIX*)
13 FORMAT(* SINGULAR MATRIX*)
14 FORMAT(* SINGULAR MATRIX*)
15 FORMAT(* SINGULAR MATRIX*)
16 FORMAT(* SINGULAR MATRIX*)
17 FORMAT(* SINGULAR MATRIX*)
18 FORMAT(//,7X,*T*,10X,*F*,19X,*F*,18X,18X,*F*,18X,*F* )

DEFINE T1 AND W SUCH THAT K=1 CORRESPONDS TO TOP OF ATMOSPHERE, K=NNP1 IS BOTTOM OF ATMOSPHERE

DO 111 K=1,NNP1
   WK=NNP1-K+1
   T(K)=TAU(NK)
111  WM(K)=OMEGA(T(K))
   DO 45 J=1,WM(K)
   E2T(K)=E2(T1(K))
   ET1(K)=E3(T1(K))
   ET1(K)=E2(T(NNP1)-T1(K))
   ET1(K)=E3(T(NNP1)-T1(K))
   EX(K)=EXP(-T1(K)/U0)
   CONTINUE
   DT=T1(NNP1)/N1
   K=0
   L=NN/N1+1

50 COMPUTE T AND W PROFILES
   T(J)=DT*(J-1)
   E3T(J)=E3(T(J))
   DO 15 J=1,N1
      SUM=0.
      DO 16 L=1,K
         SUM=SUM+WM(K)*ET1(K)*T(J/L)
      K=L+1
   15 SUM=SUM/L
   10 CONTINUE
   DO 46 K=1,NNP1
      SO(K)=0.5*WM(K)*ET1(K)*EX(K)
   46 CONTINUE
   CALL RMAT
   M(J,N)=FF(J)
   DO 20 J=1,N1
      FF(J)=M(J,N)
   20 CONTINUE
   IF (LNEQN(N-1)) GO TO 100
   DO 25 J=1,N1
      TA=(T(J)+T(J+1))*.5
   25 CONTINUE
   THIS IS T AVERAGE FOR EACH LAYER

   A(J)=M(J,J)
   THIS IS SOLUTION TO MATRIX EQN
   AA(J)=SQRT(W(J))
   THIS IS AVERAGE SOURCE IN THE INTERVAL

   25 CONTINUE
   GO TO 400
   WRITE(6,9)
   100 WRITE(6,10)
   200 JJ=J
   300 JJ=JP1
   SS2(J)=AA(J)*(E3(T(N)-T(JP1))-E3(T(N)-T(J))
   S2=S2+SS2(J)
   40 CONTINUE
   DO 30 K=1,NNP1
      *(K)
      K=1
      *(K)
S1(K) = S1(K)
G(K) = S0(K) + 5 * NN(K) * S1(K) + 5 * NN(K) * RE1 * E2T(K) * S2
CONTINUE

RESULT OF 1ST ITERATION

II = 2

30 DIFF = 0.
CALL COMP(SG)
DO 35 K = 1, NN1
GG(K) = G(K)
G(K) = S0(K) + 5 * NN(K) * S1WT(K) + 5 * NN(K) * RE1 * E2T(K) * S2
DEL = ABS((GG(K) - G(K)) / G(K))
WRITE (6, 14) T(I), G(K), GG(K), DEL
35 DIFF = DIFF + DEL
IF (DIFF .LE. 1) GO TO 400
II = II + 1
IF (II .LE. 10) GO TO 300

400 CONTINUE
Y = EXP(-T(N) / U0)
CALL COMP(SG)
DO 50 K = 1, NN1
F0(K) = EX(K)
F1(K) = 2. * S1WT(K)
X = 2. * RE1 * E2T(K)
F2(K) = X * SG2
F3(K) = X * U0 * Y
F(K) = F0(K) + F1(K) + F2(K) + F3(K)
50 CONTINUE
DO 333 K = 1, NN1
NK = NN1 + K
333 FLX(K) = F(NK)
END

SUBROUTINE RMATI
REAL M
COMMON /MATRX/M(N, N)
COMMON /PARA/U0, NN1, NN2, MN, NN1P, REF
COMMON /MATRX/T(MT, NN1, NN2)
COMMON /EFUN/ ESTM(N1), ESTT(N1), ESTM(N1), ESTT(N1)
DIMENSION T(J1, J2)
DO 10 J1 = 1, N1
10 JPI = J1
DH(J) = T(JPI) - T(J)
M(J, J) = DH(J) - M(J, J) * (DH(J) + E3(DH(J))) / 2
10 CONTINUE
IF (N .EQ. 3) GO TO 100
DO 20 J = 1, N2
20 JPI = J
DO 20 J = JPI, N1
JPI = J1
EE = E3(T(J1)) - T(J1) - T(J1P1) + T(J1P1) + E3(T(JPI) - T(J1) - T(J1P1))
10 IF (EE) M(J1J) = M(J1J) * EE
20 M(J, J) = M(J1J)
GO TO 200
200 M(J, J) = M(J1J)
GO TO 200
100 M(J, J) = M(J1J)
M(J2, J) = M(J2, J)
200 DO 30 J = 1, N1
30 JPI = J
TU(J) = T(J)
30 CONTINUE
RETURN
END

LOGICAL FUNCTION LINEQN(N)

C GAUSSIAN ELIMINATION METHOD IS USED

94
COMMON/MATRIX/A(20,21)
IF (N.GT.1) GO TO 10
IF (A(I,1).EQ.0) GO TO 500
A(I,1)=A(I,2)/A(I,1)
GO TO 620
10 SUM=0.
DO 20 I=1,N
DO 20 J=1,N
20 SUM=SUM+ABS(A(I,J))
TOLER=(SUM/FLOAT(N))*2*1.E-08
N1=N-1
NPI=N+1
DO 300 K=1,N1
TEMP=ABS(A(K,K))
IF(NP1=K) GO TO 100
KPI=K+1
DO 100 I=KPI,N
IF(ABS(A(I,K)) .LE. TOLER) GO TO 100
TEMP=ABS(A(I,K))
ITEMP=I
END
100 CONTINUE
IF (TEMP .LE. TOLER) GO TO 500
IF (ITEMP .GE. K) GO TO 200
30 DO 100 I=1,N
L=Ψ(I)-J
400 A(K,Ψ(I))=A(K,L)*A(L,Ψ(I))
500 L=Ψ(I)-J
420 GO TO 600
500 LINE=FALSE.
GO TO 500
600 RETURN
FUNCTION E2(X)
IF (X.LE.1.0E-6) GO TO 1
E2=EXP(-X)-X*E(X)
RETURN
1 E2=1.0
RETURN
FUNCTION E3(X)
IF (X.LE.1.0E-6) GO TO 1
E3=EXP(-X)-X*EXP(-X)-X*E(X)))*0.5
RETURN
1 E3=0.5
RETURN
FUNCTION E4(X)
IF (X.GE.10.) GO TO 200
IF (X.GE.1.0) GO TO 100
A1=.57721566
A2=.16615055
A3=.05918668
END
400 SE=EQ2(K—T(J+1))—EQ2(X—T(J)) 027130
RETURN 027140
100 IF(I.GE.T(2)) GO TO 500 027150
SE=EQ2(X—T(2))—EQ2(T(2)—X) 027160
RETURN 027170
500 SE=EQ2(K—T(2))—EQ2(X) 027180
RETURN 027190
200 IF(I.GE.T(N-1)) GO TO 600 027200
SE=EQ2(T(N-1)—K)—EQ2(T(N)—X) 027210
RETURN 027220
600 SE=EQ2(X—T(N-1))—EQ2(X—T(N)) 027230
RETURN 027240
END 027250
FUNCTION SINT(I) 027260
DIMENSION GM(101) 027270
COMMON /MESH/ T(21),G(101),H(21) 027280
COMMON /FUN/ EQ(T(21),EQ(T(101),EQ(T(101),EQ(T(101),EQ(T(101) 027290
COMMON /PARAM/ J0,M1,H2,NN,NNP1,REF 027300
SUM1=0. 027310
SUM2=0. 027320
DO 10 K=1,N4 027330
K1=K+1 027340
10 GM(K)=G(K)+G(K1) 027350
IF(I.EQ.1) GO TO 100 027360
I1=I+1 027370
DO 20 K=1,I1 027380
20 SUM1=SUM1+GM(K)*EQ2(I-K)—EQ2(I+K)) 027390
IF(I.EQ.NNP1) GO TO 200 027400
100 DO 30 K=1,NN 027410
30 SUM2=SUM2+GM(K)*EQ2(K—I+2)—EQ2(K—I+1)) 027420
200 SINT=(SUM1—SUM2)*5 027430
RETURN 027440
END 027450
** BLOCK DATA ** 027460
** CHLORINE MODEL STUDY PROGRAM - VERSION 4 ** 027470
** ** 027480
** BLOCK DATA ** 027490
** ** 027500
** VERSION 4.0 ** 027510
** LEVEL 770214 ** 027520
** E.R. T., INC. ** 027530
** L. PERRY, N. TRIPP ** 027540
** ** 027550
** REAL TITLE(6) ** 027560
** ** 027570
** COMMON /HEAD/ TITLE,ICODE,VER,LEVEL,DATE,IRUN,NPAGE,NLOG ** 027580
** COMMON /EDDY/ FKK,II,P11,P22,NE30Y ** 027590
** COMMON /MODEL/ ALT(41),TEMP(41),DM(41),U(41),DA2(41) ** 027600
** COMMON /MOL/ YO/XH(81),XH2O(81),P420,Q42,X11(81) ** 027610
** COMMON /MST/ SCNO2,SCCL03,SCCH22,SCCH205 ** 027620
** REAL J02,J03,J33,JHPO,JNO2,JNO3,JNO4,JCFC3,JHCL,JH232,JHOC ** 027630
** ** 027640
** COMMON /PARM/ ISWT,ISTEP,TSTOP,TLOOP,TPRM,ISIZE,ISCATT ** 027650
** COMMON /RAT/ JO2(41),JO3(41),JO4(41),JN20(41),JN203(41) ** 027660
** X JN205(41),JN206(41),JN207(41),JN208(41),JN209(41) ** 027670
** Y JN210(41) ** 027680
** REAL JNO3 ** 027690
** COMMON /RATES/ RATE(65,81),RA(65),RB(65),JN03,PJ03 ** 027700
** COMMON /KLON/ R20,RNOX,RCH4,RF11,RF12,RCH3,RLCL,RRCL4,R03 ** 027710
** COMMON /SFAC/ FCL,FM20,FCLNO3,WM0 ** 027720
** COMMON /SOLCM1/ ML(180),FL(180),QO3(100) ** 027730
** COMMON /SOLCM2/ QCF2(100),QCF1(100),QCC(100),QCH2(100) ** 027740
** X QCLNO3(100),QNO2(100),QNO3(100),QNO4(100),QNO5(100) ** 027750
** Y QCL1(100),QHCL(100),QNO2(100),QNO3(100) ** 027760
** REAL NO2,N0X,N03,N2O5 ** 027770
** COMMON /SPECIE/ M(41),DM(41),MO2(41),MO3(41),O16(41),O18(41) ** 027780
** ** 027790

97
| DATA Q02/5.2000E+18, 5.9000E-18, 5.5000E-18, 4.0000E-17, 2.0000E-18 | 028450 |
| 21.9000E-18, 1.9000E-18, 1.5000E-18, 1.0000E-18, 0.5000E-18 | 028450 |
| 34.0000E-19, 3.5000E-19, 4.6000E-19, 1.0000E-19 | 028450 |
| 44.0000E-19, 1.8000E-19, 2.4000E-19, 2.0000E-18 | 028450 |
| 54.3000E-19, 1.5000E-19, 3.0000E-19, 3.5000E-18 | 028450 |
| 62.0000E-21, 1.3000E-21, 2.2000E-21, 4.0000E-21 | 028450 |
| 74.0000E-24, 3.0000E-24, 1.0000E-24, 7.0000E-25, 3.0000E-25 | 028510 |

DATA Q03/24*6.83500E+19, 5.3500E+19, 1.4190E+19, 1.2070E+19 | 028540 |

DATA TEMP/3.0458E+02, 2.6595E+02, 2.5362E+02, 2.4541E+02, 1.9770E+02 | 026670 |

DATA DM/2.4110E+19, 1.3400E+19 | 02750 |

DATA 03/6.2500E+11, 6.4000E+11, 1.7000E+11, 1.4900E+11, 028330 |

DATA 01.5110E+01, 2.1500E+01, 9.6600E+00, 2.1800E+00, 0.5700E+00, 028110 |

DATA OZ/2.8900E+03, 2.0900E+03, 3.4000E+03, 3.5000E+03, 6.1000E+03 | 028950 |

DATA H/1.2100E+01, 0.6500E+01, 0.6000E+01, 0.6000E+01, 0.6000E+01, 029050 |
<p>| DATA H2O2/2.0000E+04 | 5.27410E+04 | 4.84110E+04 | 4.9.0940E+04 | 1.10800E+05 | 1.5000E+05 | 1.5000E+05 | 0.10800E+05 | 2.7500E+05 | 3.1000E+05 | 0.291100 |
| DATA H2O2/2.0000E+04 | 6.32010E+05 | 5.90600E+05 | 4.13000E+05 | 5.19500E+05 | 2.7500E+05 | 2.6900E+05 | 3.5900E+05 | 3.9000E+05 | 6.3000E+05 | 0.291200 |
| DATA H2O2/2.0000E+04 | 7.30000E+05 | 6.60600E+05 | 5.10000E+05 | 6.19000E+05 | 2.7500E+05 | 2.6900E+05 | 3.5900E+05 | 3.9000E+05 | 6.3000E+05 | 0.291300 |
| DATA H2O2/2.0000E+04 | 8.30000E+05 | 7.58000E+05 | 6.10000E+05 | 7.19000E+05 | 2.7500E+05 | 2.6900E+05 | 3.5900E+05 | 3.9000E+05 | 6.3000E+05 | 0.291400 |
| DATA H2O2/2.0000E+04 | 9.30000E+05 | 8.58000E+05 | 7.10000E+05 | 8.19000E+05 | 2.7500E+05 | 2.6900E+05 | 3.5900E+05 | 3.9000E+05 | 6.3000E+05 | 0.291500 |
| DATA H2O2/2.0000E+04 | 1.00000E+06 | 9.18000E+05 | 8.10000E+05 | 9.19000E+05 | 2.7500E+05 | 2.6900E+05 | 3.5900E+05 | 3.9000E+05 | 6.3000E+05 | 0.291600 |
| DATA H2O2/2.0000E+04 | 1.10000E+06 | 1.00000E+06 | 9.10000E+05 | 1.01000E+06 | 2.7500E+05 | 2.6900E+05 | 3.5900E+05 | 3.9000E+05 | 6.3000E+05 | 0.291700 |
| DATA H2O2/2.0000E+04 | 1.20000E+06 | 1.10000E+06 | 1.01000E+06 | 1.01000E+06 | 2.7500E+05 | 2.6900E+05 | 3.5900E+05 | 3.9000E+05 | 6.3000E+05 | 0.291800 |
| DATA JcF2/F-0.3033-29.6,792E-26, 24.653E-25, 3.307E-15, 0.3048 |
| 23.393E-10, 13.950E-13, 6.866E-12, 6.200E-11, 13.574E-10, 0.3049 |
| 51.956E-07, 7.2127E-07, 3.7010E-07, 4.1109E-07, 5.1436E-07, 0.3051 |
| 56.772E-07, 7.1330E-07, 6.765E-07, 7.452E-07, 9.097E-07, 0.3052 |
| 61.069E-06, 1.164E-05, 1.266E-05, 1.371E-05, 1.491E-05, 0.3053 |
| 71.685E-06, 1.737E-05, 1.856E-05, 1.913E-05, 0.3054 |
| DATA JCF3/2, 4.85E-27, 3.22E-26, 24.529E-25, 1.444E-24, 0.3056 |
| 24.303E-19, 1.829E-13, 6.02E-12, 7.075E-11, 6.305E-10, 0.3057 |
| 4.134E-08, 9.414E-08, 1.916E-07, 7.740E-07, 5.914E-07, 0.3058 |
| 4.579E-06, 2.281E-06, 3.398E-06, 3.863E-06, 4.593E-05, 0.3059 |
| 55.797E-06, 6.275E-06, 6.689E-06, 7.069E-06, 7.429E-06, 0.3060 |
| 68.100E-06, 9.510E-06, 6.666E-05, 9.225E-05, 6.990E-05, 0.3061 |
| 71.023E-06, 9.251E-05, 9.752E-05, 1.096E-05, 1.114E-05, 0.3062 |
| DATA M2O/F1, 2.27E-02, 1.109E-02, 6.762E-02, 3.543E-02, 0.3064 |
| 24.017E-02, 1.081E-04, 1.632E-05, 4.200E-05, 6.120E-05, 0.3065 |
| 3.280E-06, 6.400E-06, 6.400E-06, 6.400E-06, 6.400E-06, 0.3066 |
| 4.569E-06, 2.200E-06, 3.300E-06, 3.300E-06, 3.300E-06, 0.3067 |
| 64.000E-06, 1.300E-06, 1.300E-06, 1.300E-06, 1.300E-06, 0.3068 |
| DATA JA3/F2, 1.806E-06, 7.610E-06, 2.712E-05, 1.934E-05, 0.3070 |
| 24.215E-02, 5.696E-19, 4.497E-17, 1.003E-15, 1.62E-13, 0.3071 |
| 37.393E-13, 1.342E-12, 1.127E-11, 3.093E-11, 7.023E-11, 0.3072 |
| 42.313E-10, 1.403E-10, 7.399E-10, 5.999E-10, 7.302E-10, 0.3073 |
| 51.072E-09, 9.138E-09, 9.275E-09, 3.979E-09, 9.590E-09, 0.3074 |
| 69.017E-09, 9.179E-09, 1.492E-09, 1.866E-09, 2.606E-09, 0.3075 |
| 77.403E-09, 1.376E-08, 2.439E-08, 3.838E-08, 7.897E-08, 0.3076 |
| DATA JA3/F2, 3.51E-02, 5.209E-19, 4.276E-17, 3.723E-15, 0.3077 |
| 20.690E-05, 1.327E-05, 1.686E-05, 2.691E-05, 3.556E-05, 0.3078 |
| 18.542E-05, 3.951E-06, 6.018E-06, 5.351E-07, 6.395E-07, 0.3079 |
| 42.022E-05, 2.819E-04, 3.933E-04, 5.777E-04, 8.554E-04, 0.3080 |
| 54.733E-05, 1.263E-03, 3.749E-03, 5.244E-03, 8.691E-03, 0.3081 |
| 69.334E-05, 1.638E-03, 2.290E-03, 3.855E-03, 5.147E-03, 0.3082 |
| 75.568E-05, 1.909E-03, 2.659E-03, 4.149E-03, 5.620E-03, 0.3083 |
| 8.32E-03, 2.3E-02, 3.2E-02, 4.3E-02, 5.6E-02, 0.3084 |
| DATA QCF2/./2.79E-19, 9.12E-19, 5.70E-19, 2.46E-19, 0.3085 |
| 1.97E-21, 2.0E-21, 3.98E-20, 0.3086 |
| DATA QCF3/2.79E-19, 2.4E-19, 1.38E-19, 6.56E-19, 1.34E-19, 0.3087 |
| 1.52E-19, 1.64E-20, 2.47E-20, 1.00E-20, 3.6E-20, 0.3088 |
| DATA QcC1/A2.79E-19, 3.36E-19, 1.87E-19, 6.92E-19, 1.29E-19, 0.3089 |
| 1.75E-19, 1.97E-19, 3.38E-19, 6.48E-19, 1.08E-19, 0.3090 |
| DATA QcC3/2.59E-19, 3.55E-19, 4.17E-19, 2.68E-19, 0.3091 |
| 2.94E-19, 3.12E-19, 10.0E-20, 2.30E-20, 5.00E-20, 0.3092 |
| DATA QcC13/2.80E-19, 8.0E-19, 5.3E-19, 1.6E-19, 4.8E-19, 0.3093 |
| 5.2E-19, 5.8E-19, 1.6E-19, 2.0E-19, 3.1E-19, 0.3094 |
| 3.8E-20, 4.2E-20, 1.6E-20, 2.1E-20, 3.4E-20, 0.3095 |
| 3.1E-21, 2.6E-21, 7.1E-21, 1.4E-21, 7.7E-21, 0.3096 |</p>
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**END**
APPENDIX B

FLOW CHARTS
CMSP Chlorine Model Study Program

Start

Read TITLE keyword card
Read data card with Title of run

Call

Subroutine ALTEGEN
   to initialize run

Return

read keyword card

Is it ENDJOB?

Yes

EOJ

No

PARAMETERS = Keyword

Call

Run

A

Subroutine INPARM
   to establish initial constants
   for each case

Return

B

Subroutine PHOCHM
   to perform calculations
   for each case

Call

Return
**A. Subroutine INPARM**

Enter

READ NAMELIST $ INPUT
to change any constants from the default values established by BLOCK DATA

Call

Subroutine WEIGHT
to compute the constants of array A used in COMTAU

Call Return

Subroutine CPHI1
to compute constants of array PHI1 used in COMPJ

Call Return

Subroutine SETUP
to select a set of eddy diffusion coefficients and to create arrays of 81 levels from the original data at 41 levels of these coefficients, and temperature and M

Call Return

Subroutine RCONST
to compute the array of reaction rates at 81 levels for each of 51 reactions

Return

Return
B1. Subroutine PHOCHM

Enter

Initialize constants for steady-state case
I = 0 - iteration counter

Call

Subroutine RJITER to calculate J-values using first-guess at ozone concentrations

Return

I = I + 1
Calculate O(^1D) concentrations for very level

I > 50 ?
Yes
WRITE 'not converge' message
502 p. B-2

No

DO for each layer in atmosphere, every 2 km, 0 - 80 km, calculate concentrations of the short-lived species (ozone calculated only at and above 30 km)

Call

Subroutine CFLOW to calculate concentrations of the long-lived species using 1-km layers, 0 - 80 km (ozone only below 30 km)

Return

Up to 30 kms, replace ozone values by average of present and previous results (for faster convergence)
Save previous J-values

Call

Subroutine RJITER to recalculate J-values, using present ozone concentrations

Return

49 p. B-2
B2. Subroutine PHOCHM (continued)

Yes: Test J-O3 and OH concentrations for convergence at every level

No: 10 → p. B-1

SO2
Print results

Return
C1. Subroutine INITIAL - Short-lived Species

Start

Enter

1st time?

Yes

Calculate initial concentrations from first-guess mixing-ratios, using scaling factors

No

Initialize variables for the system of simultaneous equations:

\[ Y_1 = H \]

and set

\[ Y_2 = OH \quad Y_4 = O_3 \]

\[ Y_3 = HO_2 \]

Call

Subroutine PCLOX to calculate concentrations of CL, CLO, and HCL

Return

Call

Subroutine PNOX to calculate concentrations of NO2, NO, HNO3, NO3, N2O5, and CLNO3

Return

Do concentrations of NO, NO2, and HNO3 converge?

No

More than 10 iters.?

Yes

Stop

Yes

Return

p. C-2
C2. Subroutine SOLVE - Short-lived Species

Subroutine SOLVE uses Newton's method

Enter

KK = 1 - iteration counter
KKK = 0 - singularity counter

Set YO(N) = Y(N) for N = 1,4

I = 1

Call Subroutine JACOB

Form Jacobian B(N,N) for N = 1,3
Form PP(N) & SS(N)
Solve for 03 = Y4 above 30 bms.

B(IN,4) = PP(IN) - SS(IN) for N = 1,3

ERR = \sum \frac{(B(IN,4))^2}{SS(IN)}

Function LINEQN - uses Gaussian elimination
Solve for B(N,4), N = 1,3

Y(N) = 0.9 * Y(N)
N = 1,3

Yes

No

Matrix Singular?

KKK \geq 3?

Return

ERR \leq 1.E-5?

Yes

Return

No

Y(N) = Y(N) * B(N,4), N = 1,3
I = I + 1

I \gt 20?

Yes

No

Return
C3. Subroutine SOLVE (continued)

Calculate concentrations of
\( H = Y(1), \, OH = Y(2), \, HO_2 = Y(3), \, O_3 = Y(4) \)
also \( O, \, H_2O_2, \)
Call PCLOX for CL, CLO, and HCL
Call PNOX for NO2, NO, HNO3, NO3, N2O5, and ClNO3
\( KK = KK + 1 \)

KK > 50 ?
Yes
Return

No
Is \( \frac{Y_0(N)}{Y(N)} \geq 1 \) for all N?

Call JACOB
to compute production
and loss terms for
printing
also O3 and O2
above 30 km

Return

Save production and loss terms
for printing

Continue
D1. Subroutine CFLOW - Long-lived Species

Enter

For necessary species, set up arrays of concentrations at each of 81 1-km levels from 41 2-km levels, by interpolation using subroutine RINTER

For each species in order:
- N2O
- NOX
- CH4
- FC11
- FC12
- CH3CL
- CCL4
- CLX
- H2

Call CSPEC (p. D-2) to calculated the 81-level array of mixing ratios

For 03, call CSPEC to calculate mixing ratios for 31 k-km levels up to and including 30 km

No
Call REPCN - have species CLO and NO2 converged in region 30 km and below?

Yes

Calculate concentrations of NOX, CH4, CLX, H2 to 80 km and O3 < 30 km

Return
D2. Subroutine CSPEC

Enter

Set boundary conditions according to input

Call CXLi (for species i) to compute the 81-level arrays: production PR, loss frequency XL, initial mixing ratio DFP (always 0 for steady state)

Call COEF to compute the coefficients for the 81-level tridiagonal system of simultaneous equations

Call TRIDIA to solve the system of equations for the array X of mixing ratios at each level

Compute 81-level array of net production or loss and store in array XL i.e. $XL = PR \cdot XL \cdot X$

(These arrays are used in subroutine PRINTX where the flux of each species is calculated by trapezoidal integration and result printed)

Return
APPENDIX C

SAMPLE TEST CASES

Case 1  Absorption Only (ISCATT = 0)
(all default values)*

Case 2  Multiple Scattering (ISCATT = 1)
(all default values)*
Surface Reflectivity = 0.2

*Exceptions:  ISWITCH = 0  (fixed sun angle)
RF11 = 8.30 E + 05
RF12 = 1.13 E + 06
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