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USER'S MANUAL FOR SAMM, SHARC AND MODTRAN MERGED

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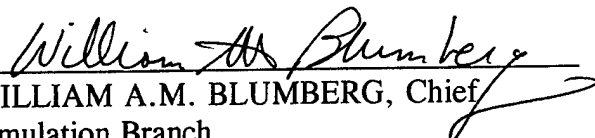
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1. INTRODUCTION

This manual describes SAMM, a new moderate spectral resolution (2 cm^{-1}) infrared (IR) atmospheric transmission and background radiance model applicable at altitudes from ground to space (300 km). SAMM, SHARC⁽¹⁾ And MODTRAN^(2,3) Merged, was developed by integrating the DOD standard lower atmosphere (2 cm^{-1} MODTRAN) and upper atmosphere (1 cm^{-1} SHARC) moderate spectral resolution models into a single, seamless code with a unified and correlated radiative transport algorithm. This manual provides an overview of the SAMM model and describes how to run SAMM by providing code implementation and execution instructions. It also discusses the newly developed radiative transport algorithm which is applicable to both the low and high altitude regimes. Frequent references are made to the SHARC,⁽¹⁾ MODTRAN,⁽²⁾ LOWTRAN 7⁽³⁾ (precursor to MODTRAN), and SAG⁽⁴⁾ (SHARC/SAMM Atmospheric Generator) manuals to avoid repetition of phenomenological descriptions, file definitions, and input instructions for users already familiar with these codes; it is helpful to have copies of these manuals on hand when initially implementing and/or running SAMM.

SAMM has five primary modules.

- INPUT - an expanded SHARC interactive input module defines file & directory names, extended & local environments, lines-of-sight (LOS), spectral bandpass parameters, and molecular radiators;
- CHEMKIN - the SHARC kinetics package solves input chemical equations to determine excited state vibrational populations in both ambient and auroral regions;
- REFGEOM - upgraded MODTRAN refractive geometry routines track altitude, latitude, and longitude;
- COLDEN - a new SAMM module calculates all optical and solar path column densities by combining MODTRAN low altitude column amounts with high altitude amounts determined through repeated calls to SHARC geometry routines; and
- RAD - a modified MODTRAN radiative transfer routine calculates spectral radiances and transmittances using a combined line-by-line (LBL) and band model equivalent width algorithm.

SAMM input and output files are a combination of those used by SHARC and MODTRAN, with some relevant modifications. This manual includes a description of the various files. Appendices contain implementation instructions, details about the source code, sample input and output files, and derivation of an upgrade made to MODTRAN's column density calculations.

2. OVERVIEW

SAMM is a model for predicting spectral radiances for selected lines-of-sight (LOS) through the atmosphere. This section presents an overview of the model, describing problem set up, code structure, and general approach.

2.1 The INPUT Module

The INPUT module defines the problem to be solved. More specifically, the module is used to set up an earth's atmosphere, to fix solar position, and to select the set of LOS and spectral bandpasses over which radiances are to be predicted.

In SAMM, the earth's atmosphere from 0 to 300 km altitude is partitioned into a single extended ambient region and localized ambient and/or auroral sub-regions. The aurora are regions whose chemistry is influenced by the bombardment of solar electrons; specification of the incident electron energy spectrum and its duration is required for modeling these aurora. Both ambient and auroral localized regions are bounded by surfaces of constant altitude, latitude, and longitude. Within each region, the user may define/select either a single set of pressure, temperature, and total molecular density profiles or multiple sets, each one associated with a particular solar earth center angle (solar earth center angle is used rather than solar zenith angle, because the former is not affected by spherical refractive geometry and therefore is altitude independent at a fixed latitude and longitude).

The SAMM input module allows the user to select the number of regions, their boundaries, and their profiles. Two generic atmospheric profile files are supplied with the code (MIDLAT.DAY and MIDLAT.NIG) along with terminator profiles for O₃ (T4Z091.ATM, T4Z093.ATM, T4Z095.ATM, T4Z097.ATM, T4Z099.ATM, T4Z101.ATM & T4Z102.ATM) and CO₂ (T5Z091.ATM, T5Z094.ATM, T5Z097.ATM, T5Z099.ATM, T5Z102.ATM, T5Z104.ATM & T5Z108.ATM). Additional atmospheric profiles can be generated using the SAG⁽⁴⁾ (SHARC/SAMM Atmospheric Generator) program.

Aerosol profiles are not defined in the atmospheric profile files, but instead are defined in an external file named HAZE.INP; these profiles are input using the MODTRAN/LOWTRAN 7 format, and they must be entered or modified by directly editing HAZE.INP.

Solar position is specified either by directly entering solar latitude and longitude or by selecting year, month, day, and Greenwich mean time.

There are three basic LOS types: observer-to-source, observer-to-space, and limb viewing. For both the observer-to-source and the observer-to-space paths, the observer location is defined by entering the observer altitude, latitude, and longitude. There are five options for specifying source location; input (1) source altitude and observer zenith & azimuth, (2) path range and observer zenith & azimuth, (3) source altitude, path range, and observer azimuth, (4) source altitude, path earth center angle, and observer azimuth, or (5) source altitude, latitude & longitude. For paths to space, the observer altitude, and either the observer zenith or the tangent altitude must be input. Limb viewing LOS are tangent paths extending from space to space; these paths are specified by entering the tangent point altitude, latitude, longitude & azimuth. For all paths, azimuth angles can be specified either by directly entering the angle (degrees East of North) or by entering a latitude and longitude in front of or behind the observer (tangent point for limb paths) location.

All spectral data are entered in wavenumber (cm^{-1}) units. The spectral range of SAMM is 250 to 10,000 cm^{-1} and the minimum spectral resolution is 1 cm^{-1} .

2.2 The CHEMKIN Module

The CHEMKIN module determines the distribution of the excited vibrational states under non-local thermodynamic equilibrium (non-LTE) conditions. At low altitudes, the time step for collisional excitation/relaxation processes is short, LTE conditions prevail, and the population of vibrational states follow a Boltzmann distribution. Spontaneous emission, chemiluminescent, and solar/thermal pumping processes compete with collisional excitation/relaxation at lower pressures. To predict vibrational state populations under these non-LTE conditions, the pertinent chemical kinetic equations must be solved explicitly.

The profiles discussed in the previous section define the total molecular densities as a function of altitude in the SAMM regions. Dominant radiators below 30 km altitude are LTE. The CHEMKIN module is used to determine vibrational state distributions between 30 and 300 km altitude. For each radiating species, a chemical mechanism (a series a chemical equations) is input to SAMM. Default kinetics files are supplied with the SAMM source. SAMM initially calculates solar and earthshine excitation rates. In ambient regions, the steady state solutions to the kinetic mechanisms are then determined layer-by-layer; for auroral regions, the time dependent chemical kinetic equations are solved. The resulting populations are then adjusted to account for self absorption.

2.3 The REFGEOM Module

The REFGEOM module tracks all required refractive paths for SAMM. The basic refractive geometry equation is

$$n_R R \sin\theta = \text{constant} \quad (1)$$

where R is the earth center distance, n_R is the real part of the refractive index, and θ is the zenith angle at R . The assumption is made that the refractive path varies insignificantly with wavelength, and refractive geometry calculations are performed for the central frequency of the spectral bandpass only. A second assumption is that the refractive index is constant above 30 km i.e., at low pressures, and straight line geometry is used for the 30 to 300 km altitude region.

Refractive paths are tracked by marching along from the initial location to the termination point. It is necessary that the altitude, latitude, longitude, path zenith, and path azimuth at the initial location all be known. If this LOS starting point information is not actual input (e.g., if path range instead of zenith angle is used to specify an observer-to-source path), then the REFGEOM module solves for the required initial data, directly if possible and iteratively when necessary.

Output from the REFGEOM module includes column densities and layer averages for both optical and scattering point-to-sun paths below 30 km. A new algorithm has been developed to calculate these quantities directly from the layer path length and boundary zenith angles, altitudes, and densities. The approach is described in Appendix H.

2.4 The COLDEN Module

The COLDEN module merges column density information from the MODTRAN and SHARC sections of the code. The MODTRAN section of the code determines all the lower altitude (< 30 km) total molecular column densities; for radiators common to both MODTRAN and SHARC (H_2O , CO_2 , CO , NO , O_3 & CH_4), densities must be partitioned into their vibrational states. At higher altitudes, the SHARC column densities must be combined with the MODTRAN path amounts for HNO_3 , SO_2 , NO_2 , NH_3 , N_2O , O_2 , and the aerosols.

Unfortunately, MODTRAN and SHARC use different conventions for molecular indices. SAMM combines the labeling schemes and places all the column density information

for the optical path into a single array (VPATH). A second array (VPATHS) contains all the column density data for scattering point-to-sun paths.

2.5 The RAD Module

The RAD module is a modification of the MODTRAN radiative transport routines, and calculates and outputs spectral radiances. The spectral bandpass is sampled in 1 cm^{-1} steps. The resulting 1 cm^{-1} data is internally degraded using a digitized triangular slit function if the user requests a FWHM (Full Width at Half Maximum) in excess of 1 cm^{-1} (FWHM must be a positive integer no greater than 50).

For each frequency, there is a loop over the optical path layers to determine their contribution to the spectral radiance. Single scatter solar/lunar radiance is included in the layer radiances by considering the contribution from L-shaped paths from the sun/moon to the layer to the observer. The multiple scattering contribution to the spectral radiance is determined by initially performing a two-flux calculation at each frequency; the required upward and downward fluxes are calculated by looping over the atmospheric layers below 100 km using a vertical path from ground to space. Details of the radiance algorithm are presented in Section 3.

3. RADIATION TRANSPORT ALGORITHM

In the lower atmosphere, below 30 km altitude, collisional processes dictate the distribution of the dominant vibrationally excited species, i.e., LTE conditions prevail. At higher altitudes, where densities are much lower, radiative pumping and spontaneous emission processes can begin to compete with the collisional processes. The deviation from LTE depends on details of the excitation reactions and varies from one molecular band to another. When the ambient temperature no longer describes the distribution of vibrationally excited states, a molecular band is said to be in non-local thermodynamic equilibrium (non-LTE). Transmittances and radiances then depend explicitly on these vibrational distributions.

3.1 Line-of-Sight Radiance

Computation of the spectral radiance for an atmospheric line-of-sight (LOS) passing through both the LTE and non-LTE regimes requires detailed information about gas kinetic temperature, pressure, species column densities, vibrational populations, solar irradiance, and surface temperature. SHARC calculates these radiances by modeling non-LTE formation processes and then performing LBL calculations, while MODTRAN uses an LTE band model approach. SAMM has adopted a hybrid approach in which the SHARC radiators (CO_2 , H_2O , O_3 , CO , OH , CH_4 , NO , & NO^+) are treated LBL and all other emitters (N_2O , O_2 , SO_2 , NO_2 , NH_3 , HNO_3 , & continuum sources) are modeled using the MODTRAN band model techniques. The LOS is represented as a series of segments, and the radiance within each (1 cm^{-1}) spectral bin is calculated as the sum of emission I^0 , single scattering I^{ss} , and multiple scattering I^{ms} terms:

$$I = \sum_{\ell} I_{\ell}^0 + I_{\ell}^{\text{ss}} + I_{\ell}^{\text{ms}} \quad , \quad (2)$$

where the sum is over the atmospheric layers traversed by the LOS. The emission from each layer is calculated as a product of the incremental transmittance $\tau_{\ell-1} - \tau_{\ell}$, one minus layer scattering albedo $1-\omega_{\ell}$, and a source term R_{ℓ} :

$$I_{\ell}^0 = (\tau_{\ell-1} - \tau_{\ell}) (1-\omega_{\ell}) R_{\ell} \quad . \quad (3)$$

The τ_ℓ are the transmittances from the observer to the far side of layer ℓ . These calculations are done at each wavenumber or spectral bin increment. Since MODTRAN is an LTE model, its source term is simply the Planck blackbody function. SAMM models both LTE and non-LTE radiators by defining the source term as an average over the individual sources (j) weighted by their incremental spectral bin equivalent widths, $\Delta W_{\ell j}$ ($= W_{\ell j} - W_{\ell-1,j}$):

$$R_\ell = \frac{c_1 \nu^3}{\pi} \sum_j \Delta W_{\ell j} \left(\frac{\rho_{\ell j}'}{\rho_{\ell j}' - \rho_{\ell j}} \right) / \sum_j \Delta W_{\ell j} , \quad (4)$$

where c_1 is the first radiation constant ($c_1 = 2\pi h c^2$, h is the Planck constant and c is the speed of light), ν is the spectral bin frequency, and $\rho_{\ell j}'$ & $\rho_{\ell j}$ are the densities of the upper & lower states, respectively. The sources of emission being summed over include SHARC molecular transitions, MODTRAN band model lines for non-SHARC species, and the MODTRAN continuum sources. This expression for the source term reduces to the blackbody function under LTE conditions, is exact in the weak line limit, and gives greatest weight to the strongest absorber in a given layer along the LOS. The equivalent width for each spectral bin is defined as a species' absorption within that bin and is given by

$$W_{\ell j} = \int_{\Delta\nu} d\nu [1 - \tau_{\ell j}(\nu)] , \quad (5)$$

where $\tau_{\ell j}$ is the spectral transmission through layer ℓ for absorber j and $\Delta\nu$ is the width of the spectral bin.

The spectrally averaged transmission arising from an ensemble of absorbers centered randomly within the spectral interval is given by

$$\tau_\ell = \prod_j \left(1 - \frac{W_{\ell j}}{\Delta\nu} \right) . \quad (6)$$

This equation implicitly includes the statistical correction for random line overlap.⁽⁵⁾ Both the single line and band model equivalent widths for a Voigt lineshape are evaluated using the Rodgers and Williams^(6,7) (RW) interpolation formula. This formula has been shown to give a peak error of 8%. The Lorentzian line tails are subtracted from the RW expression to obtain the Voigt equivalent width within a spectral bin.^(2,8) This correction is important for lower altitudes where the total equivalent width of a strong line can easily exceed the typical bin width of 1 cm^{-1} . The RW interpolation formula requires evaluation of equivalent widths in the Lorentz, Doppler, and weak-line limits. Standard approximations⁽⁹⁾ involving

Curtis-Godson^(2,7) path averages are used to evaluate these widths. Curtis-Godson path averages are used to approximate paths through multiple layers by a single homogeneous path.

An upgraded formulation for the single scattering solar radiance has been integrated into both MODTRAN and SAMM. The single scatter component can be written

$$I_{\ell}^{ss} = \pi F^{\text{sun}} \int_{\tau_{\text{sct } \ell}}^{\tau_{\text{sct } \ell-1}} \frac{P_{\ell}}{4\pi} \tau_{\text{abs}}^L(\tau) \tau_{\text{sct}}^{\text{sun}}(\tau) d\tau \quad (7)$$

F^{sun} is the extraterrestrial solar flux and P_{ℓ} is the scattering phase (angular cross-section) function. Since the variation in scattering angle along the LOS is negligible, a layer averaged phase function can be factored out of the integral. The question remains as to how the L shaped path (observer to scattering point to sun) transmittance from absorption τ_{abs}^L varies with the LOS scattering transmittance. In deriving an expression for the layer thermal emission, Cornette⁽¹⁰⁾ assumed that transmission from absorption and scattering both varied exponentially across a layer. This is equivalent to Minschwaner's assumption⁽¹¹⁾ of equal effective absorption and scattering scale heights within a layer. We similarly assume that

$$\tau_{\text{abs}}^L(\tau) = \tau_{\text{abs } \ell-1}^L \left[\frac{\tau_{\text{abs } \ell}^L}{\tau_{\text{abs } \ell-1}^L} \right]^z \quad (8)$$

where

$$z = \frac{\ln [\tau / \tau_{\text{sct } \ell-1}]}{\ln [\tau_{\text{sct } \ell} / \tau_{\text{sct } \ell-1}]} \quad (9)$$

With this assumption, the single scatter solar integral can be evaluated analytically yielding

$$I_{\ell}^{ss} = \frac{F^{\text{sun}} P_{\ell}}{4} \ln\left(\frac{\tau_{\text{sct } \ell-1}}{\tau_{\text{sct } \ell}}\right) \frac{\tau_{\ell-1}^L - \tau_{\ell}^L}{\ln [\tau_{\ell-1}^L / \tau_{\ell}^L]} \quad (10)$$

The first logarithm term equals the layer scattering optical depth, and the final term can be interpreted as an averaged L shaped path total transmittance divided by the extinction (absorption plus scattering) layer optical depth.

In MODTRAN and hence SAMM, the molecular and aerosol single scatter solar radiance contributions are treated separately. The total single scatter solar radiance is a sum of the two terms. Three choices are available for the aerosol phase function: user-supplied, Henyey-Greenstein, or Mie generated internal database,⁽³⁾ CARDS 3A1 and 3A2 of the MODTRAN/LOWTRAN 7 input stream.⁽³⁾ The L shaped path transmission terms, τ_{ℓ}^L , are

calculated for all the SHARC and MODTRAN absorbers, rigorously determining the column density through the multiple higher altitude regions.

The MODTRAN LTE treatment of multiple scattering

$$I_{\ell}^{\text{ms}} = (\tau_{\ell-1} - \tau_{\ell}) \omega_{\ell} [(1-\beta_{\ell}) F_{\ell}^{\mp} + \beta_{\ell} F_{\ell}^{\pm}] / \pi \quad , \quad (11)$$

has not been altered because multiple scattering is only significant at the lower altitudes where LTE conditions prevail. At each layer boundary, the upward and downward fluxes, $F_{\ell}^{\pm}$, the scattering albedo, ω_{ℓ} , and the backscatter fraction, β_{ℓ} are calculated. The two flux calculation, which uses a vertical path, is performed for the atmosphere defined at the observer's latitude and longitude and with its high altitude boundaries fixed at 30, 35, 40, 45, 50, 70, and 100 km; multiple scattering is not included above 100 km. When multiple scattering is not requested, the scattering albedo in Equations (3) and (11) is set to zero.

3.2 Low Altitude Solar Attenuation

Since SHARC-3, MODTRAN and SAMM calculate LOS radiances in the region of the solar terminator, solar zenith angles that are greater than 90° must be accommodated. Under these conditions, the solar irradiance passes through parts of the atmosphere that are below the lower boundary of the chemical kinetics module (50 km in SHARC-3, 30 km in SAMM). Since some of this radiation is absorbed by the lower atmosphere, its intensity, and spectral structure are modified. The amount of absorption at any wavenumber is a function of the solar zenith angle, or equivalently the minimum altitude through which the sunlight passes, and of the aerosol and molecular content of the lower atmosphere.

SHARC-3 and SAMM distinguish the attenuation of solar irradiance by "line center" and "continuum" sources. Both codes model the line center attenuation of solar irradiance by performing LBL calculations for each vibrational transition. They use an approximate distribution of lines from a BANDS file (Section 6.3 of the SHARC 3 Manual)⁽¹⁾ to describe each transition. Curtis-Godson averages are used to define Doppler and collision broadened half-widths for the solar paths. The "continuum" sources here denote all sources of absorption other than the particular vibrational band under consideration.

In SHARC-3 lower atmosphere continuum transmittances and Curtis-Godson sums are pre-stored for three fixed aerosol profiles and for one fixed molecular profile (derived from the US Standard Atmosphere). Since SAMM input includes profile information for the lower

atmosphere, the continuum transmittances, and Curtis-Godson sums are calculated as needed by making the necessary calls to MODTRAN. Thus, the solar attenuation is sensitive to variations in aerosol and cloud conditions.

4. RUNNING SAMM

This section serves as a reference for the user who wants to get SAMM running without making modifications to the kinetics supplied with the code. The instructions are written assuming SAMM is being installed on a UNIX based system; some adjustments are necessary for PC installations. The required files and auxiliary programs are discussed, allowing preparation for the first run. The menu system used by the INPUT module to communicate with the user is outlined in some detail. If modifications to the kinetics files are required, the user should read Sections 6 and 7 of the SHARC-3 manual.⁽¹⁾

4.1 Data File Preparations for Running SAMM

The specific tasks which must be completed before initially running SAMM are:

- compile interp.f to create the executable interp, and run the command file interp.run to create the link files containing the chemical kinetic schemes;
- compile and run dirac.f to create the lines file SHARC.H92 (must be created even if a SHARC-3 lines file already exists because the files have different access);
- compile and run ufmake.f to create the band model parameter file UFTAPE and the subroutine samblk.f; and
- move samblk.f into the source directory, and compile the SAMM source.

After completing these steps, a user can perform basic SAMM runs. Additional preparations are required if the user wishes (1) to use atmospheric profiles other than those supplied with the code, (2) to include aerosol profiles, or (3) to define scattering phase functions other than those internal to the code. This section describes all the above preparations.

4.1.1 NECESSARY DATA FILES

Prior to any SAMM calculation, kinetic "linking" files must be created. This is accomplished by running the INTERPRETER once for each radiator; the command file interp.run can be used to perform these multiple run of the INTERPRETER in a single step. The INTERPRETER reads chemical equations and rate constant information. The procedure is detailed in Section 7.1 of SHARC-3 manual;⁽¹⁾ the result is binary linking files for each radiator. As discussed below, these files and their associated states and bands files need not be

in the same directory as the executable version of SAMM; rather, they can be placed in a separate kinetics directory for convenience. Indeed, these files can be shared with a stand-alone version of SHARC-3.

The LBL calculations in SAMM are performed using the SHARC-3 lines file: this file contains line parameters from HITRAN92 along with auxiliary data for hot O_3 , NO, and NO^+ . The SAMM band model calculations use data from the MODTRAN band model parameter tape. Both these data files must be converted to binary for use by SAMM. Note that even though the SAMM ascii data files are identical to the ascii versions from SHARC and MODTRAN, the binary files are different and presently can not be used interchangeably.

The direct-access, binary file SHARC.H92 is created from the sequential, formatted SHARC.ASC file by compiling and executing the `dirac.f` FORTRAN program. The large SHARC.ASC file can be deleted once SHARC.H92 has been created (if needed, SHARC.ASC can be regenerated from SHARC.H92 by running program `linasc.f`). A copy of the FORTRAN block data file `RECDAT.f` is also created when `dirac.f` is run. Routine `RECDAT.f` is already included in `modblk.f` and does not have to be integrated into SAMM.

The direct-access, binary band model parameter file UFTAPE is created by compiling and executing the `ufmake.f` FORTRAN program. UFTAPE.ASC can be deleted once UFTAPE has been created (if needed, UFTAPE.ASC can be regenerated from UFTAPE and `samblk.f` by running program `bmasc.f`). SAMM requires that UFTAPE and SHARC.H92 be stored in the same directory.

The program `ufmake.f` also creates the block data routine `samblk.f`. This block data contains a data statement defining LREC, the logical record length used to create UFTAPE. Since the value of LREC is machine dependent, `samblk.f` must be moved to the directory containing the SAMM source code. No version of `samblk.f` is delivered with the source to avoid use of an incorrect logical record length!

4.1.2 OPTIONAL DATA FILES

As noted in Section 2.1, the SAMM tape contains a number of default atmospheric profiles. Additional profiles can be generated using the SAG program. Input to this routine includes temporal, geographic location, and solar activity data. Best guess profiles in the SAMM/SHARC format are output and can be used directly. A user may input customized profiles, based for example on radiosonde data, by creating an atmospheric file in the SAMM/SHARC format. A description of the format of the atmospheric files is included in Section 6.6 of the SHARC-3 manual⁽¹⁾. The SAG manual⁽⁴⁾ details the assumptions and data

sources used in SAG, and provide user instructions. The user instructions for SAG are also included in Section 7.3 of the SHARC-3 user's manual.⁽¹⁾ Note that for SAMM, input atmospheric profiles must extend all the way to the ground.

The MODTRAN parameters for selecting aerosol profile models, including clouds and rain, are input to SAMM through the HAZE.INP file. If this file does not exist, SAMM will run assuming no aerosols. HAZE.INP contains CARD2, CARD2A, CARD2B, and CARD2D from the MODTRAN/LOWTRAN 7 input file. Their format and description are described in detail in Section 3 of the LOWTRAN 7 manual.⁽³⁾ If aerosols are to be included, minimally CARD2 is necessary. CARD2 assigns pre-stored altitude and seasonal-dependent aerosol profiles and aerosol extinction coefficients. The optional aerosol inputs are used for calculations involving cirrus clouds (CARD2A), the Army Vertical Structure Algorithm (CARD2B), and user-specified attenuation coefficients (CARD2D).

If a user chooses to input a user-defined aerosol phase function, the data is input through a PHASE.INP file. PHASE.INP contains the MODTRAN inputs CARD3B1 and CARD3B2. The format and description of these inputs are described in detail in Section 3 of the LOWTRAN 7 manual.⁽³⁾

4.2 The Interactive Input Module - Modifications to SHARC-3

Once necessary/optional input data files have been created, the user must define the calculation scenario. The scenario is input to SAMM through a SAMM.INP file. The SAMM.INP file has three primary sections. The first section contains the SHARC inputs (in fact, a SAMM.INP file can be converted to a SHARC-3 input file with only minor modifications; see Section 5.2). The second section of SAMM.INP begins with the line "CMOS-00 MOSART INPUTS: ..." and contains MOSART input information. MOSART is a low altitude and backgrounds code⁽¹²⁾ that is currently being integrated into SAMM; since this work is not completed, the MOSART inputs presently have no effect on SAMM calculations, and this section of SAMM.INP should be ignored. The third and final section of SAMM.INP begins with the line "CM-00 MODTRAN INPUTS: ..." and contains MODTRAN input information not already defined in the SHARC section of the input stream.

The user updates a SAMM.INP file by running SAMM interactively. If no SAMM.INP file is found, a default SAMM.INP (TEST CASE 1) is initially created. The user then makes desired changes to SAMM.INP by responding to a menu-query system. For more experienced users, SAMM can be executed by circumventing the input module and directly

entering changes to the SAMM.INP file with an editor. After SAMM.INP has been created/updated, SAMM calculations can be performed in either interactive or batch mode.

A successful SAMM calculation produces considerable output. The files are:

- Journal file - "SAMM.LOG" (Section 5.1),
- SAMM input file - "rootname.INP" (Section 5.2),
- SHARC general output file - "rootname.OUT" (Section 5.3),
- Population files (Section 5.4),
- Spectral radiance file - "rootname.SPC" (Section 5.5),
- Transmittance file - "rootname.TRN" (Section 5.6),
- Bandpass file - "rootname.RAD" (Section 5.7),
- MODTRAN input file - "rootname.TP5" (Section 5.8),
- MODTRAN standard output file - "rootname.TP6" (Section 5.9),
- MODTRAN plotting file - "rootname.TP7" (Section 5.10), and
- MODTRAN auxiliary output file - "rootname.TP8" (Section 5.11).

The user can choose to have the program delete any of the "rootname.extension" files prior to completion to save disk space. If no warnings, cautions or errors are written to the journal file, SAMM.LOG is deleted just prior to program completion. The user should always check if the journal file was saved and, in that case, read it to insure the calculation was performed correctly. During auroral calculations, several warning messages are given stating that different molecular species were not found. Since auroral excitation is only calculated for CO₂, NO, and NO⁺, this is reasonable, but the user should check that these were not inadvertently omitted too.

The SAMM input module is derived from the SHARC-3 input module. A menu-query system walks the user through the required inputs. In general, typing a 0 or carriage return will take the user up a level in the menu system; otherwise, the user may input new information or enter a sub-menu. When a sub-menu is entered, current values of the input variables are displayed. This allows the user to scan the current values and decide if anything needs to be changed. In this section, differences between the SHARC and SAMM input modules will be highlighted; further details are described in Sections 4.2 and 4.3 of the SHARC-3 manual.

At the start of an interactive run, the top-level menu appears, Figure 1. Other than header information, the only difference between the SHARC and SAMM top-level menus is the addition in SAMM of Entry 11. MODTRAN PARAMETERS.

SHARC-3 AND MODTRAN-2 MERGED, SAMM
REVIEW OR MODIFY INPUT PARAMETERS
1) TITLE FOR CALCULATION
2) REGION DEFINITION
3) LOS GEOMETRY
4) SPECTRAL INTERVAL, RESOLUTION AND SPECIES
5) OUTPUT DATA
6) STANDARD SET-UP FOR FILE NAMES
7) INSTALLATION SETUP
8) UPDATE DEFAULT FILE AND EXIT FOR BATCH EXECUTION
9) UPDATE DEFAULT FILE AND EXIT
10) EXIT WITH NO UPDATE OF DEFAULT FILE
11) MODTRAN PARAMETERS
ENTER # OF ITEM TO BE CHANGED OR 999 TO CONTINUE SAMM EXECUTION

Figure 1. The Top-Level SAMM Menu.

4.2.1 TITLE

The SAMM and SHARC title specifications are identical. A calculation may be given a title containing up to 68 characters.

4.2.2 REGION DEFINITION

The REGION DEFINITION menus in SAMM and SHARC-3 (described in Section 4.2 of the SHARC-3 manual⁽¹⁾) are identical with one exception. Each atmospheric profile in the two codes is associated with a fixed solar earth center angle (solar earth center angle is used rather than solar zenith angle, because the former is not affected by spherical refractive geometry and therefore is altitude independent at a fixed latitude and longitude). When that angle is between 90.0° and 107.1984° , SHARC requires a "LOWER ATMOSPHERE AEROSOL NUMBER" which is used to estimate the effect of aerosol attenuation on solar

irradiances. Since SAMM models the lower atmospheric attenuation explicitly, SAMM does not require this input.

4.2.3 LOS GEOMETRY

The SAMM LOS GEOMETRY menu, Figure 2, differs from SHARC-3's in two respects. Entry 2, the SUN LOCATION, requires specification of the year and outputs the day of year, the year, and the time of day. The year is used to determine leap years. MODTRAN uses the day of year to determine sun-to-earth distance. If solar angles are directly input, SAMM prompts the user to select from the two days of the year for which the sun is at the input latitude (there is no prompting of the user at the extrema, $\pm 23.45^\circ$ latitude). Also, the allowed path parameters differ somewhat between SAMM and SHARC-3. Since SHARC-3 is strictly a high-altitude code, no LOS passing below 50 km altitude is permitted.

3) REVIEW OR MODIFY LINE-OF-SIGHT GEOMETRY

CURRENT LOS DEFINITION:

1. COORDINATE SYSTEM CENTERED AT GEOGRAPHIC NORTH POLE

2. SUN LOCATION

SOLAR LATITUDE: 0.00 DEG NORTH

SOLAR LONGITUDE: 0.00 DEG EAST OF GREENWICH

DAY OF YEAR: 80 (MAR 21,1993)

GREENWICH MEAN TIME: 0.061 (Decimal Hours)

3. SPHERICAL EARTH ASSUMED

4. ABSOLUTE LOS LOCATION SPECIFICATION

DIRECT INPUT OF LATITUDE/LONGITUDE INFORMATION

5. PATH TYPE IS LIMB VIEWING PATH

TANGENT POINT INFORMATION

TANGENT HEIGHT: 10.00 KM

TANGENT LONGITUDE: 0.000 DEGREES EAST OF GREENWICH

TANGENT LATITUDE: 0.000 DEGREES NORTH

LOCAL AZIMUTH AT TANGENT POINT

AZIMUTH ANGLE: 0.000 DEGREES EAST OF NORTH

ENTER # OF ITEM TO CHANGE OR
0 TO CONTINUE

Figure 2. LOS GEOMETRY Sub-Menu.

SAMM allows LOS down to the ground. If the input path intersects the earth, the radiance/transmission calculation is performed for the path terminating at the earth's surface. SAMM does not support the MODTRAN ITYPE=1 option, a homogeneous horizontal path.

Three additional points should be made regarding the LOS geometry:

- (1) Upon exiting from the LOS section of the interactive module, a "SUMMARY OF LINE-OF-SIGHT GEOMETRY" is written to the screen. This information is provided to enable the user to check inputs, but the displayed calculated parameters are determined using straight line geometry (once inputs have been set, SAMM calculates column densities using spherical refraction geometry and the user-specified LOS parameters).
- (2) SAMM, unlike SHARC-3, does not give a warning if the selected LOS does not pass through a local (auroral or ambient) region. Even if a LOS misses a local region, the region can influence observed radiance if intersected by single scatter solar paths.
- (3) SHARC-3 and MODTRAN use different conventions for describing longitude. SHARC-3 measures longitude in degrees East of Greenwich, while MODTRAN longitudes are in degrees West of Greenwich. SAMM explicitly prompts for longitudes in degrees East of Greenwich.

4.2.4 SPECTRAL INTERVAL, RESOLUTION, AND SPECIES

If Entry 4 is selected from the top-level menu, Figure 1, the SPECTRAL INTERVAL, RESOLUTION AND SPECIES sub-menu, Figure 3, is displayed. This menu differs from the SHARC version in that all frequency inputs are integers. In fact, the spectral interval minimum and maximum must be multiples of 5, and the highest resolution available is 1 cm^{-1} . Resolution is defined as in MODTRAN, equal to the FWHM (Full Width at Half Maximum) for a triangular slit created from rectangular 1 cm^{-1} bins. The SPECTRAL INTERVAL, RESOLUTION AND SPECIES sub-menu has one new input. Entry 5 prompts for output step size. This input allows, for example, one to select a 2 cm^{-1} triangular slit function and have radiances output each wavenumber. Since SHARC-3 employs a non-overlapping rectangular slit function, spectral comparisons between SAMM and SHARC-3 are strictly equivalent only if resolution and step size are set to 1 cm^{-1} in both codes (all test cases are run with 1 cm^{-1} resolution and step size). The SPECIES list selects which SHARC non-LTE species are to be included in the radiance/transmission calculation; selection of MODTRAN molecular radiators not supported by SHARC-3 is made from the MODTRAN PARAMETERS sub-menu (Section 4.3.7).

4) REVIEW OR MODIFY SPECTRAL INPUTS...

CURRENT VALUES ARE:

1. MINIMUM WAVENUMBER :	1500
2. MAXIMUM WAVENUMBER :	4000
3. SPECTRAL RESOLUTION (MINIMUM OF 1 CM-1) :	1
4. SPECIES INCLUDED IN RADIANCE CALCULATION	
NO ISOTOPE 14N 16O	AFGL ISOTOPE # 1
NO+ ISOTOPE 14N 16O +	AFGL ISOTOPE # 1
5. SPECTRAL STEP SIZE FOR OUTPUT	1
ENTER # OF ITEM TO BE CHANGED OR	
0 TO CONTINUE	

Figure 3. SPECTRAL INTERVAL, RESOLUTION, AND SPECIES Sub-Menu.

4.2.5 OUTPUT DATA

SAMM has eliminated the line-of-sight (Entry 9) and spectral radiance (Entry 10) output options from the SHARC-3 OUTPUT DATA sub-menu. SAMM performs the LOS and radiative transport calculations in the MODTRAN section of the code, and uses MODTRAN inputs (Sections 4.3.2 and 4.3.3) to determine which LOS and spectral data are to be printed.

4.2.6 STANDARD SET-UP FOR FILE NAMES

The STANDARD SET-UP FOR FILE NAMES sub-menu in SAMM differs from the corresponding sub-menu in SHARC-3 in that it allows the user to determine which output files are to be saved, and which are to be deleted at the completion of a run. Figure 4 contains a sample of this sub-menu. After entering 1 from this menu, the user is prompt for a new root name for the output files. The keep/delete status of an output file is toggled by entering the letter at the beginning of the line containing the output file name (A-J). Since SAMM output can be large, disk space can be saved by deleting unneeded output. This is especially convenient if numerous SAMM runs are being performed sequentially.

6) REVIEW OR MODIFY STANDARD I/O FILE NAMES
AND THEIR STATUS

1	A.	KEEP	SPECTRAL RADIANCE FILE	TEST1.SPC
	B.	KEEP	TRANSMISSION FILE	TEST1.TRN
	C.	KEEP	STANDARD OUTPUT FILE	TEST1.OUT
	D.	KEEP	STANDARD INPUT FILE	TEST1.INP
	E.	KEEP	BANDPASS FILE	TEST1.RAD
	F.	KEEP	MODTRAN INPUT FILE	TEST1.TP5
	G.	KEEP	MODTRAN STANDARD OUTPUT FILE	TEST1.TP6
	H.	KEEP	MODTRAN PLOTTING FILE	TEST1.TP7
	I.	KEEP	MODTRAN AUXILIARY OUTPUT FILE	TEST1.TP8
	J.	DELETE	MOSART INPUT FILE	TEST1.INM

2. CASE SELECTION FOR FILE NAMES UPPER

3. DIRECTORY PATH FOR OUTPUT FILES
OUTDIR/

ENTER # OF ITEM TO BE CHANGED OR
LETTER TO TOGGLE FILE STATUS OR
0 TO CONTINUE

Figure 4. STANDARD SET-UP FOR FILE NAMES Sub-Menu.

4.2.7 INSTALLATION SETUP

The INSTALLATION SETUP sub-menus from SAMM and SHARC are essentially identical. The only caveat is that the directory name selected for the SHARC lines files is also the directory name for the band model parameter file. Thus, these two data files must be in the same directory. Also, SAMM permits the user to input the name of the unformatted, direct-access band model parameter tape (the default name is UFTAPE).

4.2.8 EXIT/CONTINUE OPTIONS

The SAMM exit/continue options, Entries 8, 9, 10 & 999 from the top-level menu, have the same meaning as in SHARC-3. However, if Entry 8, 9, or 999 is selected and a repeat run is requested (see MODTRAN PARAMETERS), the interactive module will not terminate until prompting for repeat run inputs is completed.

4.3 The Interactive Input Module - MODTRAN PARAMETERS

Selecting Entry 11 from the top-level menu, Figure 1, displays the MODTRAN PARAMETERS sub-menu, Figure 5. The inputs are primarily those from CARD1 and CARD5 of MODTRAN.

4.3.1 RUNMOD

The character*1 string "RUNMOD" replaces the logical variable "MODTRN" from the MODTRAN program. RUNMOD is used to select the mode in which SAMM is to be run. The current choices are:

- "S" SAMM mode, combined LBL/band model calculations;
- "M" MODTRAN mode, an LTE band model calculation; or
- "G" GEOMETRY mode, a calculation of column densities only.

11) MODTRAN VARIABLES THE USER CAN MODIFY AND THEIR CURRENT VALUES ARE:			
1)	RUNMOD =	S	SAMM COMBINED LBL/BAND MODEL CALCULATION
2)	IEMSCT =	2	THERMAL+SOLAR RADIANCE CALCULATION
	IPH =	0	HENYEY-GREENSTEIN AEROSOL PHASE FUNCTION
	G =	0.900000	HENYEY-GREENSTEIN ASYMMETRY FACTOR
	IMULT =	1	MULTIPLE SCATTERING TO BE CALCULATED
3)	NOPRT =	0	NORMAL OUTPUT PRINTED
4)	TBOUND =	0.000 K	(NO SOURCE AT END OF LOS)
5)	SALB =	0.000000	GROUND SCATTERING ALBEDO
6)	IRPT =	0	THIS WILL BE THE FINAL CALCULATION
7)	LMOL =	N2O EXCLUDED	O2 EXCLUDED
		SO2 EXCLUDED	NO2 EXCLUDED
		NH3 EXCLUDED	HNO3 EXCLUDED
ENTER # TO MODIFY			
0 TO CONTINUE			

Figure 5. MODTRAN PARAMETERS Sub-Menu.

4.3.2 IEMSCT, IPH, G, and IMULT

Entry 2 from the MODTRAN PARAMETERS sub-menu determines the type of radiance/transmittance calculation to be performed. Following MODTRAN, the four options controlled by IEMSCT are:

- "T" Transmittance only (IEMSCT=0),
- "R" Thermal Radiance (IEMSCT=1),
- "S" Solar + Thermal Radiance (IEMSCT=2), and
- "I" Transmitted Solar Irradiance (IEMSCT=3).

Although the radiance calculations do output total transmittance, the layer loop for each frequency is terminated once the total transmittance drops below 10^{-5} ; the transmittance option loops over all layers allowing the user to calculate smaller total transmittances and to separate out the contributions to transmittance from each of the extinction sources. When radiance calculations are performed, multiple scattering can be included. If single or multiple scattering is turned on, either a Henyey-Greenstein, a user-defined, or a pre-stored MIE phase function may be selected. An asymmetry factor is input for use with the Henyey-Greenstein function, and a PHASE.INP file must be supplied if a user-defined phase function is requested. It is advised that users avoid the pre-stored MIE phase functions for band radiance profile studies that pass through 30 km altitude; these phase functions can introduce a false discontinuity. The LOWTRAN 7 manual⁽³⁾ provides additional details about the phase function inputs.

4.3.3 NOPRT

The NOPRT input determines the amount of output generated in the MODTRAN standard output file, rootname.TP6. It is recommended that this input generally be set to 1 (enter "S" in the interactive mode) so that the Small (minimal) output is generated. Minimal output includes a listing of the MODTRAN inputs, optical path column densities for all extinction sources, and spectral & bandpass radiance/transmittance data. Entering "M" sets NOPRT to 0, and the Medium (so-called normal) output is produced, which includes all MODTRAN molecular and aerosol profiles (0-100 km) and column densities for the scattering point to sun paths. A value of -1 is assigned to NOPRT when "L" for Large is entered, and then optical and sun path column densities for each vibrationally excited state of the included SHARC radiators is output.

When NOPRT equals -1, additional data is also output to the MODTRAN auxiliary file, rootname.TP8. For a transmission run (IEMSCT=0), the contribution to spectral transmission from each species is printed out; for multiple scattering runs (IMULT=1), weighting function data, i.e., the change in total transmittance with segment length along the LOS, is output.

4.3.4 TBOUND

When the MODTRAN variable TBOUND is non-zero, a blackbody source is placed at the end of the input LOS. If TBOUND exceeds zero, its value is taken to be the blackbody temperature in Kelvin (the emissivity is determined from SALB, Section 4.3.5). When TBOUND is less than or equal to zero, a blackbody source is placed at the end of the LOS only if the PATH terminates at the earth's surface; in that case, the atmospheric profile temperature at 0 km altitude is assumed to be the surface temperature (note that TBOUND is never used as the earth's surface temperature for multiple scattering calculations).

4.3.5 SALB

SALB is a wavelength independent scattering albedo, and its allowed values range from zero and one, inclusive. When TBOUND exceeds zero, 1-SALB is the source emissivity. SALB is also the ground scattering albedo used in the multiple scattering calculations and used to determine the surface blackbody and reflected solar contributions for LOS terminating at the earth's surface.

4.3.6 IRPT

The IRPT option enables a user to perform multiple calculations in a fixed environment without having to rerun SAMM for each calculation. This option has many applications such as comparing MODTRAN and SAMM results for an identical LOS (TEST CASE 6), or determining bandpass radiance profiles (TEST CASE 7). Repeat runs are not permitted following a geometry only run (RUNMOD='G').

If IRPT equals zero, a single LOS calculation is performed. IRPT must be set to 1 or 4 to run an additional calculation. No new column densities are calculated when IRPT=4. This "old column densities" option can be used

- to switch from a combined LBL/band model calculation, RUNMOD="S", to a straight band model calculation, RUNMOD="M", or vice versa,
- to change spectral bandpass parameters, or
- to follow a radiance calculation, IEMSCT=1 or IEMSCT=2, by a transmittance calculation, IEMSCT=0, (the reverse order is not permitted since the transmission calculation does not generate all the column densities required for a radiance run).

When IRPT equals 1, a repeat run calculation is performed in which all new column densities are generated. Any new LOS can be run. The primary restrictions are that the ambient and auroral environments remain fixed, the sun location is held constant, and no changes are made in the radiator list (this last requirement will be dropped in future versions of SAMM).

Determining when IRPT should be set to 1 and when it can be set to 4 might seem confusing. In fact, the interactive model automatically determines whether new column densities need to be calculated by examining the LOS inputs, and assigns the proper value to IRPT. It is only important for the user to understand the difference if he or she is modifying the SAMM input stream by directly editing the SAMM.INP file. In that case, it is critical that the user specifies the correct value.

When a repeat run is requested and the user types Entry 8, 9, or 999 from the top-level menu, Figure 1, the interactive module does not terminate. Instead the new menu shown in Figure 6, appears, prompting the user for the first repeat run inputs. If the original

REVIEW OR MODIFY INPUT DATA FOR REPEAT RUN # 1 1) EXIT WITH REPEAT RUN # 1 ELIMINATED 2) MODTRAN PARAMETERS 3) LOS GEOMETRY 4) SPECTRAL INTERVAL AND RESOLUTION ENTER # OF ITEM TO BE CHANGED OR 5 TO CONTINUE (REPEAT RUN INPUT COMPLETED)

Figure 6. REPEAT RUN # 1 Menu.

SAMM.INP file included inputs for a repeat run, those inputs are the assumed defaults. On the other hand, if the specification of a repeat run is new, the default parameters for the repeat run are those from the prior calculation.

The REPEAT RUN sub-menus are identical to the corresponding top-level sub-menus except for necessary omissions. Since repeat runs must include the same radiator lists, Entry 7 from the MODTRAN PARAMETERS sub-menu, Figure 5, and Entry 4 from the SPECTRAL INTERVAL sub-menu, Figure 3, have been deleted. The LOS GEOMETRY sub-menu differs in that the SUN LOCATION option, Entry 2 from Figure 2, is removed.

In the MODTRAN PARAMETERS sub-menu, the IRPT variable always refers to the next repeat run. Thus, if IRPT is not set to 0 and the user responds 5 from the REPEAT RUN # 1 menu, Figure 6, a REPEAT RUN # 2 menu will appear. To terminate the interactive session after a single repeat run, either set IRPT to 0 in the MODTRAN PARAMETERS sub-menu, or let the REPEAT RUN # 2 menu appear and then enter a 1. This entry eliminates the current repeat run. If 1 were to be entered directly from REPEAT RUN # 1 menu, no repeat run would be performed.

SAMM presently allows "approximately" 50 repeat runs (the actual number of allowed repeat runs depends on the number of lines of input in the first calculation, and this varies depending on the number of radiators, the number of regions, etc.). If more runs are requested, an error will appear in the rootname.LOG file to indicate that parameter "NDMAXM" must be increased in file PARMS.H. This parameter should be increased by 5 for each additional run requested.

4.3.7 LMOL

The array LMOL is used to determine which of the six band model radiators (N_2O , O_2 , SO_2 , NO_2 , NH_3 & HNO_3) are to be included in a LOS radiance/transmittance calculation. Any combination of the radiators may be included in a calculation. However, even if a molecule is excluded from a radiance calculation, its attenuation of solar irradiance from below 30 km is still included in the calculation of solar attenuation rates. This is true even though this attenuation is not modeled when calculating single and multiple scatter solar radiance contributions.

5. SAMM OUTPUT FILES

Entry 6 of the top-level menu, Figure 1, prompts the user for an output root name. This root name is used along with appropriate suffixes to name all SAMM output files except the journal file and population files.

5.1 Journal File

The SAMM journal file (SAMM.LOG) contains various informational statements generated during SAMM execution of the SHARC-3 routines. The majority of messages are due to improper preparation of the input files. An "error" message during execution is considered fatal, and execution will stop after the error message is written to the journal file. A "warning" or "caution" message is not fatal (that is, does not terminate execution), but it should inform the user that input files are inconsistent, that only a partial calculation has been performed, or that numerical difficulties have been encountered and fixed in one of the SHARC-3 modules. The user should monitor the journal file after each SAMM run to insure that the desired calculation was properly performed. The journal file is deleted just prior to code completion if no messages were written to the file.

During auroral calculations, several warning messages are routinely given stating that different molecular species were not found. Since auroral excitation is only calculated for CO₂, NO, and NO⁺, these messages are reasonable, but the user should check that these species were not inadvertently omitted too.

5.2 SAMM Input File

When SAMM is run, a copy of the input file (SAMM.INP) is written to the output directory as rootname.INP. This helps avoid the possibility of losing the original input. If SAMM.INP contains extraneous information at the end of the file, that information will be lost. Also, if the user happens to choose "SAMM" for the root name, the copy of SAMM.INP is written to SAM.INP to avoid writing over the original input file.

The rootname.INP file can be used as a SHARC-3 input file by copying the file into SHARC.INP and appending the lines containing the population file solar zenith angles with the appropriate lower atmosphere aerosol number. SHARC-3 will ignore the MOSART and MODTRAN input parameters which are located at the end of the rootname.INP file. For

SHARC, the LOS must not drop below 50 km. Also, the atmospheric profile, the population and the binary lines files for SHARC-3 and SAMM are different; an error will be logged if SAMM profile, population or line files are used as input to SHARC-3.

5.3 SHARC General Output File

The SHARC general output file "rootname.OUT" contains a summary of selected output from each of the SHARC-3 modules in SAMM. The format of this file is identical to that of SHARC-3. The SAMM version is different, however, in that no column density or radiance information is included; the SHARC-3 column density and radiance modules are not part of SAMM. A description of the SHARC-3 general output file is included in Section 5.2 of the SHARC-3 manual.⁽¹⁾

5.4 Population File

For a given set of radiators and kinetic schemes, the excited-state populations for each atmospheric layer will change only when a new model atmosphere is used, a new solar zenith angle is defined, or auroral conditions change. Thus, the excited-state populations and the information necessary to uniquely characterize them are written to a binary "population" file. This allows the user to perform multiple SAMM calculations without re-calculating the populations each time. Since these calculations are usually the most cpu intensive part of a SAMM run, using previously saved population files can be a great benefit. The information saved in a population file is:

- The model atmosphere file name,
- The molecular radiators and the associated "linking", "states", and "bands" file names,
- The list of species for each molecular radiator,
- The molecular states file for each molecular radiator,
- The state populations and associated temperatures for each radiator, and
- The auroral parameters when the auroral option is used.

The populations directory and population file names are defined by the user in the interactive input session from sub-menus 7 and 2 of the top-level menu, respectively. If not suppressed, the population file names will be appended with the root of the atmospheric profile name and with the solar zenith angle written as a three digit integer (000 to 180). Thus, if the

"MIDLAT.DAY" atmosphere is used with a 45° solar zenith angle and the input root population name is "P", the output population file will have the name "PMIDLAT.045".

5.5 Spectral Radiance File

The ASCII file "rootname.SPC" is a simple two column file. The frequency (cm^{-1}) and the spectral radiance ($\text{W}/\text{sr}/\text{cm}^2/\text{cm}^{-1}$) are written as an (x,y) ordered pair. This format is convenient for either plotting the calculated spectral radiance directly or reducing these data further. For example, the user may wish to apply a specific filter function to the spectral radiance or to convert to a set of units other than those used in SAMM (these manipulations can be performed using DEGRAD.f, a FORTRAN program included on the SAMM tape). The data is printed at a constant frequency interval equal to the step size defined in the spectral bandpass data sub-menu, Section 4.2.4. A "\$" delimiter in column 2 is used to separate data generated from repeat runs, Section 4.3.6; the delimiter lines also list the bandpass radiance and the frequency and value of the spectral radiance maximum. For transmission only runs (IEMSCT = 0 or 3), no data is output to rootname.SPC, even though the file is created.

5.6 Spectral Transmittance File

The ASCII file "rootname.TRN" contains the calculated spectral transmittance. As with the spectral radiance file, this plot file contains two columns with the frequency (cm^{-1}) and transmittance written as an (x,y) ordered pair (conversion to wavelengths or application of a filter function can be performed using the DEGRAD.f program). The data is printed at a constant frequency interval, the step size defined in the spectral data sub-menu, Section 4.2.4. A "\$" delimiter in column 2 is used to separate data generated from repeat runs, Section 4.3.6. For radiance calculations (IEMSCT = 1 or 2), the total transmittance is output with only five decimal places since the loop over LOS segments at any given frequency is terminated once total transmittance drops below 10^{-5} . For transmittance calculations, results are output with ten decimal places; these values generally contain three or four significant digits.

5.7 Bandpass Radiance File

The ASCII file "rootname.RAD" contains in-band (top hat) radiances for the spectral interval of the calculation. Values from multiple calculations can be used to plot bandpass radiance profiles. Each line contains three numbers followed by a descriptive character string. The numbers in order are the bandpass radiance ($\text{W}/\text{cm}^2\text{-sr}$), the minimum LOS altitude (km)

and the observer altitude (km). For a series of limb, half-limb or zenith calculations, the minimum LOS altitude is the pertinent ordinate (y coordinate) for plotting; for a series of nadir calculations, the observer altitude is the key ordinate. If no repeat SAMM runs are performed, rootname.RAD contains only a single line of data. For transmission only runs (IEMSCT = 0 or 3), no data is written to rootname.RAD, even though the file is created.

5.8 MODTRAN Input File

SAMM creates a MODTRAN standard input stream, "rootname.TP5". This file can generally be used to run the standard MODTRAN externally from SAMM. The results should be similar but not necessarily identical to those obtained by running MODTRAN within SAMM, RUNMOD = "M" (Section 4.3.1). MODTRAN within SAMM has an upgraded column density calculation (Appendix H), uses different layering, and allows the possibility of multiple regions and/or multiple profiles above 30 km.

The "rootname.TP5" file differs from the MODTRAN "TAPE5" file in a few respects. The character in column 1 of CARD 1 is no longer a logical variable, T for MODTRAN and F for LOWTRAN. Instead, it is the character variable "RUNMOD" described in Section 4.3.1. Also, column 11 of CARD 1 contains a letter indicating the specific geometry inputs; the letters correspond to the letters on page 36 of the LOWTRAN 7 manual,⁽³⁾ (a & b for horizontal paths; a, b, c & d for slant paths; and a & b for paths to space). CARD 3 has additional geometry input in columns 66 through 120. Column 70 contains the character string "DIR", equal to "T" or "B" depending on whether "LONG2" and "LAT2" are "T"oward or "B"ehind the LOS from the observer. The longitude (degrees West of Greenwich) and latitude (degrees North of the Equator) of the observer are specified in columns 71 through 90, formatted 2F10.3. The next 20 columns, also formatted 2F10.3, contain "LONG2" and "LAT2", the longitude and latitude of an auxiliary point used to specify path azimuth. If the path azimuth is directly specified, its value in degrees East of North is written in columns 111 through 120, formatted F10.3.

To convert "rootname.TP5" into a MODTRAN "TAPE5" file for direct use by MODTRAN, two changes are necessary on the first line of the file (CARD 1). The character in column 1 must be replaced with "T", and the character in column 11 replaced with a blank, " ". If repeat runs are requested, these same changes must be made to the additional CARD 1's. The TAPE5 file can not be converted directly to a valid MODTRAN input for limb calculations (ITYPE in column 10 of CARD 1 equal to 4) or for slant paths defined by specifying the latitude and longitude of the source point ("2E" in columns 10-11 of CARD 1).

5.9 MODTRAN Standard Output File

The SAMM output file "rootname.TP6" is similar to the MODTRAN "TAPE6" output file. The input parameter NOPRT determines the amount of information written to the file, as described in Section 4.3.3. The major difference between the SAMM and MODTRAN versions is that the SAMM file tracks the latitude and longitude along the LOS. Also, the SAMM file enables the user to output vibrational state column densities. "rootname.TP6" and "TAPE6" use the same format for the tables of radiances and/or transmittances vs frequency. The column 66 through 120 CARD 3 input described in the previous section is also included as output in the "rootname.TP6" file.

5.10 MODTRAN Plotting File

The file "rootname.TP7" is SAMM's version of MODTRAN's "TAPE7" file. The "rootname.TP7" file can be used as input to MODTRAN's plotting package. One change has been made to this file for radiance calculations (IEMSCT = 1 or 2). In this case four columns have been added to the frequency dependent output. They contain the layer number at which the radiance calculation was terminated (i.e., the layer at which transmission dropped below 10^{-5}) and the corresponding terminating altitude (km), latitude (degrees North of the Equator), and longitude (degrees West of Greenwich).

5.11 MODTRAN Auxiliary Output File

The file "rootname.TP8" is SAMM's version of MODTRAN's "TAPE8" file. One change has been made to this file. For transmission only calculations (IEMSCT = 0), the transmission for HNO_3 , OH and NO^+ has been added to the output.

6. SAMM DATA FILES

In general, the SAMM data files have the same format as the corresponding SHARC-3 data files. Information on the content and structure of all these files is presented in Section 6 of the SHARC-3 manual.⁽¹⁾ As noted above (Subsection 3.2), the Curtis-Godson files for solar irradiance are not used by SAMM; solar attenuation by the lower atmosphere is directly calculated using the MODTRAN module.

The SAMM atmospheric profiles differ from those of SHARC-3 in that the former begin at 0 km (ground level) whereas the latter begin at 50 km. Also, the SAMM profiles contain 5 additional species: N_2O , SO_2 , NO_2 , NH_3 & HNO_3 . SAG, the SHARC/SAMM Atmosphere Generator, can still be used to generate the desired atmospheric profiles; the SAG interactive module prompts the user to determine whether SHARC or SAMM profiles are to be generated. For SAMM, standard atmospheric profiles are layered in 1 km increments from 0 to 25 km, in 2 km increments from 30 to 150 km, and in 10 km increments from 160 to 300 km for a total of 102 layer boundaries. Different layer structuring can be input, but SAMM currently restricts the number of layers below 30 km to 26.

7. AUXILIARY PROGRAMS

The SAMM module is delivered with two auxiliary programs. They are sag.f, the SHARC/SAMM Atmospheric Generator, and DEGRAD.f, a filter function routine.

7.1 The SAG Program

The SAG program generates atmospheric profiles given temporal, geographic location, and solar activity inputs, basing predictions on existing knowledge of the chemical constituent variabilities. Extensive use is made of the MSISE-90⁽¹³⁾ and the NRL climatology⁽¹⁴⁾ models. SHARC, MODTRAN and SAMM atmospheric profile data files are standard outputs of the SAG module. User instructions for the code are included in Section 7.3 of the SHARC-3 manual⁽¹⁾ and in the SAG manual.⁽⁴⁾ The SAG manual also contains a discussion of the required assumptions and data sources used in developing the SAG module.

7.2 The DEGRAD Program

The DEGRAD program is used to degrade the spectral resolution of SAMM spectral radiance and transmittance data. DEGRAD is an internal SSI code delivered as a courtesy. DEGRAD accepts as input the SAMM spectral radiance and spectral transmittance files, and enables the user to pass any of a variety of filter functions over the data. The program interactively prompts the user for all required inputs using a menu driven system. Default inputs are stored in a DEGRAD.INP file; if no such file exists, one is created when the program is executed.

8. REFERENCES

1. R. D. Sharma, J. W. Duff, R. L. Sundberg, J. H. Gruninger, L. S. Bernstein, D. C. Robertson and R. J. Healey (1990), Description of SHARC-2, The Strategic High-Altitude Radiance Code, PL-TR-91-2071, ADA239008
2. A. Berk, L. S. Bernstein and D. C. Robertson (1989), MODTRAN: A Moderate Resolution Model for LOWTRAN 7, GL-TR-89-0122, ADA214337
3. F. X. Kneizys, E. P. Shettle, L. W. Abreu, J. H. Chetwynd, G. P. Anderson, W. O. Gallery, J. E. A. Selby and S. A. Clough (1988), Users Guide to LOWTRAN 7, AFGL-TR-88-0177, ADA206773
4. S. M. Adler-Golden (1993), Description of the SHARC Atmospheric Generator, Scientific Report No. 2 under contract F19628-91-C-0083, Spectral Sciences Inc, PL-TR-93-2123
5. G. N. Plass (1958), Models for Spectral Band Absorption, J. Opt. Soc. Am., 48, 690
6. C. D. Rodgers and A. P. Williams (1974), Integrated Absorption of a Spectral Line With the Voigt Profile, J. Quant. Spectrosc. Radiat. Trans., 14, 319
7. R. M. Goody and Y. L. Yung (1989), Atmospheric Radiation: Theoretical Basis, 2nd Edition, New York, Oxford University Press
8. D. C. Robertson, L. S. Bernstein and R. Haines (1980), Addition of a 5 cm^{-1} Spectral Resolution Band Model Option to LOWTRAN 5, ARI-RR-232, Aerodyne Research Inc, Billerica, MA
9. C. B. Ludwig, W. Malkmus, J. E. Reardon and J. A. L. Thomson (1973), Handbook of Infrared Radiation From Combustion Gases, NASA SP-3080, Washington, DC, NASA Scientific and Technical Information Office
10. W. M. Cornette (1992), Robust Algorithm for Correcting the Layer Problem in LOWTRAN, Appl. Opt., 31, 5767
11. Personal Communication (1993) with Ken Minschwaner and Gail Anderson
12. Prabhat Acharya, David Robertson, Gail Anderson, W. M. Cornette (1994), Moderate Spectral Atmospheric Radiance and Transmittance Program (MOSART), PL-TR-94-2244, Vol I ADA204038, Vol II ADA304180, Vol III ADA204072, Vol IV ADA204073

13. A. E. Hedin (1991), Extension of the MSIS Thermospheric Model into the Middle and Lower Atmosphere, J. Geophys. Res., **96**, 1159
14. M. E. Summers (1993), Zonally Averaged Trace Constituent Climatology, Rep. NRL-MR-7641-93-7416, Naval Research Laboratory, Washington, DC

APPENDIX A
IMPLEMENTATION INSTRUCTIONS

APPENDIX A

IMPLEMENTATION INSTRUCTIONS

SAMM, SHARC And MODTRAN Merged, is delivered with the FORTRAN source code, input data sets, and seven test cases. The SAMM package contains 232 files. The files are:

SAMM EXECUTABLE DIRECTORY

1	Samdrv.f	Main program	FORTAN	1715 lines
2	ambien.f	Ambient environment	FORTAN	2963 lines
3	aurora.f	Auroral environment	FORTAN	591 lines
4	chmkin.f	CHEMKIN subroutines	FORTAN	4043 lines
5	geolos.f	SHARC-3 LOS geometry subroutines	FORTAN	4740 lines
6	geoseg.f	SHARC-3 Segment geometry subroutines	FORTAN	946 lines
7	inactv.f	Interactive subroutines	FORTAN	6538 lines
8	input.f	SHARC-3 Input subroutines	FORTAN	3393 lines
9	inutil.f	Input utilities subroutines	FORTAN	2778 lines
10	modaer.f	MODTRAN aerosol subroutines	FORTAN	1681 lines
11	modblk.f	Block data subroutines	FORTAN	4417 lines
12	moddrv.f	MODTRAN driver subroutine	FORTAN	1725 lines
13	modgeo.f	MODTRAN geometry subroutines	FORTAN	2089 lines
14	modlay.f	MODTRAN layer loop subroutines	FORTAN	3723 lines
15	modrad.f	Radiance subroutines	FORTAN	4835 lines
16	modssg.f	MODTRAN solar scatter path subroutines	FORTAN	458 lines
17	mosinp.f	MOSART input subroutines	FORTAN	3788 lines
18	output.f	SHARC-3 Output subroutines	FORTAN	1379 lines
19	saminp.f	SAMM input subroutines	FORTAN	2776 lines
20	samseg.f	SAMM column density subroutines	FORTAN	2091 lines
21	AMBIEN.H	Ambient NLTE calculations common	FORTAN	22 lines
22	BMCOM.H	Band model data common	FORTAN	7 lines
23	CARD1.H	MODTRAN card 1 common	FORTAN	3 lines
24	CARD2.H	MODTRAN card 2 common	FORTAN	2 lines
25	CARD2D.H	MODTRAN card 2D common	FORTAN	2 lines
26	CARD3.H	MODTRAN card 3 common	FORTAN	2 lines
27	CG.H	Curtis-Godson sums common	FORTAN	4 lines
28	CNSTNS.H	Constants common	FORTAN	3 lines
29	CNTRL.H	MODTRAN column densities common	FORTAN	5 lines
30	DIRPKA.H	Directory & file names common	FORTAN	27 lines

31	FILES.H	File unit number parameters	FORTTRAN	35 lines
32	HIALT.H	SAMM geometry array common	FORTTRAN	12 lines
33	IFIL.H	MODTRAN file unit numbers common	FORTTRAN	1 lines
34	INPDAT.H	MOSART input strings common	FORTTRAN	5 lines
35	ISOTP.H	Isotope array common	FORTTRAN	11 lines
36	KNETIC.H	Chemical kinetic common	FORTTRAN	22 lines
37	LAY5.H	Continuum transmittance common	FORTTRAN	3 lines
38	LNDAT.H	Line data common	FORTTRAN	5 lines
39	LOS GEO.H	SHARC-3 LOS geometry common	FORTTRAN	32 lines
40	MODEL.H	Model atmosphere common	FORTTRAN	2 lines
41	MOSINP.H	MOSART input variables common	FORTTRAN	16 lines
42	PARMS.H	SHARC-3 parameters	FORTTRAN	43 lines
43	PARMTR.H	MODTRAN geometry data common	FORTTRAN	1 lines
44	PTH.H	MODTRAN path length common	FORTTRAN	1 lines
45	RDAMAR.H	SHARC-3 vibrational labels common	FORTTRAN	8 lines
46	RECORD.H	Input records common	FORTTRAN	8 lines
47	REG GEO.H	Region definition common	FORTTRAN	26 lines
48	RFP TH.H	MODTRAN refractive path common	FORTTRAN	3 lines
49	SM.H	SHARC-3/MODTRAN variable common	FORTTRAN	17 lines
50	SOLS.H	Solar paths common	FORTTRAN	2 lines
51	TAPE5.H	MODTRAN inputs common	FORTTRAN	25 lines
52	Makefile	Sample SAMM make file	MAKE FILE	90 lines

ATMOSPHERIC PROFILES DIRECTORY

53	MIDLAT.DAY	1976 Standard Day	DATA	444 lines
54	MIDLAT.NIG	1976 Standard Night	DATA	444 lines
55	T4Z091.ATM	High Latitude with 90.85° SZA	DATA	426 lines
56	T4Z093.ATM	High Latitude with 93.06° SZA	DATA	426 lines
57	T4Z095.ATM	High Latitude with 95.27° SZA	DATA	426 lines
58	T4Z097.ATM	High Latitude with 97.01° SZA	DATA	426 lines
59	T4Z099.ATM	High Latitude with 98.65° SZA	DATA	426 lines
60	T4Z101.ATM	High Latitude with 100.88° SZA	DATA	426 lines
61	T4Z102.ATM	High Latitude with 101.68° SZA	DATA	426 lines
62	T5Z091.ATM	High Latitude with 91.43° SZA	DATA	426 lines
63	T5Z094.ATM	High Latitude with 94.38° SZA	DATA	426 lines
64	T5Z097.ATM	High Latitude with 96.67° SZA	DATA	426 lines
65	T5Z099.ATM	High Latitude with 99.32° SZA	DATA	426 lines
66	T5Z102.ATM	High Latitude with 101.9° SZA	DATA	426 lines
67	T5Z104.ATM	High Latitude with 104.5° SZA	DATA	426 lines
68	T5Z108.ATM	High Latitude with 107.97° SZA	DATA	426 lines

LINE AND BAND MODEL DATA DIRECTORY

69	SHARC.ASC	ASCII SHARC-3 line data	DATA	303802 lines
70	UFTAPE.ASC	ASCII MODTRAN band model data	DATA	67761 lines
71	dirac.f	Creates binary line file	FORTRAN	103 lines
72	ufmake.f	Creates binary band model files	FORTRAN	134 lines
73	linasc.f	Creates ASCII line file	FORTRAN	60 lines
74	bmasc.f	Creates ASCII band model files	FORTRAN	63 lines

ATMOSPHERE GENERATOR DIRECTORY

75	sag.f	SAG source	FORTRAN	4257 lines
76	drivht.mod	Standard MODTRAN altitudes for SAG	DATA	9 lines
77	drivht.sam	Standard SAMM altitudes for SAG	DATA	24 lines
78	drivht.sha	Standard SHARC altitudes for SAG	DATA	16 lines
79	sag.run	Creates test case atmospheres	BATCH	29 lines
80	sag.inp	Input to makatm	DATA	2 lines
81	drT4Z091.dat	High latitude, 90.85° SZA input	DATA	4 lines
82	drT4Z093.dat	High latitude, 93.06° SZA input	DATA	4 lines
83	drT4Z095.dat	High latitude, 95.27° SZA input	DATA	4 lines
84	drT4Z097.dat	High latitude, 97.01° SZA input	DATA	4 lines
85	drT4Z099.dat	High latitude, 98.65° SZA input	DATA	4 lines
86	drT4Z101.dat	High latitude, 100.88° SZA input	DATA	4 lines
87	drT4Z102.dat	High latitude, 101.68° SZA input	DATA	4 lines
88	drT5Z091.dat	High latitude, 91.43° SZA input	DATA	4 lines
89	drT5Z094.dat	High latitude, 94.38° SZA input	DATA	4 lines
90	drT5Z097.dat	High latitude, 96.67° SZA input	DATA	4 lines
91	drT5Z099.dat	High latitude, 99.32° SZA input	DATA	4 lines
92	drT5Z102.dat	High latitude, 101.9° SZA input	DATA	4 lines
93	drT5Z104.dat	High latitude, 104.5° SZA input	DATA	4 lines
94	drT5Z108.dat	High latitude, 107.97° SZA input	DATA	4 lines

NRL DATA SUB-DIRECTORY

95	CH4.NRL	CH ₄ climatology data	DATA	1443 lines
96	CO.NRL	CO climatology data	DATA	1443 lines
97	H2O.NRL	H ₂ O climatology data	DATA	1443 lines
98	HNO3.NRL	HNO ₃ climatology data	DATA	1443 lines
99	N2O.NRL	N ₂ O climatology data	DATA	1443 lines
100	NO2.NRL	NO ₂ climatology data	DATA	1443 lines
101	O3D.NRL	O ₃ daytime climatology data	DATA	1443 lines
102	O3R.NRL	O ₃ night-to-day climatology data	DATA	1443 lines
103	OAT.NRL	O atom climatology data	DATA	1443 lines
104	TEMP.NRL	temperature climatology data	DATA	1443 lines

FILTER FUNCTION DIRECTORY

105	DEGRAD.f	Filter function source	FORTTRAN	967 lines
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CHEMICAL KINETICS DIRECTORY

106	interp.f	Chemical kinetics interpreter source	FORTTRAN	2080 lines
107	interp.run	Creates test case link files	BATCH	31 lines
108	ACO2.KIN	CO ₂ auroral kinetics file	DATA	637 lines
109	ACO2.OUT	CO ₂ auroral interpreter output	DATA	702 lines
110	ACO2.STA	CO ₂ auroral states/transitions file	DATA	10 lines
111	ANO.KIN	NO auroral kinetics file	DATA	667 lines
112	ANO.OUT	NO auroral interpreter output	DATA	729 lines
113	ANO.STA	NO auroral states/transitions file	DATA	41 lines
114	ANOP.KIN	NO ⁺ auroral kinetics file	DATA	626 lines
115	ANOP.OUT	NO ⁺ auroral interpreter output	DATA	689 lines
116	ANOP.STA	NO ⁺ auroral states/transitions file	DATA	32 lines
117	CH4.BND	CH ₄ band information file	DATA	163 lines
118	CH4.KIN	CH ₄ kinetics file	DATA	91 lines
119	CH4.OUT	CH ₄ interpreter output	DATA	141 lines
120	CH4.STA	CH ₄ states/transitions file	DATA	30 lines
121	CO.BND	CO band information file	DATA	55 lines
122	CO.KIN	CO kinetics file	DATA	23 lines
123	CO.OUT	CO interpreter output	DATA	52 lines
124	CO.STA	CO states/transitions file	DATA	11 lines
125	CO21.BND	CO ₂ 1st isotope band information file	DATA	651 lines
126	CO21.KIN	CO ₂ 1st isotope kinetics file	DATA	326 lines
127	CO21.OUT	CO ₂ 1st isotope interpreter output	DATA	457 lines
128	CO21.STA	CO ₂ 1st isotope states/transitions file	DATA	72 lines
129	CO22.BND	CO ₂ 2nd isotope band information file	DATA	492 lines
130	CO22.KIN	CO ₂ 2nd isotope kinetics file	DATA	319 lines
131	CO22.OUT	CO ₂ 2nd isotope interpreter output	DATA	446 lines
132	CO22.STA	CO ₂ 2nd isotope states/transitions file	DATA	70 lines
133	CO23.BND	CO ₂ 3rd isotope band information file	DATA	405 lines
134	CO23.KIN	CO ₂ 3rd isotope kinetics file	DATA	301 lines
135	CO23.OUT	CO ₂ 3rd isotope interpreter output	DATA	422 lines
136	CO23.STA	CO ₂ 3rd isotope states/transitions file	DATA	67 lines

137	H2O1.BND	H ₂ O 1st isotope band information file	DATA	213 lines
138	H2O1.KIN	H ₂ O 1st isotope kinetics file	DATA	68 lines
139	H2O1.OUT	H ₂ O 1st isotope interpreter output	DATA	110 lines
140	H2O1.STA	H ₂ O 1st isotope states/transitions file	DATA	27 lines
141	H2O2.BND	H ₂ O 2nd isotope band information file	DATA	113 lines
142	H2O2.KIN	H ₂ O 2nd isotope kinetics file	DATA	56 lines
143	H2O2.OUT	H ₂ O 2nd isotope interpreter output	DATA	98 lines
144	H2O2.STA	H ₂ O 2nd isotope states/transitions file	DATA	21 lines
145	H2O3.BND	H ₂ O 3rd isotope band information file	DATA	84 lines
146	H2O3.KIN	H ₂ O 3rd isotope kinetics file	DATA	54 lines
147	H2O3.OUT	H ₂ O 3rd isotope interpreter output	DATA	96 lines
148	H2O3.STA	H ₂ O 3rd isotope states/transitions file	DATA	20 lines
149	H2O4.BND	H ₂ O 4th isotope band information file	DATA	97 lines
150	H2O4.KIN	H ₂ O 4th isotope kinetics file	DATA	54 lines
151	H2O4.OUT	H ₂ O 4th isotope interpreter output	DATA	96 lines
152	H2O4.STA	H ₂ O 4th isotope states/transitions file	DATA	20 lines
153	NO.BND	NO band information file	DATA	55 lines
154	NO.KIN	NO kinetics file	DATA	18 lines
155	NO.OUT	NO interpreter output	DATA	44 lines
156	NO.STA	NO states/transitions file	DATA	11 lines
157	O3.BND	O ₃ band information file	DATA	574 lines
158	O3.KIN	O ₃ kinetics file	DATA	244 lines
159	O3.OUT	O ₃ interpreter output	DATA	412 lines
160	O3.STA	O ₃ states/transitions file	DATA	80 lines
161	OH.BND	OH band information file	DATA	428 lines
162	OH.KIN	OH kinetics file	DATA	87 lines
163	OH.OUT	OH interpreter output	DATA	120 lines
164	OH.STA	OH states/transitions file	DATA	39 lines

TEST CASE DIRECTORY

165	TEST1.INP	Test case 1 general input	DATA	695 lines
166	TEST1.OUT	Test case 1 SHARC-3 general output	DATA	2234 lines
167	TEST1.RAD	Test case 1 bandpass radiance output	DATA	1 lines
168	TEST1.SPC	Test case 1 spectral radiance output	DATA	2502 lines
169	TEST1.TP5	Test case 1 MODTRAN input	DATA	105 lines
170	TEST1.TP6	Test case 1 MODTRAN general output	DATA	3403 lines
171	TEST1.TP7	Test case 1 MODTRAN plotting	DATA	2513 lines
172	TEST1.TP8	Test case 1 MODTRAN auxiliary output	DATA	11 lines
173	TEST1.TRN	Test case 1 transmission data output	DATA	2502 lines

174	TEST2.INP	Test case 2 general input	DATA	770 lines
175	TEST2.OUT	Test case 2 SHARC-3 general output	DATA	5412 lines
176	TEST2.RAD	Test case 2 bandpass radiance output	DATA	1 lines
177	TEST2.SPC	Test case 2 spectral radiance output	DATA	9752 lines
178	TEST2.TP5	Test case 2 MODTRAN input	DATA	105 lines
179	TEST2.TP6	Test case 2 MODTRAN general output	DATA	11321 lines
180	TEST2.TP7	Test case 2 MODTRAN plotting	DATA	9763 lines
181	TEST2.TP8	Test case 2 MODTRAN auxiliary output	DATA	11 lines
182	TEST2.TRN	Test case 2 transmission data output	DATA	9752 lines
183	TEST3.INP	Test case 3 general input	DATA	725 lines
184	TEST3.LOG	Test case 3 journal output	DATA	40 lines
185	TEST3.OUT	Test case 3 SHARC-3 general output	DATA	12602 lines
186	TEST3.RAD	Test case 3 bandpass radiance output	DATA	1 lines
187	TEST3.SPC	Test case 3 spectral radiance output	DATA	9752 lines
188	TEST3.TP5	Test case 3 MODTRAN input	DATA	105 lines
189	TEST3.TP6	Test case 3 MODTRAN general output	DATA	11233 lines
190	TEST3.TP7	Test case 3 MODTRAN plotting	DATA	9763 lines
191	TEST3.TP8	Test case 3 MODTRAN auxiliary output	DATA	11 lines
192	TEST3.TRN	Test case 3 transmission data output	DATA	9752 lines
193	TEST4.INP	Test case 4 general input	DATA	623 lines
194	TEST4.LOG	Test case 4 journal output (empty)	DATA	5 lines
195	TEST4.OUT	Test case 4 SHARC-3 general output	DATA	5576 lines
196	TEST4.RAD	Test case 4 bandpass radiance output	DATA	1 lines
197	TEST4.SPC	Test case 4 spectral radiance output	DATA	142 lines
198	TEST4.TP5	Test case 4 MODTRAN input	DATA	105 lines
199	TEST4.TP6	Test case 4 MODTRAN general output	DATA	817 lines
200	TEST4.TP7	Test case 4 MODTRAN plotting	DATA	153 lines
201	TEST4.TP8	Test case 4 MODTRAN auxiliary output	DATA	11 lines
202	TEST4.TRN	Test case 4 transmission data output	DATA	142 lines
203	TEST5.INP	Test case 5 general input	DATA	653 lines
204	TEST5.OUT	Test case 5 SHARC-3 general output	DATA	13202 lines
205	TEST5.RAD	Test case 5 bandpass radiance output	DATA	1 lines
206	TEST5.SPC	Test case 5 spectral radiance output	DATA	162 lines
207	TEST5.TP5	Test case 5 MODTRAN input	DATA	105 lines
208	TEST5.TP6	Test case 5 MODTRAN general output	DATA	885 lines
209	TEST5.TP7	Test case 5 MODTRAN plotting	DATA	173 lines
210	TEST5.TP8	Test case 5 MODTRAN auxiliary output	DATA	11 lines
211	TEST5.TRN	Test case 5 transmission data output	DATA	162 lines

212	TEST6.HAZ	Test case 6 aerosol input	DATA	1 lines
213	TEST6.INP	Test case 6 general input	DATA	793 lines
214	TEST6.OUT	Test case 6 SHARC-3 general output	DATA	4869 lines
215	TEST6.RAD	Test case 6 bandpass radiance output	DATA	2 lines
216	TEST6.SPC	Test case 6 spectral radiance output	DATA	19504 lines
217	TEST6.TP5	Test case 6 MODTRAN input	DATA	110 lines
218	TEST6.TP6	Test case 6 MODTRAN general output	DATA	23118 lines
219	TEST6.TP7	Test case 6 MODTRAN plotting	DATA	19517 lines
220	TEST6.TP8	Test case 6 MODTRAN auxiliary output	DATA	13 lines
221	TEST6.TRN	Test case 6 transmission data output	DATA	19504 lines
222	TEST7.HAZ	Test case 7 aerosol input	DATA	1 lines
223	TEST7.INP	Test case 7 general input	DATA	1340 lines
224	TEST7.LOG	Test case 7 journal output	DATA	21 lines
225	TEST7.OUT	Test case 7 SHARC-3 general output	DATA	11252 lines
226	TEST7.RAD	Test case 7 bandpass radiance output	DATA	16 lines
227	TEST7.SPC	Test case 7 spectral radiance output	DATA	14432 lines
228	TEST7.TP5	Test case 7 MODTRAN input	DATA	1680 lines
229	TEST7.TP6	Test case 7 MODTRAN general output	DATA	28875 lines
230	TEST7.TP7	Test case 7 MODTRAN plotting	DATA	14608 lines
231	TEST7.TP8	Test case 7 MODTRAN auxiliary output	DATA	176 lines
232	TEST7.TRN	Test case 7 transmission data output	DATA	14432 lines

The FORTRAN source code for SAMM resides in the SAMM EXECUTABLE directory along with a sample make file. All "rootname.H" files are read into the source with include statements. The make file lists which files are included for each source routine. All the FORTRAN files should be compiled and linked to make the executable version of SAMM. Since details of make files are system-dependent, users will probably need to edit "Makefile" to conform with their particular system's standards. The open statements may need to be changed, again depending upon system standards. Files are opened in the Samdrv.f, ambien.f, inactv.f, inutil.f, modrad.f and saminp.f FORTRAN routines.

Atmospheric profiles are found in the ATMOSPHERIC PROFILES directory. The test case 4 and 5 profiles are all outputs from sag.f, the atmospheric generator program.

The LINE AND BAND MODEL DATA directory contains four separate FORTRAN programs. The programs dirac.f and ufmake.f must be compiled, linked and run to execute SAMM. The ufmake.f program will output a file named "samblk.f". "samblk.f" should be copied to the SAMM executable directory; it is part of SAMM's source code. "ufmake.f" will also create the direct-access, binary file "UFTAPE"; "UFTAPE.ASC" can be removed once "UFTAPE" has been generated. The dirac.f program will output a file named "RECDAT.f"; this file can be deleted since it is not used. "dirac.f" will also create the direct-access, binary

file "SHARC.H92"; "SHARC.ASC" can be removed once "SHARC.H92" is created. The programs linasc.f and bmasc.f can be used to retrieve the ASCII files. These programs make it unnecessary to keep the large ASCII files once the binary files are created. Note, bmasc.f reads samblk.f as input, so a copy of samblk.f should be kept in the LINE AND BAND MODEL DATA directory.

The ATMOSPHERE GENERATOR directory contains the SHARC/SAMM Atmosphere Generator (SAG) program. Required data files are stored in the NRLDAT sub-directory. The source is named sag.f, and the climatology data files all have "NRL" (Naval Research Laboratory) as a suffix. Executing the SAG program requires a general input file named "drivstor.dat" and an altitude file. A typical altitude profile for SAMM is included in "drivht.sam". The files with a "dat" suffix are drivstor.dat files for test cases 4 and 5. Anyone of these files can be copied into "drivstor.dat" and then altered interactively to obtain the desired profile. The UNIX batch program "sag.run" generates the test case 4 and 5 profiles found in the atmospheric profiles directory. The batch file assumes the SAG executable has the name "sag.exe".

DEGRAD.f is a filter function routine which is found in the FILTER FUNCTION directory. DEGRAD.f is designed to process the "rootname.SPC" and "rootname.TRN" SAMM output files.

The INTERPRETER in the chemical kinetics directory should be compiled as a stand alone program. The INTERPRETER subroutines are described in Appendix B of the SHARC-3 manual⁽¹⁾, and use of the program is discussed in Section 7 of the manual, Appendix I.

The output files for the seven test cases are all included in the TEST CASE directory. To run a test case, the "rootname.INP" file must be copied into the SAMM EXECUTABLE directory as "SAMM.INP" and the "rootname.HAZ" file must be copied into the SAMM EXECUTABLE directory as "HAZE.INP". If no "rootname.HAZ" file exists (TEST CASE 1 through 5), there should be no HAZE.INP in the SAMM EXECUTABLE directory when the code is run. This means the calculations are being run without aerosols.

REFERENCES

1. R. D. Sharma, J. W. Duff, R. L. Sundberg, J. H. Gruninger, L. S. Bernstein, D. C. Robertson, S. M. Adler-Golden, M. W. Matthew and R. J. Healey (1996), User's Manual for SHARC-3, The Strategic High-Altitude Radiance Code, PL-TR-96-2104

APPENDIX B
SAMM PARAMETERS

APPENDIX B

SAMM PARAMETERS

For each "rootname.H" file, a list of the parameters is provided along with a brief definition. These parameters are included in the various subroutines via FORTRAN "include" statements.

CNTRL.H

KMAX (=63) The number of LOWTRAN absorption/scattering sources.

FILES.H

NINP	(=9)	Unit number for MOSART input file.
LDEF	(=10)	Unit number for problem definition input file.
LATM	(=11)	Unit number for atmospheric profile data file.
LINK	(=12)	Unit number for linking (chemical kinetics) data file.
LBAND	(=13)	Unit number for bands data file.
LRAD	(=14)	Unit number for states/transitions data file.
LINE	(=15)	Unit number for SHARC-3 lines data file.
LSAVE	(=16)	Unit number for populations data file.
LHAZE	(=18)	Unit number for aerosol data file.
LPHASE	(=19)	Unit number for user-supplied phase function data file.
NDEF	(=20)	Unit number for writing out new SAMM.INP file.
NERR	(=21)	Unit number for journal output file.
NSPEC	(=22)	Unit number for spectral radiance output file.
NOUT	(=23)	Unit number for SHARC-3 general output file.
NSCR	(=25)	Unit number for scratch file.
NSAVE	(=26)	Unit number for saved population file.
NCHK	(=27)	Unit number for file checking.
NTAPE5	(=28)	Unit number for MODTRAN input file.
NTRAN	(=29)	Unit number for spectral transmission output file.
NUWIJ	(=30)	Unit number for W_{ij} matrix output file.

HALT.H

MXLAY	(=284)	Maximum number layer boundaries along LOS.
MXRAD	(=13)	Maximum number of SHARC radiator, isotopes counted separately.
MAXIV	(=31)	Maximum number of vibrational states for a SHARC-3 radiator, or maximum number of MODTRAN radiators, which ever is larger.
NSPECS	(=12)	Number of species on the band model parameter tape.

LNDAT.H

MXLIN	(=412)	Maximum number of lines on the SHARC-3 lines file in 1 cm ⁻¹ bin.
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MOSINP.H

NOPT	(=13)	Number of MOSART input stream sections.
NANTMX	(=25)	Maximum number of lines of antecedent input data.
MLMAX	(=100)	Maximum number of MOSART layer boundaries.

PARMS.H

NPOPMX	(=7)	Maximum number of profiles/population files for each region.
NREGMX	(=5)	Maximum number of regions.
NENVMX	(=2)	Maximum number of environments for each region.
NBYMAX	(=106)	Maximum number of layer boundaries.
NRDMX	(=16)	Maximum number of SHARC-3 molecular emitters.
NMOLMX	(=8)	Maximum number of distinct radiating molecules.
NISOMX	(=8)	Maximum number of isotopes for each species.
NMMAX	(=30)	Maximum number of atmospheric species.
NVMAX	(=35)	Maximum number of vibrational states for each molecular emitter.
NSMAX	(=20)	Maximum number of bins for band distributions.
NBMAX	(=46)	Maximum number of bands.
NTMPMX	(=5)	Maximum number of temperatures for band distributions.
NWMAX	(=200)	Maximum number of frequency bins for the Voigt line shape function.
NVARMX	(=20)	Maximum number of variables for generic interactive read.
NCHMAX	(=80)	Maximum length of reaction input string.
NWRTMX	(=20)	Maximum number of types of output.
NDMAX	(=400)	Maximum number of non-comment lines in a SAMM.INP file.
NSEGMX	(=18)	Maximum number of major segments along a line of sight.
NSECMX	(=4)	Maximum number of intersections through a single region.
NEDGMX	(=4)	Maximum number of region edges.

NSTRMX	(=80)	Maximum length of a character string in the defaults file.
NSINMX	(=5)	Maximum number of Curtis-Godson LOS through lower atmosphere.
NDMAXM	(=260)	Maximum number of non-comment MODTRAN lines in a SAMM.INP file.
MOSDMX	(=200)	Maximum number of non-comment MOSART lines in a SAMM.INP file.
NBY2MX	(=232)	Maximum number of layer boundaries along LOS in SHARC region
NLYMAX	(=105)	Maximum number of layers
NMOL	(=29)	Maximum number of molecules.
NW	(=200)	Maximum number of items read from a single line of the input file.
NWUSED	(=10)	Maximum number of items presently expected to be read from a single line of the input file.
NFIX	(=36)	The first NFIX data lines in the input file, defining information expected in the same sequence in every input file.
NFILES	(=3)	Number of types of kinetics files (linking, states, bands).
NEDGE	(=4)	Number of region edges.
NKMAX	(=95)	Maximum number of species allowed.
NIMAX	(=750)	Maximum number of reactions.
NLNMAX	(=15)	Maximum length of a species symbol.
NSPMAX	(=8)	Maximum number of species allowed in any given reaction.
NTBMAX	(=6)	Maximum number of third bodies allowed in any given reaction.
NRWMAX	(=9902)	Dimension of CHEMKIN double precision work matrix.
NIWMAX	(=115)	Dimension of CHEMKIN integer work matrix.
SMLLMX	(=10)	Maximum number of characters in prefix/suffix names.
NAMLMX	(=32)	Maximum number of characters for input/output file names.
DIRLMX	(=64)	Maximum number of characters for directory names.
LNGLMX	(=64)	Maximum number of characters for population file names.
LFILMX	(=132)	Maximum number of characters for full path name of population files.
FILLMX	(=96)	Maximum number of characters for full path name of files.

SM.H

MXCG	(=52)	Maximum number of layers for lower atmosphere LOS path.
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TAPE5.H

MXLYRS	(=33)	Maximum number of MODTRAN layer boundaries.
MXIREG	(=4)	Maximum number of aerosol profiles.
MXNANG	(=50)	Maximum number of angles in a user-defined phase function.
MX4	(=4)	Maximum number of different user-defined phase functions.
MX47	(=47)	Maximum number of wavelengths used for tabulating optical data.

APPENDIX C
SAMM SUBROUTINES

APPENDIX C

SAMM SUBROUTINES

A list of the subroutines comprising the various SAMM modules is given below.

Samdrv.f: The DRIVER Module

SAMM	Drives SAMM calculation. Makes primary calls to the SHARC and MODTRAN modules, defines input file as "SAMM.INP", and deletes unwanted output files.
SHARC3	Drives the SHARC calculations in SAMM.
MODTRN	Contains MODTRAN comments and calls the MODTRAN driver routine.

ambien.f: The AMBIENT ENVIRONMENT Module

AMBDRV	Calls the appropriate CHEMKIN/NEMESIS subroutines to compute the enhanced vibrationally excited state populations.
ARATE	Solves the two-state steady-state equation for the atmospheric excitation rate constant.
CGSUMS	Increments Curtis-Godson sums.
COLDEN	Computes the total column density for each atmospheric layer for the radiating species.
CPF12	Calculates the real part of the complex probability function for a Voigt line shape.
DEWV	Computes the equivalent width for a single isolated Voigt line.
WIDTHD	Calculates the Doppler halfwidth.
E2	Computes the second exponential integral as a function of optical depth.
EMISS	Locates the Einstein A coefficient for the current transition and calculates the sum of all Einstein A coefficients for all transitions from the upper vibrational state.
ERATE	Calculates the earthshine excitation rate for each atmospheric layer.

ESCPRB	Normalizes the escape probabilities calculated by subroutine PATH for each layer.
ESHINE	Calculates the earthshine flux for the current transition using the specified effective earthshine temperature.
FORMV	Calculates the Voigt line shape function.
WIDTHL	Calculates the Lorentz halfwidth.
MULSCT	Calculates the nth-order multiple scattering enhancement to the excited-state number density using the single-scattering enhancement matrix.
NEMDRV	Drives computation of the escape probabilities and enhanced excited-state number densities for each atmospheric layer using Monte Carlo integration of atmospheric layers, line strengths, and frequencies.
NEMFAC	Computes the probability of escaping a specified layer and the excitation of the layer from all other layers. These quantities are used for the subsequent auroral calculation.
NEMRXN	Identifies the excitation and relaxation processes in the chemical kinetics mechanism for the current transition being considered by NEMESIS.
N2FAC	Computes the effective rate constant for the $\text{CO}_2(00011) + \text{N}_2(0)$ quenching process and the excited state populations for N_2 following Kummer and James.
PATH	Integrates through the atmospheric layers to determine the escape probabilities and single-scattering enhancements.
PICKSJ	Determines the line strength selected from the line strength distribution function.
PICKZ	Finds the initial location and the corresponding layer for photon emission.
POPLTE	Computes the LTE populations for N_2 and O_2 which are subsequently used in the calculation of vibrationally excited states for CO and H_2O .
QUENCH	Computes the total quenching rate for the upper state of the transition.
RANF	Generates uniformly distributed random numbers between 0 and 1 (machine-dependent).
SINTRP	Performs a linear interpolation to obtain the line strength distribution function for the appropriate layer temperature.

SOLAR	Calculates the solar flux at the transition frequency assuming a 5500 K blackbody.
CGDAT	Calculates Curtis-Godson sums for determining attenuation of solar irradiance by repeated calls to MODTRAN.
SRATE	Calculates the solar excitation rate for each atmospheric layer.
STEADY	Sets up the steady state rate equations and then uses LUDCMP and LUBKSB to solve the set of linear algebraic equations for the number densities c_k . The major limitation to the steady-state procedure used here is the assumption that the rate equations are linear in the unknown vibrational population, that is, there is no energy exchange among the emitting species. This restriction can be easily relaxed by using an algorithm which solves nonlinear equations (as opposed to LUDCMP/LUBKSB).
VOIGT	Determines the emission frequency using a Voigt line shape function. The absorption cross section at this frequency is also computed.
GVLOAD	Transfers the number densities, vibrational transitions, and related information from the regional arrays into global arrays, which are ultimately used by radiative transport routines.
GVZERO	Initializes all of the global variable arrays.
RVLOAD	Transfers the number densities, vibrational transitions, and related information from the local environment arrays into regional arrays.
RVZERO	Initializes all of the regional variable arrays.

aurora.f: The AURORAL ENVIRONMENT Module

ALAM	Computes Grun's universal energy-dissipation function using a linear interpolation of tabulated values.
AURDRV	Drives the time-dependent auroral calculation. The auroral species number densities are returned to SHARC main at the observation time specified by the user.
CKLOAD	Loads the populations computed during the ambient calculation as the initial number densities for the auroral species.
EPFLUX	Calculates the primary energy flux assuming either a Gaussian or Maxwellian distribution function for the electron spectra.

- IPPRAT Calculates the ion pair production rate as a function of altitude for the specified auroral energy parameters.
- RATMOD Modifies the Einstein A-coefficients and loads the layer excitation rates into the appropriate rate constant arrays. These quantities are computed by the ambient calculation.
- TIMDEP Controls the time dependent integration of the auroral rate equations.

chmkin.f: The CHEMICAL KINETICS Module

- ARTCON Uses the kinetic data from the auroral linking file to compute the rate constants as a function of temperature in exactly the same manner as RATCON (see below). However, ARTCON identifies primary electron processes and uses the input ionization efficiencies and the ion pair production rate to compute rate constants for secondary electron formation.
- FUN Supplies LSODE with the species production rates obtained from PRAT.
- JAC Supplies LSODE with the Jacobian of the species production rates obtained from PRATJ.
- LUBKSB/LUDCMP Solve a set of simultaneous linearly independent algebraic equations (the steady-state equations) using a LU (lower/upper) decomposition procedure.
- PRAT Uses the data obtained from the "linking" file to set up the differential equations for the species production rates.
- PRATJ Uses the data obtained from the "linking" file to set up the Jacobian of the species production differential equations with respect to the species number densities.
- RATCON Uses the kinetic data from the linking file to compute the rate constants as a function of temperature. The assumed form of the rate constant is

$$k = A T^{\beta} \exp(-E/T - C/T^{1/3}) \quad ,$$

where A is the pre-exponential factor, β is the exponent of the temperature term, E is the activation energy (can also be used to write a reverse rate constant in terms of the forward rate constant via detailed balance), and C is the (historic) SSH $T^{1/3}$ coefficient.

LSODE	Numerically integrates the auroral rate equations. The package uses Gear's method for stiff differential equations and is supplied with the Sandia Livermore CHEMKIN code. The following subroutines/functions are used by the LSODE package: INTDY, STODE, CFODE, PREPJ, SOLSY, EWSET, VNORM, DGEFA, DGESL, DGBFA, DGBSL, DAXPY, DSCAL, DDOT, IDAMAX, D1MACH, XERRWV. For a brief description of these routines, see SUBROUTINE LSODE.
INTDY	See LSODE.
STODE	See LSODE.
CFODE	Integrates the differential equations expressing the auroral model. See LSODE.
PREPJ	See LSODE.
SOLSY	See LSODE.
EWSET	See LSODE.
VNORM	See LSODE.
DGEFA	See LSODE.
DGESL	See LSODE.
DGBFA	See LSODE.
DGBSL	See LSODE.
DAXPY	See LSODE.
DSCAL	See LSODE.
DDOT	See LSODE.
IDAMAX	See LSODE.
D1MACH	See LSODE.
XERRWV	Prints LSODE-related error and warning messages. See LSODE.
LSODED	See LSODE.

geolos.f: The SHARC LINE-OF-SIGHT GEOMETRY Module

INGEOM	Reads LOS geometry information from the default file and allows the user to review/change the parameters.
SHOGEO	Writes to the screen the current line-of-sight geometry input.
SHOLOS	Writes to the screen all line-of-sight information at the end of a line-of-sight menu session.

GETLOC	Interactively determines a line-of-sight in either latitude, longitude representation or solar zenith, azimuth terms.
GETSOL	Handles interactive input of the point beneath the sun in latitude and longitude.
SUBSOL	Computes solar latitude and longitude from the date and time of day, during interactive input.
RELABS	Performs conversions between relative and absolute line-of-sight specifications.
GETAZI	Handles interactive input of local azimuth angles for a line-of-sight.
ARCCOS	Checks argument of arccosine to make sure it is between 1.0 and -1.0, then computes ACOS.
ARCSIN	Checks argument of arcsine to make sure it is between 1.0 and -1.0, then computes ASIN.
ARCTAN	Returns an angle between 0 and 2π given the end coordinates of a line with one vertex at the origin.
AZI	Computes the local azimuth given the latitude of two points and the angle between them.
CHECKG	Checks the geometry inputs prior to an calculation.
CONDTR	Converts all angles to radians and transforms coordinates to geographic coordinates.
CONRTD	Converts all angles to degrees and transforms coordinates to magnetic north pole coordinates.
CONMTG	Converts coordinates based on magnetic north pole to geographic north pole coordinates.
CONGTM	Converts coordinates based on geographic north pole to magnetic north pole coordinates.
CONREL	Converts a line-of-sight specified in terms of solar zeniths and azimuths to latitude and longitude specifications.
CONABS	Converts a line-of-sight specified in latitudes and longitudes to representation in terms of solar zeniths and azimuths.
CROSS	Takes the cross product between two vectors using the right hand rule.
DOT	Takes dot product of two vectors.
DAZI	Computes the local azimuth given the latitude of two points and the angle between them (double precision).

DLATI	Computes the latitude of point "I" in radians given the latitude of another point, "II" and the latitude of point I to II (double precision).
DLONGI	Computes the longitude of point "I" in radians given the longitude of another point, "II" and the longitude of point I to II (double precision).
FNDDAY	Determines days of year corresponding to solar latitude.
FNDGMT	Determines Greenwich Mean Time from day of year and solar longitude.
GEOMEX	Completes the full (over complete) set of variables which describe the line-of-sight.
INSIDE	Determines whether the local region forms a proper convex spherical pyramid.
LATI	Computes the latitude of point "I" in radians given the latitude of another point, "II" and the latitude of point I to II.
LATPHI	Calculates the latitude and longitude of vector 2 relative to vector 1, given the latitudes and longitudes of vectors 1 and 2 relative to a common vector.
LONGI	Computes the longitude of point "I" in radians given the longitude of another point, "II" and the longitude of point I to II.
LOS	Determines the line-of-sight vector.
MAJSEG	Determines the major segments of the LOS through a region.
NORM	Normalizes a vector of length 3.
ORDKEY	Determines the relative order of the elements of a vector, and returns an integer vector key containing the element indices in order of increasing element magnitude.
ORDRS	Determines the order of occurrence of intersections of the line of sight with region boundaries.
OPSANG	Computes the supplemental angle.
PLSECT	Determines the intersection of a line-of-sight vector with a plane.
PYRINT	Computes the segment boundaries of the LOS that are within a spherical pyramid.
RADE	Computes the earth radius as a function of latitude.
RANGER	Computes the over complete set of LOS geometry parameters.
REGANG	Maps an arbitrary angle to a specified interval of 2π .

REGDTR	Converts edge latitudes and longitudes to radians and converts to geographic coordinates if necessary.
REGLOS	Determines if observer or source is inside the angular region.
SETGEO	Initializes geometry parameters.
UNIVEC	Determines the unit vector from latitude and longitude.
VECPOL	Determines a cartesian vector from an altitude, latitude and longitude.
VECVRT	Determines polar coordinates from a cartesian vector.

geoseg.f: The SHARC SEGMENT GEOMETRY Module

SEGEN	Generates minor segments for each major segment along the specified line-of-sight.
SEGMNT	Computes major segment properties, including the major segment lengths, the number of major segments, and identifies the lower boundary for each segment.
PROCAL	Calculates the line-of-sight properties for a major segment in a single region.
ZNFDGE	Determines the appropriate profile column densities for each segment of the line-of-sight.

inactv.f: The INTERACTIVE INPUT Module

PROBDF	Drives the interactive menu or batch execution of SAMM, and determines all of the input parameters.
ADDREG	Reviews, edits and adds regional information.
ADDRAD	ADDRAD is the input routine which is used to add radiative species to the ambient and auroral population calculations.
CHKREG	Checks all regional information, such as filenames and input variable prior to an calculation.
CHKLYR	Checks that sets of boundary altitudes of multiple profiles within a region are the same.
CHKPOP	Compares population file content information for consistency with region data and other profiles specified in SHARC.INP.
ALLOLD	Determines whether or not all population files are old.
INATM	Interactively reviews/changes the user's choice of model atmosphere.
INAUR	Interactively reviews/changes the user's choice of auroral conditions.

INBOND	Interactively inputs the parameters which define a local region.
INMOL	Interactively reviews/changes the radiators included in the population calculations.
INNAME	Interactively reviews/changes the names for the standard input and output files.
INNEM	Interactively reviews/changes the input parameters for the Monte Carlo radiation trapping module.
INOUT	Allows the user to review and/or modify the amount of output written to the general output file.
INPOP	Interactively reviews/changes the population file names and status.
GENTAB	Generates the proper character string for appending to a standard population file name.
INREGN	Interactively reviews/changes regional information.
RMREG	Removes an unwanted region.
RMRAD	Eliminates a radiator from the list of species desired for population calculation.
INSOL	Interactively changes/reviews the solar zenith angle.
INSPEC	Interactively changes and/or modifies the spectral range, resolution and species included in spectral radiance calculation.
SPCCHK	Checks to ensure that populations exist for all species selected for spectral calculation.
INSTDS	Supplies the menus for input of name patterns and directories for kinetics, atmospheric, population and lines files.
INTITL	Interactively reviews/changes the title of the calculation.
INTYPE	Interactively changes the environment type. SAMM currently has two environments: ambient and auroral.
OPNFLS	Opens output and line files.
POLL	Writes the main interactive menu for running SAMM.

input.f: The INPUT Module

ATMDEN	Loads atmospheric profile into the appropriate local arrays.
ATMIN	Identifies the atmospheric species in the general species list, and reads atmospheric profile (containing the species number densities and kinetic temperature).

ATMLYR	Computes the atmospheric properties for each layer.
ATMSYM	Sets up the character arrays identifying the atmospheric species and an indexing array which relates the atmospheric species to the species read by CKLINK.
BANDIN	Reads the molecular bands file (Subsection 3.3), which describes the line strength distribution function parameters for each vibrational transition.
BLKDTS	Sets numerous parameters concerning molecular data.
BOTCHK	Checks that the lowest altitude in an atmospheric profile matches that defined in block data. This assures consistency within the layer to layer pumping routine.
CKLINK	Reads the "linking" file created by INTERP, and defines the arrays containing information on species names, chemical kinetics mechanism (that is, the stoichiometric coefficients) and the rate constants.
POPIN	Reads in population file data for CHKPOP.
RADIN	Reads the molecular states file (Subsection 3.2), which contains the molecular radiator, the vibrational states included in the mechanism and the transitions to be considered by NEMESIS.
REGCHK	Checks region altitude boundaries for consistency with profile boundaries.
RETREV	Reads the saved population file data.
XNUM	Translates an alphanumeric character string containing N integer, real, or exponential numbers into their respective real values.

inutil.f: The INPUT UTILITIES Module

LOADDE	Opens and loads the input data found in SAMM.INP into the array DFLTS. If SAMM.INP is not found, this routine calls NODFTS to load in a set of default parameters.
DUMPDE	Writes the current values of the input variables into the defaults file.
NODFTS	Loads the default values for a calculation into SHARC.INP when an SHARC.INP is not found.
COMOUT	Prints standard comments into the defaults file.
DFLTSG	Reads the regional information found in the defaults file.
PARSEC	Separates text and numerical input parameters from an input character string.

RCHECK	Checks the range of the variable to verify that the variable value is between the given bounds.
MCHECK	Checks the range of the variable to verify that the variable value is between the given bounds.
REDCHR	Reads user response to queries that require character string answers.
REDINT	Reads user response to queries that require integer answers.
REDREL	Reads user response to queries that require real variable answers.
SRTMOL	Sorts molecular radiators according to AFGL molecule number.
STUFFD	Fills dflts array with regional input information.
UPCASE	Converts a character string to all upper case characters.
LOCASE	Converts a character string to lower case.
CPYSTR	Copies one character string into another.
LENSTR	Determines the non-blank length of a character string.
CATSTR	Concatenates two character strings.
ITOASC	Converts an integer to its ASCII representation.
WRTSTR	Writes a character string to an internal file.
ACTIVE	Reads the first data line in the default file to determine if the calculation is interactive or batch.
FCHECK	Opens files and checks their status against the expected status. For example, does a new file already exist.
DCHECK	Checks for the existence of a directory.
KEEPI	Stores a copy of an integer vector.
KEEPR	Stores a copy of a real vector.
LENREC	Determines the length of records in a direct access file.
MRGSTR	Merges a character string with another string.
VIBTRN	Translates the vibrational state designation found in the sharc line file data base to the appropriate index for the population arrays.
VIBES	Converts 1982 HITRAN vibrational assignments to 1985 format when ICHOIC=1, and converts 1985 format to 1982 vibrational assignments when ICHOIC=2. This routine is from the HITRAN line selection program.

modaer.f: The MODTRAN AEROSOLS Module

AERNSM	Defines the lower atmosphere molecular, aerosol and cloud profiles.
CIRR18	Defines the new cirrus and optically thin cirrus profiles.
FLAYZ	Determines the final lower atmosphere altitude boundaries.
JOU	Interprets the JCHAR character inputs.
CHECK	Converts pressure and temperature to MODTRAN standards.
DEFAULT	Chooses a stored atmospheric profile and interpolates default values for a specific altitude.
CONVRT	Accommodates uniform data for MODEL 0 or 7.
WATVAP	Computes water vapor number density (mol/cm^3) to accommodate "JCHAR" definitions specified by user.
VSANSM	Drives Vertical Structure Algorithm routines.
LAYVSA	Determines atmospheric layering for the Vertical Structure Algorithm.
LAYCLD	Determines atmospheric layering for MODTRAN cloud models.
MARINE	Determines aerosol extinction and absorption coefficients for the Navy maritime model.
DESATT	Determines aerosol extinction and absorption coefficients.
CLDPRF	Defines standard cloud profiles.
AERPRF	Computes density profiles for aerosols.

modblk.f: The MODTRAN BLOCK DATA Module

BLKDAT	Defines constants and routing arrays (conversions between SHARC, HITRAN and MODTRAN labeling schemes).
BLKMOD	Initializes fixed MODTRAN inputs.
MLATMB	Defines model atmospheric data for six stored atmospheric models.
RECDAT	Defines the frequency to record array for the direct-access SHARC lines file.
TITLE	Defines titles for MODTRAN output.
EXTDTA	Defines aerosol and cloud extinction, absorption and asymmetry parameters.
PHSDTA	Defines 70 averaged phase functions and truth table identifying correct phase function.

MDTA	Defines cloud and rain modeled atmospheric data.
DSTDTA	Defines desert aerosol extinction, absorption coefficients and asymmetry parameters for 4 wind speeds.
CPTRCG	Defines Pierluissi band model absorption coefficients for trace gases.
CPUMIX	Defines Pierluissi band model absorption coefficients for uniformly mixed gases.
CPH2O	Defines Pierluissi band model absorption coefficients for water vapor.
CPO3	Defines Pierluissi band model absorption coefficients for ozone.

moddrv.f: The MODTRAN DRIVER Module

DRIVR	Drives MODTRAN calculation and read control cards.
PATHAZ	Calculates the path azimuth based on latitude and longitude data.
PSIECA	Calculates earth centered angle and path azimuth from an observer to a source point given latitude and longitude data.
RDNSM	Reads user input data when user-defined molecular profiles and Vertical Structure Algorithm options are selected.
RDEXA	Reads user-defined aerosol or cloud input.
CIRRUS	Generates altitude profiles of cirrus cloud density.
VSA	Drives Army Vertical Structure Algorithm calculations of aerosol extinction and relative humidity for low visibility/low ceiling conditions.
STDMDL	Sets up scaled densities for the model atmosphere.
AERTMP	Defines temperature for each aerosol altitude region.
EXABIN	Loads aerosol extinction, absorption and scattering.
EQULWC	Calculates liquid water content of standard aerosols.

modgeo.f: The MODTRAN REFRACTIVE GEOMETRY Module

GEOM	Drives the low altitude air mass subroutines, and calculates attenuation amounts for slant paths.
GEOMIN	Translates geometry input parameters into the standard set.
FNDHMN	Calculates the minimum altitude along a path and the zenith angle at termination.

REDUC	Eliminates slant path segments that extend into the high altitude regime.
LOCATE	Locates latitude and longitude of point given latitude and longitude of observer, earth centered angle and path azimuth at observer.
FBETA	Calculates the zenith angle at the observer given observer and source altitude and the earth centered angle.
RPATH	Drives calculation of refractive path from observer to source.
TANHT	Calculates tangent height along a refractive path.
FILLS	Defines the boundaries of the slant path and interpolates densities at these boundaries.
LAYERS	Calculates path length through one layer.
RADREF	Computes the reciprocal of the radius of curvature as a function of altitude.
FINDSH	Finds the scaling parameters for refractive index within a layer.
SCALHT	Calculates coefficient and scale height for index of refraction.
ANDEX	Computes index of refraction at a specific height.
EXPINT	Performs exponential interpolations.
FNDH2	Finds the termination point altitude and zenith angle given the observer altitude, zenith angle and range.
FTRANG	Finds zenith angles at observer and source given their range and altitudes.
DENFAC	Evaluates the integral from $x=0$ to $x=1$ of $\exp[-R(Bx + 2Ax)]$.
DAWSON	Evaluates the integral from $t=0$ to $t=x$ of $\exp(t^2 - x^2)$.
FACFNC	Evaluates $0.5 \sqrt{\pi} \exp(z^2/b^2) \operatorname{erfc}(z/b) / b$ where $\operatorname{erfc}(x)$ is the complement of the error function evaluated at x .

modlay.f: The RADIATIVE TRANSPORT LAYER LOOP Module

LOOP	Loops over layers for each frequency calculating radiances and transmittance.
BBFN	Calculates the Planck black body function $[W/cm^2-sr-\mu m]$.
LAY5DT	Fetches the layer dependent 5 cm^{-1} resolution data.
RAIN	Fetches the extinction, absorption and scattering coefficients and the asymmetry factor for rain.
TNRAIN	Calculates the extinction due to rain as a function of rain rate.

GMRAIN	Computes attenuation of condensed water in the form of rain.
AITK	Performs aitken interpolation.
RNSCAT	Calculates extinction, scattering and asymmetry parameter due to rain in the microwave region.
RNTAB	Contains tables of rain data.
BS	Performs a binary search to determine bracketed values.
DBLTX	Calculates transmittance from the double exponential band model.
SSRAD	Performs the layer by layer single scattering radiance sum.
PHASEF	Chooses correct phase function based on relative humidity, frequency, scattering angle and model.
HENGNS	Calculates the phase function using the Henyey-Greenstein method.
SOURCE	Calculates solar intensity date and calculates lunar intensity.
BMLOAD	Loads band model parameter data.
BMFLUX	Calculates upward and downward fluxes at 1 cm^{-1} resolution.
FLXADD	Calculates upward and downward fluxes at 5 cm^{-1} resolution using the k-distribution method.
BETABS	Supplies the back scatter fraction for a given asymmetry factor and cosine.
SAMMOD	Calculates molecular transmittance at 1 cm^{-1} resolution.
SAMLP	Determines the band model contributions to molecular transmittance for a multiple scattering path.
SAMLPO	Determines the band model contributions to molecular transmittance for an optical path.
SAMWID	Calculates the spectral bin Voigt equivalent width.
SAMERF	Returns a value for " $\exp(-y*y) + \sqrt{\pi} * y * \text{erf}(y) - 1$ " where y is the argument and erf is the error function.
SUN	Evaluates the extraterrestrial solar irradiance.

modrad.f: The RADIATIVE TRANSPORT Module

TRANS	Drives radiative transport calculations and writes out results.
MAPMS	Maps LOS layer indices into vertical path indices.
SAMDAT	Calculates frequency-independent data needed for the band model and line-by-line molecular transmittance calculations.

FRQ5DT	Calculates the layer independent 5 cm^{-1} data.
CXDTA	Locates coefficient for double exponential band model.
C4DTA	Returns N_2 continuum absorption coefficient at required wavenumber.
ABCDTA	Moves double exponential coefficients into new arrays.
SLF296	Loads self-broadened water vapor continuum at 296 K.
SLF260	Loads self-broadened water vapor continuum at 260 K.
FRN296	Loads foreign-broadened water vapor continuum at 296 K.
C6DTA	Returns Rayleigh molecular scattering attenuation coefficient at required wavenumber.
C8DTA	Returns Chappuis ozone visible absorption coefficient at required wavenumber (13000 to 24200 cm^{-1}).
HNO3	Determines nitric acid absorption coefficient at required wavenumber.
FUDGE	Calculates a fudge factor based on the sum of exponentials.
AEREXT	Interpolates aerosol attenuation coefficients and asymmetry factors to required wavenumber.
GAMFOG	Computes attenuation of equivalent liquid water content in clouds.
INDX	Calculates the real and imaginary part of refractive of the refractive index of water.
DEBYE	Calculates the wavenumber dependence of the dielectric constant of water.
DOP	Describes the real part of the dielectric constant for water.
HERTDA	Defines the UV O_2 Herzberg continuum using an analytic function.
SCHRUN	Determines the UV O_2 Schumann-Runge band model parameters.
O3HH0	Returns the constant term in the UV O_3 Hartley band (24370 to 40800 cm^{-1}) temperature dependent absorption coefficient expansion.
O3HH1	Returns the linear term in the UV O_3 Hartley band (24370 to 40800 cm^{-1}) temperature dependent absorption coefficient expansion.
O3HH2	Returns the quadratic term in the UV O_3 Hartley band (24370 to 40800 cm^{-1}) temperature dependent absorption coefficient expansion.
O3UV	Interpolates UV O_3 data for the 40800 to 54054 cm^{-1} region.
O2CONT	Interpolates the O_2 continuum for the 1395 to 1760 cm^{-1} region.

modssg.f: The SOLAR SCATTERING GEOMETRY Module

SSGEOM	Obtains attenuation amounts for the lower atmosphere from scattering points along optical path to the extraterrestrial source.
SAVRES	Saves and restores optical path geometry and amount parameters in preparation for solar path calculations.
FNDSUN	Determines subsolar angles when solar zenith and azimuth at the observer are input.
PSI	Returns solar azimuth relative to LOS at current scattering location.
SCTANG	Returns the scattering angle at any point along the optical path.

mosinp.f: The MOSART INPUT Module

CHRCBD	Initializes MOSART character strings.
DEVCBD	Assigns MOSART file unit numbers.
F5FMT	Determines the x (0 to 4) in format f5.x such that input altitudes (km) are printed with the maximum possible number significant figures.
GETATM	Determines pressure, temperature and MOSART species densities at an input altitudes.
GETVAR	Reads a free format real variable from an input character string.
INITL	Finds the location of the first non-blank character in a character string.
INMOS	Reads MOSART inputs from array "DFLMOS" and allows the user to change the data using a menu-query system.
INPTBD	Contains the MOSART sample input file.
INSERT	Inserts one character string into another eliminating leading blanks and truncating if necessary.
LCTRIM	Trims any leading blanks from an input character string.
MOSIN	Writes out the MOSART input file.
OPTNS	Reviews and/or modifies MOSART input options.
PROMPT	Changes MOSART input data in interactive mode.
RDALTS	Prompts user for MOSART user-defined altitude grid.
RDANTE	Prompts user for MOSART antecedent input data.
RDATM	Prompts user for MOSART user-defined atmosphere data.

RDET	Prompts user for MOSART extraterrestrial source input options.
RDH2O	Prompts user for MOSART hydrometer data.
RDKEEP	Prompts user for MOSART keep/delete file status data.
RDNAMS	Prompts user for MOSART optional data file names.
RDOBS	Prompts user for MOSART observer parameters.
RDTBCK	Prompts user for MOSART terrain material temperatures.
RDterr	Prompts user for MOSART terrain specifications.
RDTHRM	Prompts user for MOSART source earth/skyshine specifications.
RDUAER	Prompts user for MOSART user-defined aerosol data.

output.f: The SHARC OUTPUT Module

AMABOUT	Prints number densities for ambient molecules.
ATMOUT	Prints the atmospheric profile.
AUROUT	Prints the time dependent number densities for an auroral calculation.
BANNER	Outputs the SHARC banner identifying the run.
BNDOUT	prints the line strength distribution function parameters.
GEMOUT	Writes out a brief summary of the LOS information to rootname.OUT.
GENOUT	Writes out a brief general description of each regional calculation.
NEMOUT	Prints out some of the inputs used by NEMESIS.
POPOUT	Outputs the number densities as a function of altitude for each vibrational state in the mechanism.
RADOUT	Outputs the information contained in the molecular states file.
RETOUT	Writes a summary of the population file to rootname.OUT when an old population file is used in a new calculation.
SAVE	Writes the population file.
SUMOUT	Prints a calculational summary at the beginning of each SAMM run.
VBTOUT	Outputs the vibrational temperatures as a function of altitude for each vibrational state in the mechanism.
VIBTMP	Calculates vibrational temperatures of excited state species.

samblk.f: The BAND MODEL PARAMETER BLOCK DATA Module

SAMBLK Defines the final frequency and number of parameter sets in each record in the direct-access band model file.

saminp.f: The LOWER ATMOSPHERE INPUT Module

CRD1 Interactively reviews/modifies MODTRAN CARD1 inputs.

CRD2 Reads in aerosol input data.

CRD2IN Reads in atmospheric profiles for use in lower atmosphere.

CRD2C Drives determination of lower atmosphere profiles.

FINDEX Determines the location of the MODTRAN molecules in the SHARC molecular density array.

XNTRP Interpolates to determine pressure, temperature and molecular densities to input altitude and solar zenith angle.

DAYMON Converts day of year to month and day of month ignoring leap year.

INMOD Reads MODTRAN inputs from default file, calls routine to prompt for changes, and stores final input selections.

INSHAR Sets array indicating which SHARC radiators are to be included in radiance calculation.

IPOPMD Finds the population files of the extended region which have earth centered angles to the sun bracketing the observer-to-sun earth centered angle.

LOCCUR Determines whether one character string is a substring of another character string ignoring upper and lower case differences.

RDIEMS Allows the user to review or modify the type radiance/transmittance calculation to be performed.

RDIRPT Allows the user to change whether or not a repeat run is to be performed.

RDLMOL Allows the user to review or modify the MODTRAN radiator list.

RDNOPR Allows the user to review or modify the amount of output generated in the MODTRAN standard output file, rootname.TP6.

RDRUNM Allows the user to review or modify whether a SAMM, MODTRAN or GEOMETRY ONLY calculation is to be performed.

RDSALB	Allows the user to review or modify the scattering albedo.
RDTBND	Allows the user to review or modify the boundary temperature.
REPEAT	Sets up repeat runs.
WTCD1	Writes MODTRAN CARD 1 data to file TAPE5.
WTCD2	Writes MODTRAN CARD 2 data to file TAPE5.
WTCD3	Writes MODTRAN CARD 3 data to file TAPE5.
WTCD45	Writes MODTRAN CARD 4 and CARD 5 data to file TAPE5.
WTTAP5	Writes MODTRAN input data to file TAPE5 for repeat runs.

samseg.f: The COLUMN DENSITY Module

NLTE	Drives column density calculations combining MODTRAN low altitude column densities with calls to SHARC routines to determine high altitude column densities.
GETPOP	fetches LOS average populations for each high altitude layer.
HIGH	determines high altitude column densities for lte radiators.
SAMSS	drives the calculation of cumulative absorber amounts from scattering points along the optical path to the extraterrestrial source.
VIBSS	calculates the vibrational state column densities for the scattering point to sun paths.
HIGHSS	calculates the lte radiator column densities for the scattering point to sun paths.
PTHOUT	prints out column density data.
VPLOW	calculates lower atmosphere column densities.
RQVIB	returns the reciprocal of the vibrational partition functions for the SHARC radiators.

APPENDIX D
TEST CASES

APPENDIX D

TEST CASES

SAMM is supplied with seven test cases to allow the user to check that it has been properly installed, and to demonstrate some of its features. The first five test cases are modeled after the five SHARC-3 test cases. The input files which define all test cases are supplied; if the user employs the data files supplied, the resulting calculation outputs should match those shipped for the cases, apart from minor roundoff error. Appendix A lists the test case files and the files are stored in sub-directory INPDIR (assuming a SAMM TAR tape). For each of the seven test cases, there is a general input file, TESTn.INP (n=1-7); a SHARC general output file, TESTn.OUT; spectral radiance, transmission and bandpass radiance files, TESTn.SPC, TESTn.TRN, and TESTn.RAD; a MODTRAN input file, TESTn.TP5; and MODTRAN standard, plotting and auxiliary output files, TESTn.TP6, TESTn.TP7, and TESTn.TP8. Since test case 6 and 7 include aerosols, the HAZE.INP files TEST6.HAZ and TEST7.HAZ are included for these cases. Test cases 3, 4, and 7 output warnings to the journal file; for these test cases, TESTn.LOG files have also been included. The main points of interest for each case are discussed here.

D.1 PREPARATIONS

To prepare for running the test cases, the SAMM executable subdirectories "DATDIR", "POPDIR", "KINDIR", "OUTDIR", and "ATMDIR" should be created if they do not already exist. Test case files (TESTn.extension) have been placed in subdirectory INPDIR to prevent them from being over written. SAMM output will be written to the OUTDIR subdirectory. All atmosphere profiles should be placed in the ATMDIR subdirectory. The user should compile, link, and run the INTERPRETER source files from subdirectory KINDIR. From DATDIR, the ASCII-to-binary source files (dirac.f and ufmak.f) should each be compiled, linked, and run, and the output file "samblk.f" should be moved up to the SAMM executable directory which should contain the rest of the SAMM FORTRAN source files. The "POPDIR" and "OUTDIR" subdirectories must exist in preparation for receiving output. If this set of subdirectories is in some way undesirable, the user will need to modify the directory paths in top-level menu item 7. Finally, the SAMM source should be compiled and linked.

D.2 THE TEST CASES

D.2.1 First Test Case

For test case 1 only, it is not necessary to copy TEST1.INP into the SAMM executable directory as SAMM.INP. The SAMM source has the inputs for test case 1 built into the code as defaults. Simply running SAMM will generate a SAMM.INP which is identical to TEST1.INP, assuming the executable directory does not have either a pre-existing SAMM.INP or HAZE.INP file. This arrangement insures that the user will never lack for an input file upon which to build. Without a HAZE.INP input file, SAMM assumes no aerosols. Once the input file is properly generated, the user can run the test case and, as for all the cases, compare the output files with those shipped. If SAMM is run interactively (entering 999 from the main menu), the journal file will contain a warning noting no SAMM.INP file was found and that the default had to be used. If the users exits the main menu with an 8, in preparation for a batch mode run, then the journal file, SAMM.LOG will again contain this warning; however, when SAMM is subsequently run in batch mode, the original journal file will be deleted (since SAMM.INP did exist for the batch run).

This first case has a nighttime auroral region embedded in an extended ambient region. The selection of radiators, NO and NO⁺, permit this case to run in a relatively brief time. Selected inputs and outputs from Test Case 1 are reproduced in Appendices E and F. This case matches SHARC-3 Test Case 1 except for differences in spectral resolution. The SAMM and SHARC-3 results are compared at the same resolution in Figure D-1.

D.2.2 Second Test Case

All remaining cases must be run from the supplied TESTn.INP files, which the user must copy to SAMM.INP in the executable directory. Again, the executable directory should not contain a HAZE.INP file since this test case does not include aerosols. The second case calculates nighttime emission from all seven SHARC radiators, but with none of the MODTRAN only radiators. There should be no journal file at the end of the run. This case is identical to the SHARC-3 Test Case 2 except for differences in spectral resolution. The SAMM and SHARC-3 results are compared at the same resolution in Figure D-2. A more detailed comparison illustrates that the only significant differences arise for the 7.65 μm CH₄ band, Figure D-3. Since SHARC-3 and SAMM use different lower boundaries for solving the chemical kinetics equations (50 km in SHARC-3 and 30 km in SAMM), they predict different amounts of earthshine pumping. Generally these differences are small. The 7.65 μm CH₄

band is an exception in this case. Preliminary comparisons to CIRRIIS data seem to indicate better agreement with SAMM, but these results are inconclusive due to uncertainties in the methane profile.

D.2.3 Third Test Case

The third test case, like the first, is a nighttime aurora, but with CO₂ added as a radiator; only NO and NO⁺ are calculated as in the first test case. The third test case demonstrates the reuse of population files. The first two cases generate new population files. Being binary, these files cannot be shipped and must be generated on the user's machine. The species population information in them can be reused once generated. The third-case auroral calculation requires both ambient and auroral population files. Instead of being generated anew, however, the ambient file is that created by the second test case. That file, POP2.180, must have been previously generated by the second case and left in the POPDIR subdirectory in order for the third case to run. The third case creates its own auroral population file POP3A.180. Test Case 3 outputs a warning in the journal file indicating that vibrational state populations have been determined for molecules not included in the radiator list. That is, POP2.180 generated vibrational distributions for all species, but only NO, NO⁺ and CO₂ have been included in the radiator list. This case matches SHARC-3 Test Case 3 except for differences in spectral resolution. The SAMM and SHARC-3 results are compared at the same resolution in Figure D-4.

D.2.4 Fourth Test Case

The fourth and fifth test cases demonstrate the use of multiple atmospheric profiles to model the terminator. The atmosphere generator was used to write seven files representing solar zenith angles from 91° to 102°, essentially bracketing the change in ozone vibration state densities at high latitudes. The atmosphere names are "T4Z(solar zenith angle).ATM" where the solar zenith angle is a 3 digit integer between 091 and 102. The test case calculates the radiance of O₃, whose concentration is sensitive to solar illumination. The LOS for the first three test cases are limb views; the LOS starts and ends at the maximum 300 km altitude, capturing radiation from the entire atmosphere above the tangent altitude. This test case uses an observer to space LOS; the observer is located at 184 km and looks downward through the tangent point at 96 km and back up to 300 km. This case matches SHARC-3 Test Case 4 except for differences in spectral resolution. The SAMM and SHARC-3 results are compared at the same resolution in Figure D-5.

D.2.5 Fifth Test Case

The fifth case also uses seven profiles to model a terminator LOS. Presently, seven is the maximum number of profiles allowed for a single region (increase NPOPMX in PARMS.H to allow for more profiles). The atmosphere names are "T5Z(solar zenith angle).ATM". The observer is in about the same location as in the fourth case, slightly higher at 250 km. The radiators are the three most prominent isotopes of CO₂. This case matches SHARC-3 Test Case 5 except for differences in spectral resolution. The SAMM and SHARC-3 results are compared at the same resolution in Figure D-6.

D.2.6 Sixth Test Case

The sixth test case is considerably different from the first five test cases. This test case includes aerosols, so it is necessary to copy TEST6.HAZ into the executable directory as HAZE.INP. Test case 6 performs a low altitude daytime calculation (limb LOS tangent at 10 meters altitude) with all SHARC and MODTRAN radiators, and uses the repeat run option to compare SAMM combined LBL/band model results to MODTRAN band model only results. Solar and thermal single and multiple scattering is included in the calculations. Agreement is excellent in all regions except the center of the 4.3 μm band, where near field hot CO₂ significantly contributes to the spectral radiance. The complete SAMM and MODTRAN results are compared in Figure D-7. In Figure D-8, the 4.3 μm region is plotted on a more expanded scale in order to show the differences between SAMM and MODTRAN.

D.2.7 Seventh Test Case

The seventh test case demonstrates how SAMM is used to calculate bandpass radiance profiles. Again for this case it is necessary to copy TEST7.HAZ into HAZE.INP. In this run, a localized auroral region is centered 65° north of the equator and at 0° longitude. The aurora extends from 80 to 160 km altitude. Sixteen limb calculations are performed with tangent heights separated by 8 km from ground to 120 km altitude. All radiators are included in the calculations. The tangent point is located at the center of the aurora, 65° North and 0° East. The LOS travels directly west at the tangent point. SAMM, SHARC, and MODTRAN predictions are compared in Figure D-9 for the bandpass extending from 1500 to 2400 cm⁻¹.

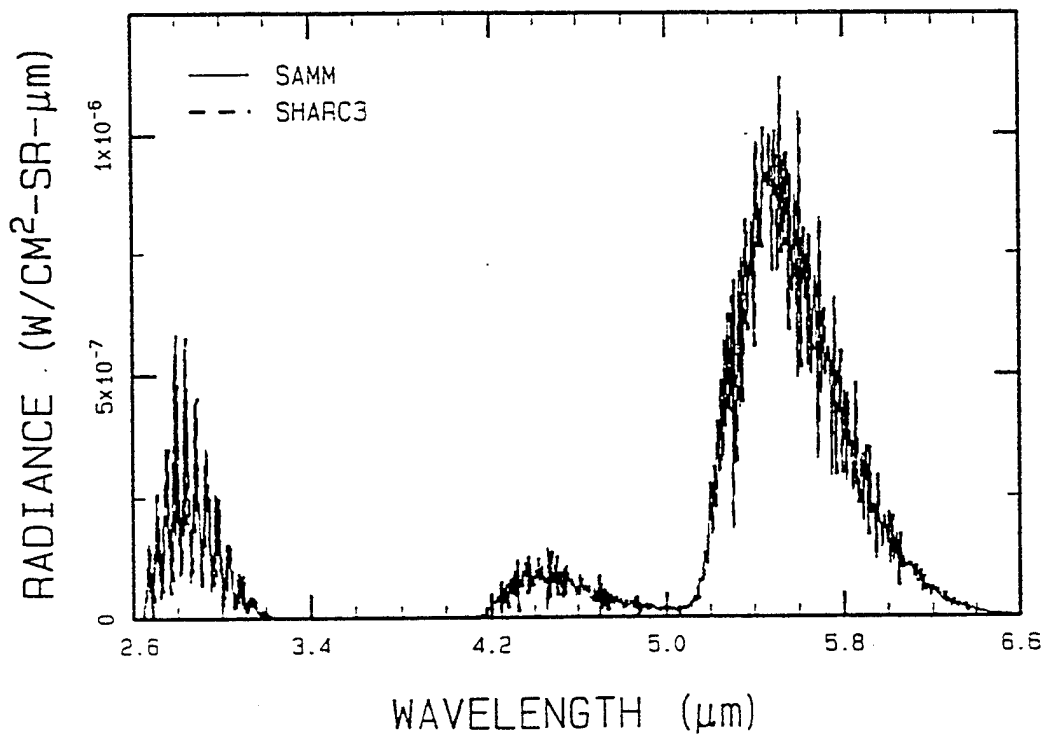


Figure D-1. SMM/SHARC Test Case 1 Comparison.

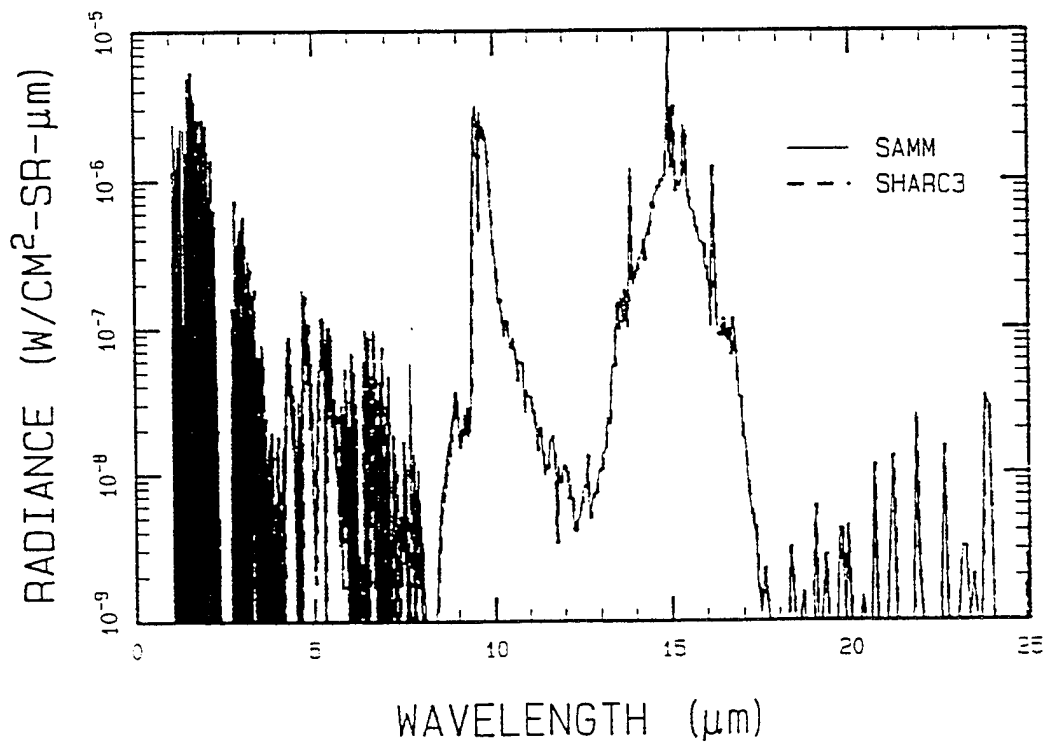


Figure D-2. SMM/SHARC Test Case 2 Comparison.

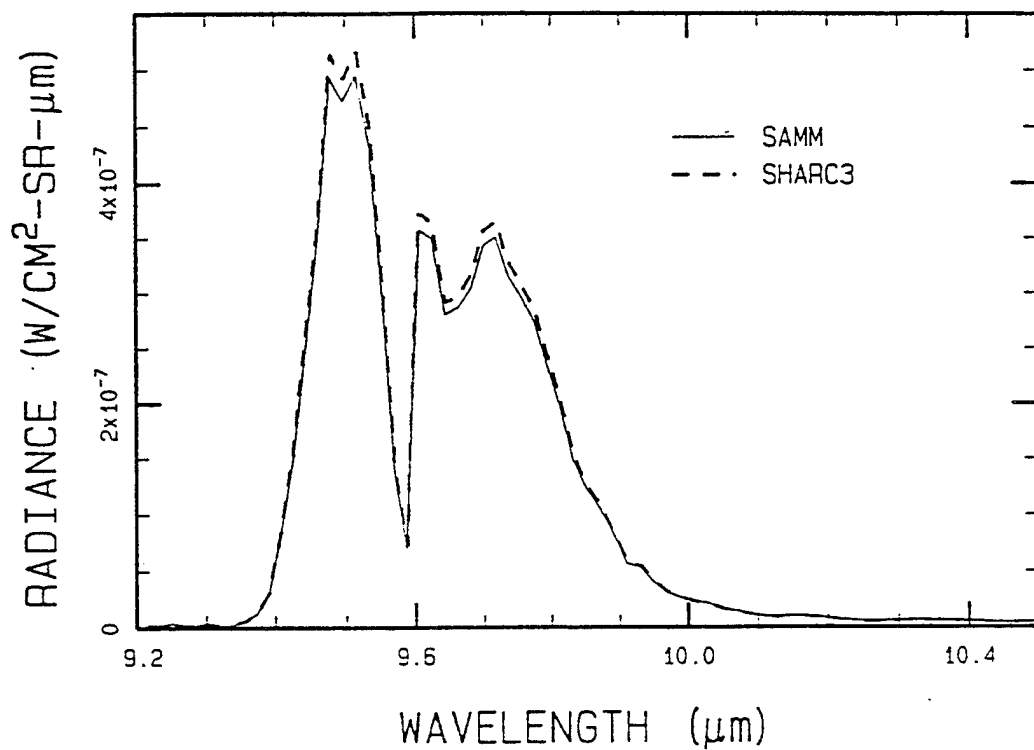


Figure D-5. SMM/SHARC Test Case 4 Comparison.

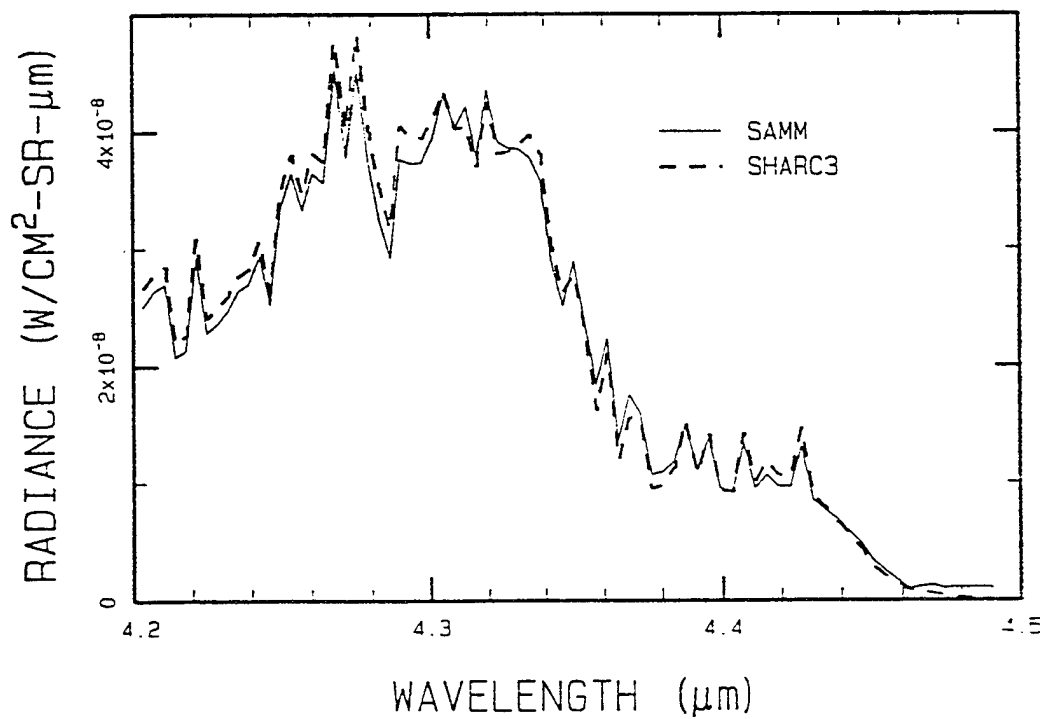


Figure D-6. SMM/SHARC Test Case 5 Comparison.

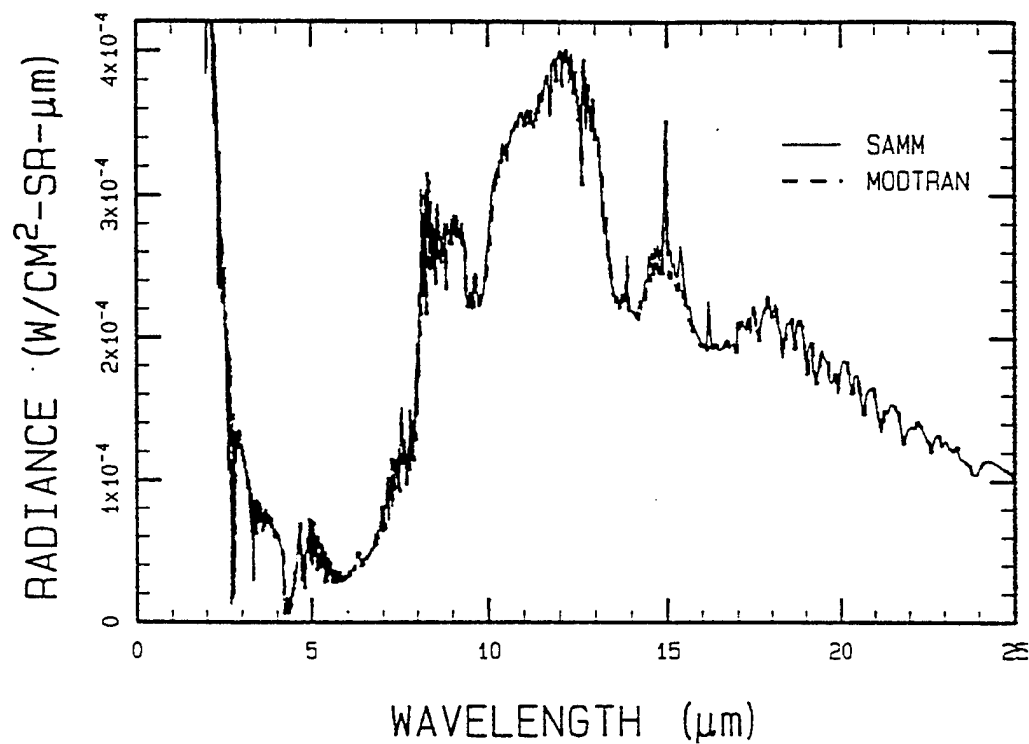


Figure D-7. SAMM/MODTRAN Test Case 6 Comparison.

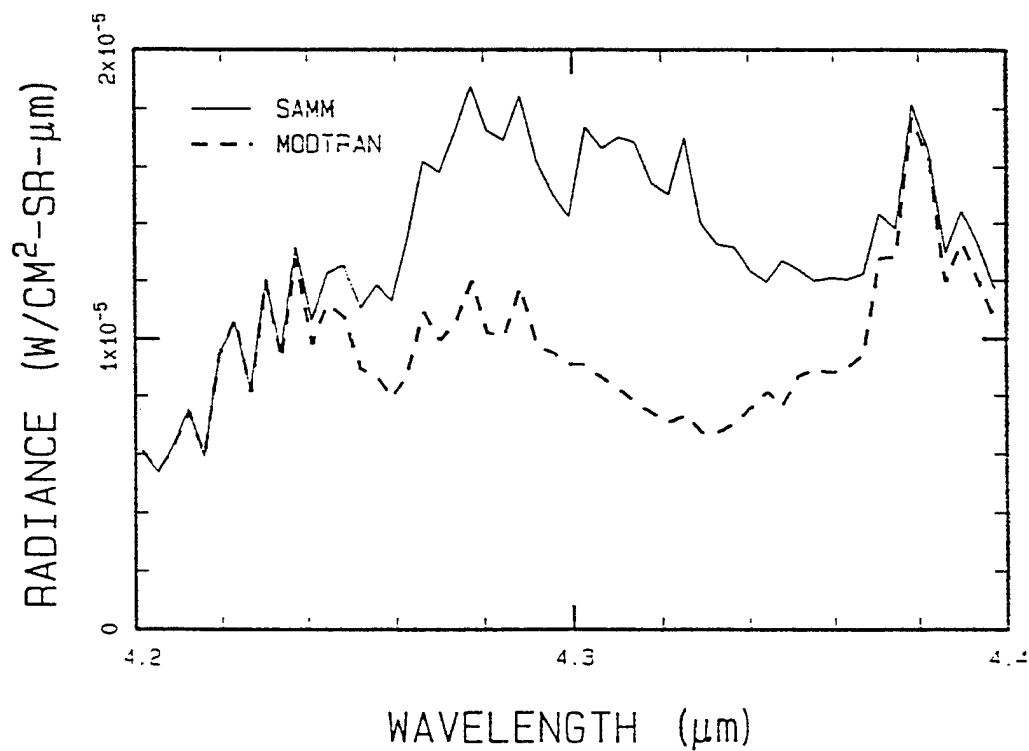


Figure D-8. SAMM/MODTRAN Test Case 6 Comparison in the 4 μm Region.

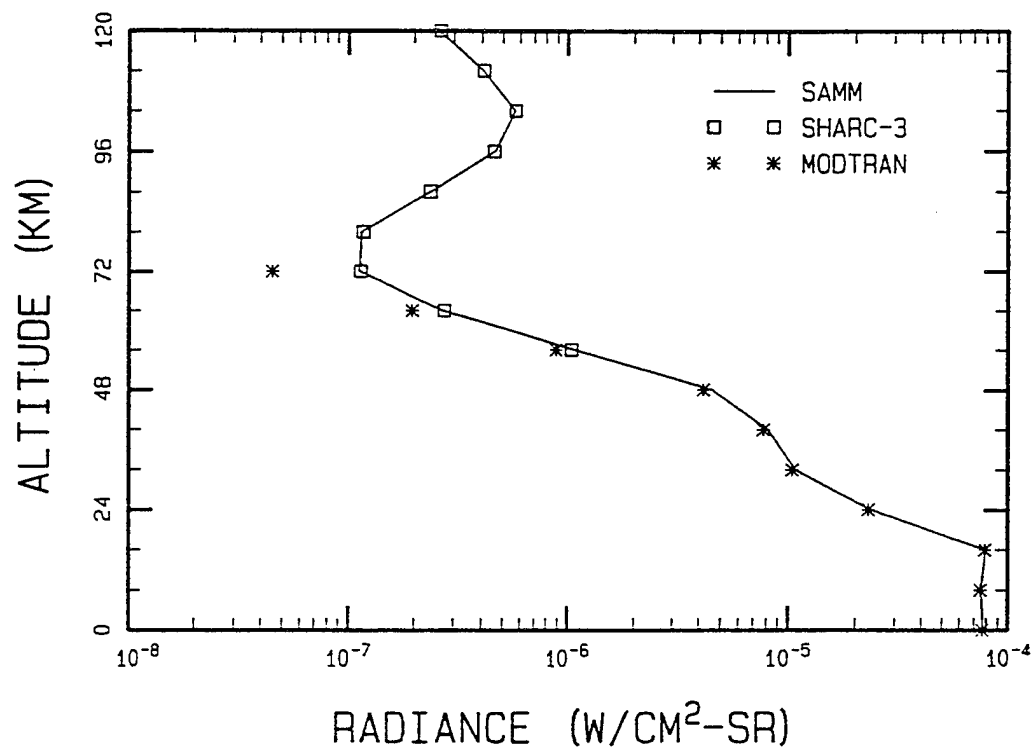


Figure D-9. SMM/SHARC/MODTRAN Test Case 7 Comparison for the 4.2 to 6.7 μm Bandpass.

APPENDIX E

SAMM MID-LATITUDE NIGHT-TIME
ATMOSPHERIC PROFILE

APPENDIX E

SAMM MID-LATITUDE NIGHT-TIME ATMOSPHERIC PROFILE

ATMOSPHERE SAMM

MIDLAT.NIG

END

NUMBER OF LAYERS

102

END

EXOATMOSPHERIC TEMPERATURE

1000.0

END

SPECIES

N2 O2 O CO2 CO H2O NO O3 H OH N2O CH4 NO2 SO2 NH3 HNO3

END

ALTITUDES

0.0	1.0	2.0	3.0	4.0
5.0	6.0	7.0	8.0	9.0
10.0	11.0	12.0	13.0	14.0
15.0	16.0	17.0	18.0	19.0
20.0	21.0	22.0	23.0	24.0
25.0				
30.0	32.0	34.0	36.0	38.0
40.0	42.0	44.0	46.0	48.0
50.0	52.0	54.0	56.0	58.0
60.0	62.0	64.0	66.0	68.0
70.0	72.0	74.0	76.0	78.0
80.0	82.0	84.0	86.0	88.0
90.0	92.0	94.0	96.0	98.0
100.0	102.0	104.0	106.0	108.0
110.0	112.0	114.0	116.0	118.0
120.0	122.0	124.0	126.0	128.0
130.0	132.0	134.0	136.0	138.0
140.0	142.0	144.0	146.0	148.0
150.0	160.0	170.0	180.0	190.0
200.0	210.0	220.0	230.0	240.0
250.0	260.0	270.0	280.0	290.0
300.0				

END

TEMPERATURES

2.8820E+02	2.8170E+02	2.7520E+02	2.6870E+02	2.6220E+02
2.5570E+02	2.4920E+02	2.4270E+02	2.3620E+02	2.2970E+02
2.2330E+02	2.1680E+02	2.1670E+02	2.1670E+02	2.1670E+02
2.1670E+02	2.1670E+02	2.1670E+02	2.1670E+02	2.1670E+02
2.1670E+02	2.1760E+02	2.1860E+02	2.1960E+02	2.2060E+02
2.2160E+02				
2.2650E+02	2.2930E+02	2.3388E+02	2.3904E+02	2.4438E+02
2.5040E+02	2.5590E+02	2.6142E+02	2.6674E+02	2.7062E+02
2.7065E+02	2.6900E+02	2.6350E+02	2.5800E+02	2.5250E+02
2.4706E+02	2.4157E+02	2.3607E+02	2.3058E+02	2.2509E+02
2.1959E+02	2.1426E+02	2.1035E+02	2.0643E+02	2.0252E+02
1.9861E+02	1.9470E+02	1.9078E+02	1.8687E+02	1.8687E+02
1.8687E+02	1.8698E+02	1.8774E+02	1.8931E+02	1.9172E+02
1.9508E+02	1.9953E+02	2.0531E+02	2.1289E+02	2.2329E+02
2.4000E+02	2.6400E+02	2.8800E+02	3.1200E+02	3.3600E+02
3.6000E+02	3.8355E+02	4.0622E+02	4.2804E+02	4.4904E+02
4.6927E+02	4.8838E+02	5.0748E+02	5.2519E+02	5.4290E+02
5.5932E+02	5.7573E+02	5.9095E+02	6.0617E+02	6.2028E+02
6.3439E+02	6.9629E+02	7.4757E+02	7.9007E+02	8.2531E+02
8.5456E+02	8.7679E+02	8.9901E+02	9.0739E+02	9.1578E+02
9.3338E+02	9.5099E+02	9.5724E+02	9.6350E+02	9.6976E+02
9.7601E+02				

END

N2 DENSITIES

1.9900E+19	1.8065E+19	1.6354E+19	1.4769E+19	1.3308E+19
1.1965E+19	1.0723E+19	9.5907E+18	8.5441E+18	7.5905E+18
6.7182E+18	5.9270E+18	5.0679E+18	4.3314E+18	3.7012E+18
3.1631E+18	2.7038E+18	2.3118E+18	1.9759E+18	1.6893E+18
1.4441E+18	1.2301E+18	1.0481E+18	8.9346E+17	7.6265E+17
6.5112E+17				
2.9912E+17	2.1427E+17	1.5883E+17	1.1945E+17	8.9279E+16
6.4901E+16	4.8696E+16	3.6741E+16	2.7915E+16	2.1423E+16
1.6700E+16	1.3200E+16	1.0400E+16	8.1700E+15	6.4000E+15
5.0401E+15	3.9179E+15	3.0285E+15	2.3272E+15	1.7774E+15
1.3487E+15	1.0158E+15	7.5547E+14	5.5885E+14	4.1110E+14
3.0067E+14	2.1859E+14	1.5792E+14	1.1335E+14	7.9150E+13
5.5470E+13	3.8860E+13	2.7150E+13	1.8940E+13	1.3200E+13
9.2100E+12	6.5080E+12	4.6090E+12	3.2730E+12	2.3270E+12
1.6410E+12	1.1580E+12	8.4220E+11	6.2850E+11	4.7940E+11
3.7260E+11	2.9470E+11	2.3680E+11	1.9300E+11	1.5920E+11
1.3260E+11	1.1160E+11	9.4600E+10	8.0800E+10	6.9470E+10
6.0090E+10	5.2250E+10	4.5650E+10	4.0070E+10	3.5310E+10
3.1240E+10	1.7740E+10	1.0700E+10	6.7400E+09	4.3850E+09
2.9250E+09	1.9890E+09	1.3730E+09	9.6000E+08	6.7780E+08
4.8260E+08	3.4590E+08	2.4940E+08	1.8060E+08	1.3140E+08
9.5930E+07				

END

O2 DENSITIES

5.3253E+18	4.8342E+18	4.3765E+18	3.9522E+18	3.5614E+18
3.2019E+18	2.8696E+18	2.5665E+18	2.2865E+18	2.0313E+18
1.7978E+18	1.5861E+18	1.3562E+18	1.1591E+18	9.9045E+17
8.4645E+17	7.2356E+17	6.1864E+17	5.2877E+17	4.5207E+17
3.8644E+17	3.2917E+17	2.8048E+17	2.3910E+17	2.0409E+17
1.7424E+17				
8.0047E+16	5.7340E+16	4.2505E+16	3.1966E+16	2.3891E+16
1.7368E+16	1.3031E+16	9.8320E+15	7.4702E+15	5.7329E+15
4.4600E+15	3.5200E+15	2.7800E+15	2.1900E+15	1.7100E+15
1.3521E+15	1.0510E+15	8.1245E+14	6.2433E+14	4.7682E+14
3.6181E+14	2.7251E+14	2.0267E+14	1.4992E+14	1.1029E+14
8.0661E+13	5.8641E+13	4.2366E+13	3.0310E+13	2.1200E+13
1.4790E+13	1.0270E+13	7.0600E+12	4.8010E+12	3.2300E+12
2.1510E+12	1.4300E+12	9.4340E+11	6.1890E+11	4.0450E+11
2.6210E+11	1.7060E+11	1.1560E+11	8.1200E+10	5.8920E+10
4.3950E+10	3.3600E+10	2.6250E+10	2.0870E+10	1.6830E+10
1.3750E+10	1.1340E+10	9.4440E+09	7.9270E+09	6.7020E+09
5.7020E+09	4.8810E+09	4.1990E+09	3.6310E+09	3.1530E+09
2.7500E+09	1.4600E+09	8.2770E+08	4.9210E+08	3.0310E+08
1.9180E+08	1.2390E+08	8.1450E+07	5.4250E+07	3.6530E+07
2.4820E+07	1.7000E+07	1.1710E+07	8.1100E+06	5.6430E+06
3.9420E+06				

END

O DENSITIES

0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00				
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1.0000E+04	2.5100E+04	6.3100E+04	1.5800E+05	3.9800E+05
1.0000E+06	2.5119E+06	6.3096E+06	1.5849E+07	3.9811E+07
1.0000E+08	2.5119E+08	6.3096E+08	1.5849E+09	3.9811E+09
1.0000E+10	2.0488E+10	4.1976E+10	8.6000E+10	1.5130E+11
2.4430E+11	3.4340E+11	4.1590E+11	4.4710E+11	4.4760E+11
4.2980E+11	4.0070E+11	3.6190E+11	3.1880E+11	2.7480E+11
2.3030E+11	1.8890E+11	1.5650E+11	1.3050E+11	1.0960E+11
9.2750E+10	7.9250E+10	6.8400E+10	5.9560E+10	5.2290E+10
4.6250E+10	4.1180E+10	3.6880E+10	3.3200E+10	3.0040E+10
2.7290E+10	2.4890E+10	2.2780E+10	2.0920E+10	1.9270E+10
1.7800E+10	1.2380E+10	8.9960E+09	6.7470E+09	5.1810E+09
4.0500E+09	3.2110E+09	2.5730E+09	2.0810E+09	1.6950E+09
1.3880E+09	1.1430E+09	9.4470E+08	7.8340E+08	6.5160E+08
5.4330E+08				

END

CO2 DENSITIES

8.4084E+15	7.6329E+15	6.9102E+15	6.2403E+15	5.6232E+15
5.0556E+15	4.5309E+15	4.0524E+15	3.6102E+15	3.2073E+15
2.8387E+15	2.5044E+15	2.1414E+15	1.8302E+15	1.5639E+15
1.3365E+15	1.1425E+15	9.7680E+14	8.3490E+14	7.1379E+14
6.1017E+14	5.1975E+14	4.4286E+14	3.7752E+14	3.2224E+14
2.7512E+14				
1.2639E+14	9.0537E+13	6.7113E+13	5.0473E+13	3.7723E+13
2.7423E+13	2.0576E+13	1.5524E+13	1.1795E+13	9.0519E+12
7.0500E+12	5.5600E+12	4.3900E+12	3.4500E+12	2.7100E+12
2.0268E+12	1.5755E+12	1.2178E+12	9.3586E+11	7.1474E+11
5.4235E+11	4.0849E+11	3.0380E+11	2.2473E+11	1.6532E+11
1.2091E+11	8.7901E+10	6.3505E+10	4.5582E+10	3.1936E+10
2.2380E+10	1.5679E+10	1.0958E+10	7.6444E+09	5.3303E+09
3.7193E+09	2.5999E+09	1.8222E+09	1.2809E+09	9.0199E+08
6.3096E+08	3.8519E+08	2.4553E+08	1.6228E+08	1.1063E+08
7.7452E+07	5.5552E+07	4.0724E+07	3.0420E+07	2.3095E+07
1.7785E+07	1.3878E+07	1.0934E+07	8.7128E+06	6.9961E+06
5.6699E+06	4.6236E+06	3.7995E+06	3.1382E+06	2.6089E+06
2.1781E+06	9.4394E+05	4.4431E+05	2.2195E+05	1.1589E+05
6.2601E+04	3.4781E+04	1.9643E+04	1.1394E+04	6.6526E+03
3.8811E+03	2.2906E+03	1.3793E+03	8.3449E+02	5.0729E+02
3.0983E+02				

END

CO DENSITIES

3.8220E+12	3.3538E+12	2.9295E+12	2.5510E+12	2.2356E+12
1.9962E+12	1.7684E+12	1.5313E+12	1.2964E+12	1.0633E+12
8.5693E+11	6.8028E+11	5.0705E+11	3.5350E+11	2.3813E+11
1.5961E+11	1.0625E+11	7.3674E+10	4.9740E+10	3.3505E+10
2.4610E+10	1.9404E+10	1.6533E+10	1.4952E+10	1.3671E+10
1.2489E+10				
6.5493E+09	4.9963E+09	3.9532E+09	3.1980E+09	2.5981E+09
2.0750E+09	1.7180E+09	1.4429E+09	1.2237E+09	1.0638E+09
9.8300E+08	9.1300E+08	8.2900E+08	7.7900E+08	7.4400E+08
9.0000E+08	1.0500E+09	1.2500E+09	1.4300E+09	1.5500E+09
1.6800E+09	1.8400E+09	1.9200E+09	1.9600E+09	1.9300E+09
1.8300E+09	1.6800E+09	1.5100E+09	1.2800E+09	1.0000E+09
7.8100E+08	6.7200E+08	5.1000E+08	4.0000E+08	3.0000E+08
2.2300E+08	1.6300E+08	1.2000E+08	8.7600E+07	6.4400E+07
4.7000E+07	3.5900E+07	2.8000E+07	2.2500E+07	1.8400E+07
1.5300E+07	1.2600E+07	1.0600E+07	9.0400E+06	7.7500E+06
6.8300E+06	5.8100E+06	5.0000E+06	4.3200E+06	3.7600E+06
3.3000E+06	2.9100E+06	2.5700E+06	2.2900E+06	2.0500E+06
1.8500E+06	1.0900E+06	7.0000E+05	4.7000E+05	2.9800E+05
1.9500E+05	1.3000E+05	9.0700E+04	6.5700E+04	4.8900E+04
3.8000E+04	3.0200E+04	2.4200E+04	1.9400E+04	1.5800E+04
1.2900E+04				

END

H2O DENSITIES

1.9734E+17	1.4042E+17	9.6973E+16	6.0172E+16	3.6772E+16
2.1402E+16	1.2706E+16	7.0242E+15	4.0117E+15	1.5385E+15
6.0180E+14	2.7419E+14	1.2368E+14	6.0174E+13	2.8088E+13
2.0250E+13	1.3675E+13	1.1396E+13	9.6773E+12	8.3275E+12
7.2111E+12	6.2606E+12	5.4552E+12	4.8048E+12	4.1989E+12
3.6891E+12				
1.8097E+12	1.3182E+12	9.9039E+11	7.5249E+11	5.6756E+11
4.1758E+11	3.1953E+11	2.4438E+11	1.8711E+11	1.4387E+11
1.1200E+11	8.7300E+10	6.8200E+10	5.2600E+10	4.1000E+10
3.3500E+10	2.6000E+10	2.0400E+10	1.5100E+10	1.0900E+10
7.9200E+09	5.7500E+09	3.8700E+09	2.6100E+09	1.6800E+09
1.0600E+09	6.5800E+08	3.5900E+08	2.0300E+08	1.1400E+08
6.1400E+07	3.4400E+07	1.8400E+07	1.0500E+07	6.3400E+06
3.7700E+06	2.3400E+06	1.4200E+06	8.4200E+05	4.8100E+05
2.5600E+05	1.3700E+05	6.6900E+04	3.3600E+04	2.6000E+04
2.0400E+04	1.6300E+04	1.3300E+04	1.0900E+04	9.1300E+03
7.7100E+03	6.5700E+03	5.6300E+03	4.8800E+03	4.2500E+03
3.7200E+03	3.2800E+03	2.9000E+03	2.5800E+03	2.3100E+03
2.0700E+03	1.2600E+03	8.2200E+02	5.6000E+02	3.9500E+02
2.8700E+02	2.1300E+02	1.6100E+02	1.2400E+02	9.6400E+01
7.6000E+01	6.0000E+01	4.8000E+01	3.9000E+01	3.2000E+01
2.6000E+01				

END

NO DENSITIES

7.6440E+09	6.9390E+09	6.2820E+09	5.6730E+09	5.1120E+09
4.5960E+09	4.1190E+09	3.6840E+09	3.2820E+09	2.9157E+09
2.5806E+09	2.2767E+09	1.9467E+09	1.6583E+09	1.3980E+09
1.1462E+09	9.2782E+08	7.4592E+08	6.0720E+08	5.2777E+08
4.7150E+08	4.3628E+08	4.1199E+08	4.1184E+08	4.4040E+08
5.7108E+08				
9.3835E+08	1.0991E+09	1.2105E+09	1.2159E+09	1.1072E+09
9.3072E+08	7.3303E+08	5.5415E+08	4.0800E+08	2.9779E+08
2.2000E+08	1.7200E+08	1.3400E+08	1.0600E+08	8.2800E+07
6.4902E+07	5.0625E+07	3.9488E+07	3.1146E+07	2.4842E+07
1.9814E+07	1.6964E+07	1.4523E+07	1.2734E+07	1.1436E+07
1.0269E+07	1.0927E+07	1.1627E+07	1.5138E+07	1.9711E+07
2.5663E+07	3.2704E+07	4.1846E+07	5.2882E+07	6.1872E+07
7.2242E+07	7.5363E+07	7.7797E+07	7.7797E+07	7.8731E+07
7.8731E+07	7.5313E+07	7.3370E+07	6.7500E+07	6.1100E+07
5.4900E+07	4.8300E+07	4.1500E+07	3.3500E+07	2.7000E+07
2.1700E+07	1.7400E+07	1.4400E+07	1.1900E+07	9.8500E+06
8.3400E+06	7.1900E+06	6.2500E+06	5.4300E+06	4.7200E+06
4.1100E+06	2.0600E+06	1.0500E+06	6.1000E+05	4.0200E+05
2.6500E+05	1.7500E+05	1.1500E+05	7.5900E+04	5.0000E+04
3.2800E+04	2.1500E+04	1.4100E+04	9.2800E+03	6.0900E+03
4.0000E+03				

END

O3 DENSITIES

6.7777E+11	6.7794E+11	6.7783E+11	6.2743E+11	5.7714E+11
5.7726E+11	5.6458E+11	6.1511E+11	6.5268E+11	8.9104E+11
1.1294E+12	1.6309E+12	2.0083E+12	2.1330E+12	2.3837E+12
2.6345E+12	3.0123E+12	3.5135E+12	4.0151E+12	4.3909E+12
4.7686E+12	4.7691E+12	4.8943E+12	4.7682E+12	4.5183E+12
4.2669E+12				
2.5098E+12	1.9757E+12	1.5554E+12	1.1964E+12	8.7991E+11
6.0663E+11	3.9941E+11	2.6397E+11	1.6998E+11	1.0635E+11
6.6400E+10	3.8400E+10	2.5500E+10	1.6100E+10	1.1200E+10
7.3000E+09	4.8000E+09	3.1000E+09	1.8000E+09	8.7000E+08
3.8000E+08	1.7000E+08	1.6000E+08	2.3000E+08	3.0000E+08
3.6000E+08	4.2000E+08	4.7000E+08	4.9000E+08	4.7000E+08
4.1000E+08	3.2000E+08	2.1000E+08	1.2000E+08	6.7000E+07
3.6000E+07	1.9000E+07	9.5000E+06	4.6000E+06	1.6000E+06
5.6500E+05	1.9000E+05	6.5000E+04	2.2000E+04	7.8000E+03
3.1000E+03	1.4700E+03	8.4000E+02	4.3000E+02	2.6000E+02
1.5000E+02	9.7000E+01	6.4000E+01	4.1000E+01	2.8000E+01
1.8000E+01	1.3500E+01	9.9000E+00	7.3000E+00	5.6000E+00
4.5000E+00	1.6000E+00	6.0000E-01	2.4000E-01	9.2000E-02
3.7000E-02	2.0000E-02	1.3000E-02	8.0000E-03	5.0000E-03
3.1000E-03	2.1000E-03	1.4000E-03	9.7000E-04	6.5000E-04
4.4000E-04				

END

H DENSITIES

0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00				
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
4.4600E-02	9.3600E-01	1.8300E+00	2.7200E+00	3.6100E+00
4.5000E+00	5.3900E+00	6.2800E+00	7.1800E+00	8.0700E+00
8.9600E+00	9.8500E+00	5.2600E+01	2.3200E+03	3.1800E+04
9.4500E+06	7.2200E+06	6.0300E+06	9.0900E+06	2.7900E+07
5.6000E+07	6.5400E+07	5.9500E+07	4.8400E+07	3.7800E+07
2.8700E+07	2.1800E+07	1.6400E+07	1.2600E+07	9.7300E+06
7.5600E+06	6.4100E+06	5.4400E+06	4.4600E+06	3.4800E+06
2.5100E+06	2.1400E+06	1.8200E+06	1.5100E+06	1.2000E+06
9.1200E+05	8.0800E+05	7.0300E+05	5.9800E+05	4.9300E+05
3.8800E+05	3.3700E+05	2.9200E+05	2.4700E+05	2.0200E+05
1.6000E+05	7.1300E+04	3.4500E+04	1.7100E+04	8.0000E+03
4.0800E+03	2.0200E+03	1.0500E+03	6.1000E+02	3.1500E+02
1.7400E+02	1.0300E+02	5.8100E+01	3.1900E+01	1.7800E+01
9.7300E+00				

END

OH DENSITIES

1.1211E+06	1.0177E+06	9.2136E+05	8.3204E+05	7.4976E+05
6.7408E+05	6.0412E+05	5.4155E+05	4.8683E+05	4.4319E+05
4.0257E+05	3.6427E+05	3.2056E+05	2.8784E+05	2.6775E+05
2.7338E+05	2.8562E+05	3.0784E+05	3.2890E+05	3.5473E+05
3.9938E+05	5.3550E+05	6.8308E+05	8.6830E+05	1.1327E+06
1.8175E+06				
4.4811E+06	7.5358E+06	1.1855E+07	1.6972E+07	2.1549E+07
2.3684E+07	2.3585E+07	2.1926E+07	1.9200E+07	1.6377E+07
1.4400E+07	1.3200E+07	1.1900E+07	1.1600E+07	1.1400E+07
1.1310E+07	1.1830E+07	1.2380E+07	1.2610E+07	1.2500E+07
1.2390E+07	1.1070E+07	9.8900E+06	8.0150E+06	5.8910E+06
4.3300E+06	2.4510E+06	1.3870E+06	6.2760E+05	2.2690E+05
8.2060E+04	3.0790E+04	1.1550E+04	4.2160E+03	1.4970E+03
5.6600E+02	2.6200E+02	1.4200E+02	8.6800E+01	5.7500E+01
4.0300E+01	3.0000E+01	2.2500E+01	1.7300E+01	1.3700E+01
1.0300E+01	8.2500E+00	6.7200E+00	5.5900E+00	4.7300E+00
3.9800E+00	3.4000E+00	2.9000E+00	2.5200E+00	2.1800E+00
1.9140E+00	1.6840E+00	1.4900E+00	1.3220E+00	1.1820E+00
1.0580E+00	6.4400E-01	4.1600E-01	2.8200E-01	1.9900E-01
1.4440E-01	1.0780E-01	8.1000E-02	6.2400E-02	4.8600E-02
3.8000E-02	3.0200E-02	2.4200E-02	1.9420E-02	1.5780E-02
1.2820E-02				

END

N2O DENSITIES

8.1536E+12	7.4016E+12	6.7008E+12	6.0512E+12	5.4528E+12
4.9024E+12	4.3936E+12	3.9296E+12	3.5008E+12	3.1052E+12
2.7346E+12	2.3829E+12	2.0083E+12	1.6904E+12	1.4212E+12
1.1923E+12	9.9602E+11	8.2377E+11	6.7576E+11	5.4659E+11
4.3729E+11	3.4556E+11	2.7524E+11	2.2502E+11	1.8309E+11
1.4640E+11				
5.4233E+10	3.3234E+10	2.0664E+10	1.2450E+10	7.0711E+09
3.7503E+09	1.8938E+09	9.3174E+08	4.6029E+08	2.2454E+08
1.0150E+08	6.6625E+07	4.3731E+07	2.9112E+07	1.9655E+07
1.3270E+07	9.0539E+06	6.1775E+06	4.2224E+06	2.8912E+06
1.9797E+06	1.3370E+06	9.0296E+05	6.0638E+05	4.0491E+05
2.7039E+05	1.8002E+05	1.1986E+05	7.8983E+04	5.1512E+04
3.3596E+04	2.1878E+04	1.4247E+04	9.2857E+03	6.0571E+03
3.9510E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00

END

4.3316E+13	3.9321E+13	3.5598E+13	3.2147E+13	2.8968E+13
2.6044E+13	2.3341E+13	2.0864E+13	1.8565E+13	1.6454E+13
1.4494E+13	1.2712E+13	1.0785E+13	9.1232E+12	7.7056E+12
6.5003E+12	5.4769E+12	4.5969E+12	3.8481E+12	3.2012E+12
2.6330E+12	2.1341E+12	1.7070E+12	1.3625E+12	1.0917E+12
8.7955E+11				
3.4991E+11	2.3213E+11	1.5833E+11	1.0876E+11	7.3266E+10
4.6852E+10	2.9945E+10	1.8799E+10	1.1652E+10	7.1950E+09
4.4450E+09	3.1890E+09	2.2830E+09	1.6780E+09	1.2640E+09
9.5910E+08	7.4560E+08	5.7630E+08	4.4290E+08	3.3820E+08
2.5670E+08	1.9330E+08	1.4380E+08	1.0640E+08	7.8240E+07
5.7230E+07	4.1610E+07	3.0060E+07	2.1270E+07	1.4470E+07
9.8740E+06	6.7260E+06	4.5700E+06	3.0960E+06	2.0920E+06
1.4150E+06	9.6670E+05	6.6220E+05	4.4990E+05	3.0300E+05
2.0270E+05	1.2000E+05	7.3320E+04	4.3900E+04	2.5660E+04
1.5280E+04	8.2020E+03	4.4730E+03	2.4750E+03	1.3860E+03
7.8400E+02	4.4800E+02	2.5800E+02	1.4970E+02	8.7440E+01
5.1390E+01	3.0370E+01	1.8030E+01	1.0760E+01	6.4470E+00
3.8780E+00	3.2080E-01	2.8280E-02	2.6120E-03	2.5020E-04
2.4640E-05	2.4830E-06	2.5480E-07	2.6560E-08	2.8040E-09
2.9920E-10	3.2240E-11	3.5020E-12	3.8300E-13	4.2140E-14
4.6620E-15				

NO2 DENSITIES

END

[illegible]

NH3 DENSITIES

END

HNO3 DENSITIES

END

APPENDIX F

SAMM "TST1.OUT" OUTPUT FILE
(EXCERPTS FROM TEST CASE 1)

APPENDIX F

SAMM "TST1.OUT" OUTPUT FILE (EXCERPTS FROM TEST CASE 1)

```

      SSSSSS  HH  HH  AAAAAA  RRRRRR  CCCCCC
      SS      HH  HH  AA  AA  RR  RR  CC
      SS      HH  HH  AA  AA  RR  RR  CC
      SSSSSS  HHHHHHHH  AAAAAAAA  RRRRRRRR  CC
      SS      HH  HH  AA  AA  RR  RR  CC
      SS      HH  HH  AA  AA  RR  RR  CC
      SSSSSS  HH  HH  AA  AA  RR  RR  CCCCCC
  
```

STRATEGIC HIGH-ALTITUDE RADIANCE CODE

VERSION 3.0

CASE 1: NO & NO+ ONLY, AURORAL REGION

1

CALCULATION SUMMARY

```

NUMBER OF REGIONS:          2
ENVIRONMENT(S) FOR REGION  1:
  1 - AMBIENT
    SAVING POPULATION FILE:    POP1.180
    SPECIES-ISOTOPE INPUT FILES:
      NO  -1 NO.LNK
      NO.STA
      NO.BND
ENVIRONMENT(S) FOR REGION  2:
  2 - AURORAL
    SAVING POPULATION FILE:    POP1A.180
    SPECIES-ISOTOPE INPUT FILES:
      NO  -1 ANO.LNK
      ANO.STA
      NO+ -1 ANOP.LNK
      ANOP.STA
  
```

RADIANCE CALCULATION

SPECIES-ISOTOPE INCLUDED:	NO -1
	NO+ -1
MINIMUM FREQUENCY:	1500.0 CM-1
MAXIMUM FREQUENCY:	4000.0 CM-1
SPECTRAL RESOLUTION:	1.0 CM-1
SPECTRAL STEP SIZE:	1.0 CM-1

SUN LOCATION

SOLAR LONGITUDE:	180.0 DEG
SOLAR LATITUDE:	-23.0 DEG
DAY OF YEAR:	2

LINE-OF-SIGHT GEOMETRY

LOS TYPE:	LIMB VIEWING PATH
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GEOGRAPHIC POLE COORDINATE SYSTEM

SPHERICAL EARTH ASSUMED

LONG PATH SOURCE RANGE:	3242.5 KM
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TANGENT POINT LOCATION

TANGENT POINT LOCAL LOS AZIMUTH:	-90.0 DEG
TANGENT ALTITUDE:	100.0 KM
TANGENT LONGITUDE:	.0 DEG
TANGENT LATITUDE:	65.0 DEG
TANGENT SOLAR EARTH CENTER ANGLE:	138.0 DEG
TANGENT SOLAR AZIMUTH:	.0 DEG

OBSERVER POINT LOCATION

OBSERVER LOCAL LOS ZENITH ANGLE:	104.1 DEG
OBSERVER LOCAL LOS AZIMUTH ANGLE:	-62.5 DEG
OBSERVER-EARTH-SOURCE ANGLE:	28.1 DEG
OBSERVER ALTITUDE:	300.0 KM
OBSERVER LONGITUDE:	30.7 DEG
OBSERVER LATITUDE:	61.5 DEG
OBSERVER SOLAR EARTH CENTER ANGLE:	136.1 DEG
OBSERVER SOLAR AZIMUTH:	-20.5 DEG

SOURCE POINT LOCATION

SOURCE ALTITUDE:	300.0 KM
SOURCE LONGITUDE:	329.3 DEG
SOURCE LATITUDE:	61.5 DEG
SOURCE SOLAR EARTH CENTER ANGLE:	136.1 DEG
SOURCE SOLAR AZIMUTH:	20.5 DEG

1

AMBIENT ATMOSPHERIC REGION NUMBER 1. PROFILE 1.

AMBIENT PARAMETERS

ATMOSPHERE FILE:	MIDLAT.NIG
NUMBER OF LAYERS:	75
LOWER BOUNDARY:	30.0 KM
UPPER BOUNDARY:	300.0 KM
EARTHSHINE EXCITATION:	Y
SOLAR ZENITH ANGLE:	138.0
RADIATING SPECIES-ISOTOPE:	NO -1

1

14N 160 RADIATIVE PROPERTIES FOR REGION 1.

STATE	ENERGY(CM-1)	DEGENERACY
NO(0)	.000	1.
NO(1)	1876.077	1.
NO(2)	3724.067	1.

	TRANSITION	FREQUENCY(CM-1)	ESHINE T(K)	RADIANCE
NO(1)	-NO(0)	1876.077	240.0	Y
NO(2)	-NO(0)	3724.067	230.0	Y
NO(2)	-NO(1)	1847.990	240.0	Y

TRANSITION		NO. OF LINES	AVERAGE STRENGTH (CM-1/MOLEC-CM-2)				
NO(1)	-NO(0)		T(K)/ 200.	250.	300.	500.	1000.
		33.	.110E-18	.999E-19	.912E-19	.661E-19	.362E-19
		28.	.379E-19	.427E-19	.455E-19	.461E-19	.329E-19
		19.	.110E-19	.163E-19	.212E-19	.328E-19	.322E-19
		15.	.355E-20	.618E-20	.928E-20	.197E-19	.249E-19
		17.	.118E-20	.250E-20	.441E-20	.132E-19	.215E-19
		15.	.344E-21	.938E-21	.197E-20	.841E-20	.180E-19
		11.	.109E-21	.357E-21	.870E-21	.512E-20	.140E-19
		12.	.365E-22	.160E-21	.464E-21	.372E-20	.126E-19
		11.	.111E-22	.657E-22	.228E-21	.260E-20	.115E-19
		10.	.346E-23	.250E-22	.101E-21	.158E-20	.884E-20
		10.	.107E-23	.994E-23	.473E-22	.102E-20	.728E-20
		8.	.345E-24	.451E-23	.261E-22	.806E-21	.738E-20
		9.	.116E-24	.152E-23	.962E-23	.386E-21	.442E-20
		8.	.353E-25	.660E-24	.510E-23	.290E-21	.424E-20
		17.	.729E-26	.186E-24	.175E-23	.152E-21	.312E-20
NO(2)	-NO(0)	33.	.174E-20	.159E-20	.145E-20	.106E-20	.614E-21
		28.	.605E-21	.680E-21	.724E-21	.737E-21	.560E-21
		19.	.174E-21	.259E-21	.337E-21	.523E-21	.546E-21
		15.	.566E-22	.985E-22	.148E-21	.316E-21	.424E-21
		18.	.182E-22	.393E-22	.697E-22	.212E-21	.372E-21
		14.	.523E-23	.139E-22	.291E-22	.126E-21	.292E-21
		12.	.167E-23	.564E-23	.140E-22	.846E-22	.249E-21
		11.	.552E-24	.234E-23	.674E-23	.550E-22	.202E-21
		12.	.170E-24	.103E-23	.361E-23	.421E-22	.200E-21
		10.	.489E-25	.349E-24	.143E-23	.234E-22	.145E-21
		10.	.150E-25	.139E-24	.673E-24	.153E-22	.121E-21
		7.	.499E-26	.636E-25	.371E-24	.118E-22	.118E-21
		7.	.188E-26	.210E-25	.124E-24	.473E-23	.573E-22
		3.	.538E-27	.364E-26	.127E-25	.138E-24	.617E-24
		6.	.114E-27	.110E-26	.483E-26	.830E-25	.522E-24
NO(2)	-NO(1)	33.	.212E-18	.193E-18	.176E-18	.127E-18	.695E-19
		28.	.739E-19	.830E-19	.883E-19	.892E-19	.633E-19
		20.	.211E-19	.315E-19	.413E-19	.639E-19	.627E-19
		16.	.637E-20	.113E-19	.173E-19	.385E-19	.502E-19
		17.	.208E-20	.435E-20	.768E-20	.236E-19	.396E-19
		14.	.609E-21	.161E-20	.337E-20	.149E-19	.327E-19
		12.	.195E-21	.650E-21	.162E-20	.100E-19	.282E-19
		11.	.651E-22	.271E-21	.777E-21	.638E-20	.223E-19
		11.	.212E-22	.123E-21	.428E-21	.490E-20	.216E-19
		10.	.654E-23	.463E-22	.187E-21	.296E-20	.167E-19
		10.	.204E-23	.187E-22	.892E-22	.195E-20	.140E-19
		9.	.620E-24	.765E-23	.439E-22	.136E-20	.125E-19
		8.	.209E-24	.304E-23	.199E-22	.836E-21	.982E-20
		8.	.695E-25	.125E-23	.957E-23	.540E-21	.785E-20
		16.	.151E-25	.367E-24	.342E-23	.293E-21	.592E-20

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14N 160 RADIATIVE EXCITATION SUMMARY PROFILE 1. REGION 1.

NEMESIS OUTPUT FOR NO(1) -NO(0)

EARTHSHINE FLUX(PHOTONS/SEC/CM2/CM-1): .865E+13
 EINSTEIN A COEFFICIENT(1/SEC): .132E+02
 SUM OF EINSTEIN A COEFFICIENTS(1/SEC): .132E+02
 TOTAL NUMBER OF PHOTONS: 10000
 MAXIMUM ORDER OF SCATTERING: 200

ALT(KM)	POPULATIONS(MOLEC/CM3)		PROBABILITIES		QUENCHING RATE(1/SEC)	EXCITATION RATES(1/SEC)			
	LOWER STATE	UPPER STATE	RE-EMISSION	ESCAPE		EARTH	SUN	ATMOSPHERE	
		INITIAL							FINAL
.310E+02	.102E+10	.731E+04	.731E+04	.731E-02	.100E+01	.179E+04	.859E-04	.000E+00	.000E+00
.330E+02	.115E+10	.999E+04	.999E+04	.100E-01	.100E+01	.130E+04	.859E-04	.000E+00	.000E+00
.350E+02	.121E+10	.133E+05	.133E+05	.134E-01	.100E+01	.968E+03	.858E-04	.000E+00	.000E+00
.370E+02	.116E+10	.163E+05	.163E+05	.178E-01	.100E+01	.726E+03	.857E-04	.000E+00	.000E+00

* * *

.275E+03	.117E+05	.312E+01	.312E+01	.996E+00	.100E+01	.585E-01	.781E-04	.000E+00	.000E+00
.285E+03	.768E+04	.174E+01	.174E+01	.996E+00	.100E+01	.486E-01	.780E-04	.000E+00	.000E+00
.295E+03	.504E+04	.975E+00	.975E+00	.997E+00	.100E+01	.405E-01	.779E-04	.000E+00	.000E+00

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14N 160 RADIATIVE EXCITATION SUMMARY PROFILE 1. REGION 1.

NEMESIS OUTPUT FOR NO(2) -NO(0)

EARTHSHINE FLUX(PHOTONS/SEC/CM2/CM-1): .199E+09
 EINSTEIN A COEFFICIENT(1/SEC): .836E+00
 SUM OF EINSTEIN A COEFFICIENTS(1/SEC): .256E+02
 TOTAL NUMBER OF PHOTONS: 10000
 MAXIMUM ORDER OF SCATTERING: 200

ALT(KM)	POPULATIONS(MOLEC/CM3)		PROBABILITIES		QUENCHING RATE(1/SEC)	EXCITATION RATES(1/SEC)			
	LOWER STATE	UPPER STATE	RE-EMISSION	ESCAPE		EARTH	SUN	ATMOSPHERE	
		INITIAL							FINAL
.310E+02	.102E+10	.623E-01	.623E-01	.183E-03	.100E+01	.453E+04	.315E-10	.000E+00	.000E+00
.330E+02	.115E+10	.102E+00	.102E+00	.252E-03	.100E+01	.329E+04	.315E-10	.000E+00	.000E+00
.350E+02	.121E+10	.172E+00	.172E+00	.337E-03	.100E+01	.246E+04	.315E-10	.000E+00	.000E+00
.370E+02	.116E+10	.268E+00	.268E+00	.447E-03	.100E+01	.184E+04	.315E-10	.000E+00	.000E+00

* * *

.275E+03	.117E+05	.325E-01	.325E-01	.326E-01	.100E+01	.562E-01	.300E-10	.000E+00	.000E+00
.285E+03	.768E+04	.184E-01	.184E-01	.326E-01	.100E+01	.466E-01	.300E-10	.000E+00	.000E+00
.295E+03	.504E+04	.104E-01	.104E-01	.326E-01	.100E+01	.388E-01	.300E-10	.000E+00	.000E+00

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14N 160 RADIATIVE EXCITATION SUMMARY PROFILE 1. REGION 1.

NEMESIS OUTPUT FOR NO(2) -NO(1)

EARTHSHINE FLUX(PHOTONS/SEC/CM2/CM-1): .993E+13
 EINSTEIN A COEFFICIENT(1/SEC): .248E+02
 SUM OF EINSTEIN A COEFFICIENTS(1/SEC): .256E+02
 TOTAL NUMBER OF PHOTONS: 10000
 MAXIMUM ORDER OF SCATTERING: 200

ALT(KM)	POPULATIONS(MOLEC/CM3)		PROBABILITIES		QUENCHING RATE(1/SEC)	EXCITATION RATES(1/SEC)			
	LOWER STATE	UPPER STATE	RE-EMISSION	ESCAPE		EARTH	SUN	ATMOSPHERE	
		INITIAL							FINAL
.310E+02	.731E+04	.626E-01	.626E-01	.543E-02	.100E+01	.453E+04	.191E-03	.000E+00	.000E+00
.330E+02	.999E+04	.103E+00	.103E+00	.746E-02	.100E+01	.329E+04	.191E-03	.000E+00	.000E+00
.350E+02	.133E+05	.173E+00	.173E+00	.998E-02	.100E+01	.246E+04	.191E-03	.000E+00	.000E+00
.370E+02	.163E+05	.269E+00	.269E+00	.133E-01	.100E+01	.184E+04	.191E-03	.000E+00	.000E+00
* * *									
.275E+03	.312E+01	.325E-01	.325E-01	.965E+00	.100E+01	.562E-01	.175E-03	.000E+00	.000E+00
.285E+03	.174E+01	.184E-01	.184E-01	.966E+00	.100E+01	.466E-01	.174E-03	.000E+00	.000E+00
.295E+03	.975E+00	.104E-01	.104E-01	.966E+00	.100E+01	.388E-01	.174E-03	.000E+00	.000E+00

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14N 160 EXCITED STATE NUMBER DENSITIES(MOLEC/CM3) PROFILE 1. REGION 1.

ALT(KM)	NO(0)	NO(1)	NO(2)
31.0	.102E+10	.731E+04	.626E-01
33.0	.115E+10	.999E+04	.103E+00
35.0	.121E+10	.133E+05	.173E+00
37.0	.116E+10	.163E+05	.269E+00

* * *

275.0	.117E+05	.312E+01	.325E-01
285.0	.768E+04	.174E+01	.184E-01
295.0	.504E+04	.975E+00	.104E-01

1

14N 160 VIBRATIONAL TEMPERATURES(K) PROFILE 1. REGION 1.

ALT(KM)	KINETIC	NO(1)	NO(2)
31.0	227.9	227.9	227.9
33.0	231.6	231.5	231.5
35.0	236.5	236.3	236.4
37.0	241.7	241.5	241.5

* * *

275.0	960.4	328.0	418.9
285.0	966.6	321.7	414.0
295.0	972.9	315.7	409.3

1

AMBIENT ATMOSPHERIC REGION NUMBER 2. PROFILE 1.

AMBIENT PARAMETERS

ATMOSPHERE FILE:	MIDLAT.NIG
NUMBER OF LAYERS:	75
LOWER BOUNDARY:	30.0 KM
UPPER BOUNDARY:	300.0 KM
EARTHSHINE EXCITATION:	Y
SOLAR ZENITH ANGLE:	138.0
RADIATING SPECIES-ISOTOPE:	NO -1

1

14N 160 RADIATIVE PROPERTIES FOR REGION 2.

STATE	ENERGY(CM-1)	DEGENERACY
NO(0)	.000	1.
NO(1)	1876.077	1.
NO(2)	3724.067	1.

	TRANSITION	FREQUENCY(CM-1)	ESHINE T(K)	RADIANCE
NO(1)	-NO(0)	1876.077	240.0	Y
NO(2)	-NO(0)	3724.067	230.0	Y
NO(2)	-NO(1)	1847.990	240.0	Y

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14N 160 EXCITED STATE NUMBER DENSITIES(MOLEC/CM3) PROFILE 1. REGION 2.

ALT(KM)	NO(0)	NO(1)	NO(2)
31.0	.102E+10	.731E+04	.626E-01
33.0	.115E+10	.999E+04	.103E+00
35.0	.121E+10	.133E+05	.173E+00
37.0	.116E+10	.163E+05	.269E+00

* * *

275.0	.117E+05	.312E+01	.325E-01
285.0	.768E+04	.174E+01	.184E-01
295.0	.504E+04	.975E+00	.104E-01

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14N 160 VIBRATIONAL TEMPERATURES(K) PROFILE 1. REGION 2.

ALT(KM)	KINETIC	NO(1)	NO(2)
31.0	227.9	227.9	227.9
33.0	231.6	231.5	231.5
35.0	236.5	236.3	236.4
37.0	241.7	241.5	241.5

* * *

275.0	960.4	328.0	418.9
285.0	966.6	321.7	414.0
295.0	972.9	315.7	409.3

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AURORAL ATMOSPHERIC REGION NUMBER 2. PROFILE 1.

AMBIENT PARAMETERS

ATMOSPHERE FILE:	MIDLAT.NIG
NUMBER OF LAYERS:	75
LOWER BOUNDARY:	30.0 KM
UPPER BOUNDARY:	300.0 KM
EARTHSHINE EXCITATION:	Y
SOLAR ZENITH ANGLE:	138.0

AURORAL PARAMETERS

MAXWELLIAN ELECTRON ENERGY SPECTRUM

CODE-SELECTED IBC CLASS:	III
TOTAL ENERGY FLUX:	100.0 ERGS/CM2/SEC
CHARACTERISTIC ENERGY:	5.0 KEV
DURATION OF AURORA:	100.0 SEC
TIME OF OBSERVATION:	100.0 SEC

RADIATING SPECIES-ISOTOPE:	NO -1
	NO+ -1

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14N 160 RADIATIVE PROPERTIES FOR REGION 2.

STATE	ENERGY(CM-1)	DEGENERACY
NO(0)	.000	1.
NO(1)	1876.174	1.
NO(2)	3724.170	1.
NO(3)	5544.125	1.
NO(4)	7336.086	1.
NO(5)	9100.091	1.
NO(6)	10836.123	1.
NO(7)	12544.098	1.
NO(8)	14223.999	1.
NO(9)	15875.815	1.
NO(10)	17499.535	1.
NO(11)	19095.146	1.
NO(12)	20662.643	1.

	TRANSITION	FREQUENCY(CM-1)	ESHINE T(K)	RADIANCE
NO(1)	-NO(0)	1876.174	240.0	Y
NO(2)	-NO(0)	3724.170	240.0	Y
NO(2)	-NO(1)	1847.996	240.0	Y
NO(3)	-NO(1)	3667.951	240.0	Y
NO(3)	-NO(2)	1819.955	240.0	Y
NO(4)	-NO(2)	3611.916	240.0	Y
NO(4)	-NO(3)	1791.961	240.0	Y
NO(5)	-NO(3)	3555.966	240.0	Y
NO(5)	-NO(4)	1764.005	240.0	Y
NO(6)	-NO(4)	3500.037	240.0	Y
NO(6)	-NO(5)	1736.032	240.0	Y
NO(7)	-NO(5)	3444.007	240.0	Y
NO(7)	-NO(6)	1707.975	240.0	Y
NO(8)	-NO(6)	3387.876	240.0	Y
NO(8)	-NO(7)	1679.901	240.0	Y
NO(9)	-NO(7)	3331.718	240.0	Y
NO(9)	-NO(8)	1651.816	240.0	Y
NO(10)	-NO(8)	3275.536	240.0	Y
NO(10)	-NO(9)	1623.720	240.0	Y
NO(11)	-NO(9)	3219.331	240.0	Y
NO(11)	-NO(10)	1595.611	240.0	Y
NO(12)	-NO(10)	3163.107	240.0	Y
NO(12)	-NO(11)	1567.496	240.0	Y

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SUMMARY OF AURORAL ENHANCEMENT PROFILE 1. REGION 2.

AURORALLY ENHANCED NUMBER DENSITIES(MOLEC/CM3)

ALT(KM)	T(SEC)	N2	O2	O	NO	N2+	O2+	O+
		N+	NO+	CH4	EP	ES(1)	ES(2)	ES(3)
		ES(4)	ES(5)	ES(6)	ES(7)	ES(8)	ES(9)	ES(10)
		ES(11)	ES(12)	ES(13)	ES(14)	N2(1)	N2(2)	N2(3)
		N2(4)	N2(5)	N2(a)	N2(A)	N2(BW)	N2(C)	N2(R)
		O2(1)	O2(a)	O2(b)	O2(A)	O2(B)	O2(R)	O(1D)
		O(1S)	O(1S)	N(2D)	N(4S)	NO(0)	NO(1)	NO(2)
		NO(3)	NO(4)	NO(5)	NO(6)	NO(7)	NO(8)	NO(9)
		NO(10)	NO(11)	NO(12)				
81.0	25.0	.260E+15	.697E+14	.152E+11	.106E+08	.610E-03	.101E+03	.384E-05
		.178E-04	.245E+02	.494E+08	.100E+01	.125E+03	.806E-03	.201E-03
		.154E-05	.166E-06	.117E-06	.409E-06	.199E-05	.565E-05	.117E-05
		.345E-06	.101E-06	.762E-07	.610E-07	.581E+05	.391E+00	.104E+00
		.233E-01	.655E-02	.175E+02	.474E-02	.547E+02	.146E+02	.633E+02
		.453E+03	.586E+02	.419E+01	.276E+02	.937E+01	.169E+02	.425E-03
		.187E+01	.125E-02	.832E-02	.846E+02	.106E+08	.587E+02	.864E-01
		.496E-01	.294E-01	.172E-01	.109E-01	.648E-02	.381E-02	.195E-02
		.954E-03	.428E-03	.138E-03				
83.0	70.0	.188E+15	.505E+14	.312E+11	.113E+08	.114E-01	.371E+04	.740E-04
		.340E-03	.952E+03	.358E+08	.100E+01	.466E+04	.154E-01	.384E-02
		.294E-04	.316E-05	.223E-05	.782E-05	.380E-04	.108E-03	.224E-04
		.658E-05	.193E-05	.145E-05	.116E-05	.177E+07	.805E+01	.212E+01
		.456E+00	.128E+00	.678E+03	.903E-01	.212E+04	.565E+03	.245E+04
		.173E+05	.227E+04	.162E+03	.107E+04	.363E+03	.655E+03	.889E-02
		.731E+02	.136E+00	.167E+00	.330E+04	.113E+08	.627E+02	.128E+01
		.747E+00	.453E+00	.273E+00	.174E+00	.105E+00	.623E-01	.320E-01
		.158E-01	.715E-02	.233E-02				
* * *								
149.0	100.0	.333E+11	.295E+10	.185E+11	.469E+07	.915E+04	.242E+06	.115E+04
		.277E+04	.120E+06	.516E+01	.100E+01	.276E+06	.840E+05	.151E+05
		.843E+02	.981E+01	.712E+01	.225E+02	.762E+02	.134E+03	.514E+02
		.171E+02	.505E+01	.399E+01	.326E+01	.275E+08	.444E+07	.150E+07
		.279E+06	.842E+05	.440E+06	.310E+05	.134E+07	.372E+06	.170E+07
		.696E+07	.634E+06	.225E+05	.147E+06	.804E+05	.150E+06	.761E+05
		.452E+06	.309E+06	.711E+06	.575E+07	.627E+07	.856E+04	.696E+03
		.400E+03	.260E+03	.174E+03	.112E+03	.721E+02	.442E+02	.233E+02
		.118E+02	.566E+01	.199E+01				
155.0	100.0	.245E+11	.211E+10	.151E+11	.329E+07	.882E+04	.224E+06	.129E+04
		.297E+04	.105E+06	.210E+01	.100E+01	.237E+06	.894E+05	.160E+05
		.890E+02	.104E+02	.753E+01	.235E+02	.775E+02	.132E+03	.528E+02
		.178E+02	.526E+01	.417E+01	.341E+01	.201E+08	.361E+07	.128E+07
		.249E+06	.789E+05	.338E+06	.293E+05	.102E+07	.286E+06	.131E+07
		.522E+07	.474E+06	.162E+05	.106E+06	.599E+05	.112E+06	.806E+05
		.351E+06	.263E+06	.685E+06	.441E+07	.435E+07	.627E+04	.501E+03
		.285E+03	.185E+03	.123E+03	.794E+02	.512E+02	.313E+02	.166E+02
		.834E+01	.401E+01	.141E+01				

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14N 160 EXCITED STATE NUMBER DENSITIES(MOLEC/CM3) PROFILE 1. REGION 2.

ALT(KM)	NO(0) NO(7)	NO(1) NO(8)	NO(2) NO(9)	NO(3) NO(10)	NO(4) NO(11)	NO(5) NO(12)	NO(6)
31.0	.102E+10 .000E+00	.731E+04 .000E+00	.626E-01 .000E+00	.000E+00 .000E+00	.000E+00 .000E+00	.000E+00 .000E+00	.000E+00
33.0	.115E+10 .000E+00	.999E+04 .000E+00	.103E+00 .000E+00	.000E+00 .000E+00	.000E+00 .000E+00	.000E+00 .000E+00	.000E+00
35.0	.121E+10 .000E+00	.133E+05 .000E+00	.173E+00 .000E+00	.000E+00 .000E+00	.000E+00 .000E+00	.000E+00 .000E+00	.000E+00
37.0	.116E+10 .000E+00	.163E+05 .000E+00	.269E+00 .000E+00	.000E+00 .000E+00	.000E+00 .000E+00	.000E+00 .000E+00	.000E+00

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275.0	.117E+05 .000E+00	.312E+01 .000E+00	.325E-01 .000E+00	.000E+00 .000E+00	.000E+00 .000E+00	.000E+00 .000E+00	.000E+00
285.0	.768E+04 .000E+00	.174E+01 .000E+00	.184E-01 .000E+00	.000E+00 .000E+00	.000E+00 .000E+00	.000E+00 .000E+00	.000E+00
295.0	.504E+04 .000E+00	.975E+00 .000E+00	.104E-01 .000E+00	.000E+00 .000E+00	.000E+00 .000E+00	.000E+00 .000E+00	.000E+00

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14N 160 VIBRATIONAL TEMPERATURES(K) PROFILE 1. REGION 2.

ALT(KM)	KINETIC	NO(1) NO(8)	NO(2) NO(9)	NO(3) NO(10)	NO(4) NO(11)	NO(5) NO(12)	NO(6)	NO(7)
31.0	227.9	227.9 .0	227.9 .0	.0 .0	.0 .0	.0 .0	.0	.0
33.0	231.6	231.6 .0	231.6 .0	.0 .0	.0 .0	.0 .0	.0	.0
35.0	236.5	236.4 .0	236.4 .0	.0 .0	.0 .0	.0 .0	.0	.0
37.0	241.7	241.5 .0	241.5 .0	.0 .0	.0 .0	.0 .0	.0	.0

* * *

275.0	960.4	328.0 .0	418.9 .0	.0 .0	.0 .0	.0 .0	.0	.0
285.0	966.6	321.7 .0	414.0 .0	.0 .0	.0 .0	.0 .0	.0	.0
295.0	972.9	315.7 .0	409.3 .0	.0 .0	.0 .0	.0 .0	.0	.0

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14N 160 + RADIATIVE PROPERTIES FOR REGION 2.

STATE	ENERGY(CM-1)	DEGENERACY
NO+(0)	.000	1.
NO+(1)	2344.160	1.
NO+(2)	4655.668	1.
NO+(3)	6934.433	1.
NO+(4)	9180.356	1.
NO+(5)	11393.349	1.
NO+(6)	13573.319	1.
NO+(7)	15720.170	1.
NO+(8)	17833.813	1.
NO+(9)	19914.141	1.
NO+(10)	21961.072	1.
NO+(11)	23974.510	1.
NO+(12)	25954.361	1.
NO+(13)	27900.529	1.

	TRANSITION	FREQUENCY(CM-1)	ESHINE T(K)	RADIANCE
NO+(1)	-NO+(0)	2344.160	240.0	Y
NO+(2)	-NO+(1)	2311.508	240.0	Y
NO+(3)	-NO+(2)	2278.765	240.0	Y
NO+(4)	-NO+(3)	2245.924	240.0	Y
NO+(5)	-NO+(4)	2212.992	240.0	Y
NO+(6)	-NO+(5)	2179.971	240.0	Y
NO+(7)	-NO+(6)	2146.851	240.0	Y
NO+(8)	-NO+(7)	2113.643	240.0	Y
NO+(9)	-NO+(8)	2080.328	240.0	Y
NO+(10)	-NO+(9)	2046.932	240.0	Y
NO+(11)	-NO+(10)	2013.438	240.0	Y
NO+(12)	-NO+(11)	1979.852	240.0	Y
NO+(13)	-NO+(12)	1946.168	240.0	Y

SUMMARY OF AURORAL ENHANCEMENT PROFILE 1. REGION 2.

AURORALLY ENHANCED NUMBER DENSITIES(MOLEC/CM3)

ALT(KM)	T(SEC)	N2	O2	O	NO	N2+	O2+	O+
		N+	NO+	CH4	EP	ES(1)	ES(2)	ES(3)
		ES(4)	ES(5)	ES(6)	ES(7)	ES(8)	ES(9)	ES(10)
		ES(11)	ES(12)	ES(13)	ES(14)	N2(1)	N2(2)	N2(3)
		N2(4)	N2(5)	N2(a)	N2(A)	N2(BW)	N2(C)	N2(R)
		O2(1)	O2(a)	O2(b)	O2(A)	O2(B)	O2(R)	O(1D)
		O(1S)	O(1S)	N(2D)	N(4S)	NO+(0)	NO+(1)	NO+(2)
		NO+(3)	NO+(4)	NO+(5)	NO+(6)	NO+(7)	NO+(8)	NO+(9)
		NO+(10)	NO+(11)	NO+(12)	NO+(13)			
81.0	5.0	.260E+15	.697E+14	.152E+11	.106E+08	.610E-03	.232E+02	.263E-03
		.178E-04	.000E+00	.494E+08	.100E+01	.251E+02	.806E-03	.201E-03
		.154E-05	.166E-06	.117E-06	.409E-06	.199E-05	.565E-05	.117E-05
		.345E-06	.101E-06	.762E-07	.610E-07	.111E+05	.379E+00	.102E+00
		.230E-01	.652E-02	.350E+01	.473E-02	.109E+02	.291E+01	.127E+02
		.906E+02	.117E+02	.838E+00	.551E+01	.187E+01	.338E+01	.438E-03
		.197E-02	.249E-03	.840E-02	.169E+02	.186E+01	.198E-03	.187E-03
		.174E-03	.158E-03	.138E-03	.114E-03	.880E-04	.573E-04	.447E-04
		.437E-04	.403E-04	.297E-04	.178E-04			
83.0	5.0	.188E+15	.505E+14	.312E+11	.113E+08	.114E-01	.321E+03	.498E-02
		.340E-03	.000E+00	.358E+08	.100E+01	.347E+03	.154E-01	.384E-02
		.294E-04	.316E-05	.223E-05	.782E-05	.380E-04	.108E-03	.224E-04
		.658E-05	.193E-05	.145E-05	.116E-05	.355E+05	.740E+01	.199E+01
		.449E+00	.127E+00	.484E+02	.902E-01	.151E+03	.403E+02	.175E+03
		.122E+04	.162E+03	.116E+02	.763E+02	.259E+02	.468E+02	.829E-02
		.770E-01	.975E-02	.162E+00	.236E+03	.260E+02	.377E-02	.356E-02
		.331E-02	.299E-02	.261E-02	.216E-02	.166E-02	.108E-02	.843E-03
		.825E-03	.760E-03	.561E-03	.336E-03			
* * *								
149.0	15.0	.333E+11	.295E+10	.185E+11	.456E+07	.912E+04	.740E+05	.910E+05
		.275E+04	.000E+00	.516E+01	.100E+01	.364E+06	.828E+05	.151E+05
		.843E+02	.981E+01	.712E+01	.225E+02	.762E+02	.134E+03	.514E+02
		.171E+02	.505E+01	.399E+01	.326E+01	.291E+07	.653E+06	.281E+06
		.759E+05	.336E+05	.660E+05	.278E+05	.200E+06	.557E+05	.254E+06
		.880E+06	.898E+05	.337E+04	.221E+05	.121E+05	.224E+05	.491E+05
		.494E+05	.464E+05	.341E+06	.515E+06	.285E+06	.214E+03	.111E+03
		.742E+02	.539E+02	.405E+02	.300E+02	.212E+02	.130E+02	.966E+01
		.916E+01	.827E+01	.604E+01	.363E+01			
155.0	20.0	.245E+11	.211E+10	.151E+11	.322E+07	.875E+04	.661E+05	.102E+06
		.294E+04	.000E+00	.210E+01	.100E+01	.366E+06	.883E+05	.161E+05
		.890E+02	.104E+02	.753E+01	.235E+02	.775E+02	.132E+03	.528E+02
		.178E+02	.526E+01	.417E+01	.341E+01	.302E+07	.681E+06	.292E+06
		.778E+05	.340E+05	.675E+05	.267E+05	.204E+06	.571E+05	.261E+06
		.886E+06	.899E+05	.323E+04	.212E+05	.120E+05	.223E+05	.541E+05
		.528E+05	.526E+05	.338E+06	.542E+06	.290E+06	.164E+03	.849E+02
		.566E+02	.412E+02	.309E+02	.229E+02	.162E+02	.990E+01	.736E+01
		.698E+01	.630E+01	.460E+01	.277E+01			

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14N 16O + EXCITED STATE NUMBER DENSITIES(MOLEC/CM3)								PROFILE 1.	REGION 2.
ALT(KM)	NO+(0)	NO+(1)	NO+(2)	NO+(3)	NO+(4)	NO+(5)	NO+(6)		
	NO+(7)	NO+(8)	NO+(9)	NO+(10)	NO+(11)	NO+(12)	NO+(13)		
* * *									
79.0	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00		
	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00		
81.0	.186E+01	.198E-03	.187E-03	.174E-03	.158E-03	.138E-03	.114E-03		
	.880E-04	.573E-04	.447E-04	.437E-04	.403E-04	.297E-04	.178E-04		
83.0	.260E+02	.377E-02	.356E-02	.331E-02	.299E-02	.261E-02	.216E-02		
	.166E-02	.108E-02	.843E-03	.825E-03	.760E-03	.561E-03	.336E-03		
* * *									
149.0	.285E+06	.214E+03	.111E+03	.742E+02	.539E+02	.405E+02	.300E+02		
	.212E+02	.130E+02	.966E+01	.916E+01	.827E+01	.604E+01	.363E+01		
155.0	.290E+06	.164E+03	.849E+02	.566E+02	.412E+02	.309E+02	.229E+02		
	.162E+02	.990E+01	.736E+01	.698E+01	.630E+01	.460E+01	.277E+01		
165.0	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00		
	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00		

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14N 16O + VIBRATIONAL TEMPERATURES(K)								PROFILE 1.	REGION 2.
ALT(KM)	KINETIC	NO+(1)	NO+(2)	NO+(3)	NO+(4)	NO+(5)	NO+(6)		
		NO+(8)	NO+(9)	NO+(10)	NO+(11)	NO+(12)	NO+(13)		NO+(7)
* * *									
79.0	200.6	.0	.0	.0	.0	.0	.0		.0
		.0	.0	.0	.0	.0	.0		
81.0	196.7	368.5	727.7	1075.5	1408.5	1723.3	2013.1		2270.6
		2469.7	2693.2	2963.9	3211.2	3380.6	3473.5		
83.0	192.7	381.6	753.0	1112.4	1456.1	1780.5	2078.4		2342.1
		2544.0	2772.1	3050.4	3304.2	3475.6	3566.7		
* * *									
149.0	627.3	468.9	853.4	1208.8	1540.9	1850.5	2132.2		2379.6
		2567.0	2783.9	3054.2	3301.7	3470.0	3561.8		
155.0	665.3	451.0	823.3	1168.0	1490.6	1792.0	2066.8		2309.2
		2494.7	2707.7	2971.0	3212.5	3379.0	3472.5		
165.0	721.9	.0	.0	.0	.0	.0	.0		.0
		.0	.0	.0	.0	.0	.0		

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APPENDIX G

SAMM "TST1.TP6" OUTPUT FILE
(EXCERPTS FROM TEST CASE 1)

APPENDIX G

SAMM "TST1.TP6" OUTPUT FILE (EXCERPTS FROM TEST CASE 1)

***** SAMM *****

CARD 1 *****S 7 4A 1 0 0 0 0 0 0 0 0 1 0 .000 .0500
CARD 2 ***** 0 0 0 3 0 0 .000 .000 .000 .000 .000
CARD 2C ***** 33 1 0

MODEL ATMOSPHERE NO. 7 ICLD = 0

MODEL 0 / 7 USER INPUT DATA

.000	9.987E-01	2.882E+02	.000E+00	.000E+00	.000E+00	BABBBB88888888
.000E+00	.000E+00	.000E+00	.000E+00	7.644E+09	.000E+00	.000E+00
.000E+00						
1.000	8.847E-01	2.817E+02	.000E+00	.000E+00	.000E+00	BABBBB88888888
.000E+00	.000E+00	.000E+00	.000E+00	6.939E+09	.000E+00	.000E+00
.000E+00						
2.000	7.813E-01	2.752E+02	.000E+00	.000E+00	.000E+00	BABBBB88888888
.000E+00	.000E+00	.000E+00	.000E+00	6.282E+09	.000E+00	.000E+00
.000E+00						
3.000	6.879E-01	2.687E+02	.000E+00	.000E+00	.000E+00	BABBBB88888888
.000E+00	.000E+00	.000E+00	.000E+00	5.673E+09	.000E+00	.000E+00
.000E+00						

* * *

50.000	7.806E-04	2.706E+02	.000E+00	.000E+00	.000E+00	BABBBB88888888
.000E+00	.000E+00	.000E+00	.000E+00	2.200E+08	.000E+00	.000E+00
.000E+00						
70.000	5.120E-05	2.196E+02	.000E+00	.000E+00	.000E+00	BABBBB88888888
.000E+00	.000E+00	.000E+00	.000E+00	1.981E+07	.000E+00	.000E+00
.000E+00						
100.000	3.135E-07	1.951E+02	.000E+00	.000E+00	.000E+00	BABBBB88888888
.000E+00	.000E+00	.000E+00	.000E+00	7.224E+07	.000E+00	.000E+00
.000E+00						

Z (KM)	P (MB)	T (K)	REL H (%)	H2O (GM M-3)	CLO AMT (GM M-3)	RAIN RATE (MM HR-1)	TYPE	AEROSOL PROFILE
.000	1011.933	288.20	.00	.000E+00	.000E+00	.000E+00	USER RAIN NO CLOUD	USER RAIN NO CLOUD
1.000	896.422	281.70	.00	.000E+00	.000E+00	.000E+00	USER RAIN NO CLOUD	USER RAIN NO CLOUD
2.000	791.652	275.20	.00	.000E+00	.000E+00	.000E+00	USER RAIN NO CLOUD	USER RAIN NO CLOUD
3.000	697.015	268.70	.00	.000E+00	.000E+00	.000E+00	USER RAIN NO CLOUD	USER RAIN NO CLOUD SPRING-SUMMER

* * *

50.000	.791	270.60	.00	.000E+00	.000E+00	.000E+00	USER RAIN NO CLOUD	USER RAIN NO CLOUD SPRING-SUMMER
70.000	.052	219.60	.00	.000E+00	.000E+00	.000E+00	USER RAIN NO CLOUD	USER RAIN NO CLOUD SPRING-SUMMER
100.000	.000	195.10	.00	.000E+00	.000E+00	.000E+00	USER RAIN NO CLOUD	USER RAIN NO CLOUD SPRING-SUMMER

CARD 3 ***** 100.000 .000 .000 .000 .000 6371.000 0 360.000 65.000 .000 .000 -90.00

CARD 4 ***** 1500 4000 1 1

PROGRAM WILL COMPUTE RADIANCE

ATMOSPHERIC MODEL

TEMPERATURE = 7

WATER VAPOR = 7

OZONE = 7

M4 = 0 M5 = 0 M6 = 0 MDEF = 0

SPACE TO SPACE LIMB PATH

HMIN = 100.000 KM

FREQUENCY RANGE

IV1 = 1500 CM-1 (6.67 MICROMETERS)

IV2 = 4000 CM-1 (2.50 MICROMETERS)

IDV = 1 CM-1

IFWHM = 1 CM-1

ATMOSPHERIC PROFILES

I	Z (KM)	P (MB)	T (K)	N2 (MOL/CM2 KM)	CNTMSLF (MOL/CM2 KM)	MOL (-)	SCAT (-)	N-1 (-)	O3 (UV) (ATM CM/KM)	O2 (UV) (ATM CM/KM)
1	.00	1011.933	288.2	7.188E-01	.000E+00	9.465E-01	2.723E-04	.000E+00	.000E+00	.000E+00
2	1.00	896.422	281.7	5.837E-01	.000E+00	8.578E-01	2.468E-04	.000E+00	.000E+00	.000E+00
3	2.00	791.652	275.2	4.714E-01	.000E+00	7.755E-01	2.231E-04	.000E+00	.000E+00	.000E+00
4	3.00	697.015	268.7	3.788E-01	.000E+00	6.993E-01	2.012E-04	.000E+00	.000E+00	.000E+00

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31	50.00	.791	270.6	4.826E-07	.000E+00	7.880E-04	2.267E-07	.000E+00	.000E+00	.000E+00
32	70.00	.052	219.6	2.840E-09	.000E+00	6.369E-05	1.832E-08	.000E+00	.000E+00	.000E+00
33	100.00	.000	195.1	1.272E-13	.000E+00	4.389E-07	1.263E-10	.000E+00	.000E+00	.000E+00

ATMOSPHERIC PROFILES

I	Z (KM)	P (MB)	T (K)	CNTMFRN (MOL/CM2 KM)	HNO3 (ATM CM/KM)	AEROSOL 1 (-)	AEROSOL 2 (-)	AEROSOL 3 (-)	AEROSOL 4 (-)	AER1*RH (-)	CIRRUS (-)	RH (PERCNT)
1	.00	1011.933	288.2	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00
2	1.00	896.422	281.7	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00
3	2.00	791.652	275.2	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00
4	3.00	697.015	268.7	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00

* * *

31	50.00	.791	270.6	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00
32	70.00	.052	219.6	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00
33	100.00	.000	195.1	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00

ATMOSPHERIC PROFILES

I	Z (KM)	P (MB)	T (K)	H2O (MOL/CM2 KM)	O3 (MOL/CM2 KM)	CO2 (MOL/CM2 KM)	CO (MOL/CM2 KM)	CH4 (MOL/CM2 KM)	N2O (MOL/CM2 KM)	O2 (MOL/CM2 KM)	NH3 (MOL/CM2 KM)	NO (MOL/CM2 KM)	NO2 (MOL/CM2 KM)	SO2 (MOL/CM2 KM)
1	.00	1011.933	288.2	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	2.84E-05	.00E+00	.00E+00
2	1.00	896.422	281.7	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	2.58E-05	.00E+00	.00E+00
3	2.00	791.652	275.2	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	2.34E-05	.00E+00	.00E+00
4	3.00	697.015	268.7	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	2.11E-05	.00E+00	.00E+00

* * *

31	50.00	.791	270.6	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	8.18E-07	.00E+00	.00E+00
32	70.00	.052	219.6	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	7.37E-08	.00E+00	.00E+00
33	100.00	.000	195.1	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	2.69E-07	.00E+00	.00E+00

GEOMIN: THE ENTIRE PATH LIES ABOVE THE TOP ZMAX OF THE ATMOSPHERIC PROFILE

ZMAXS = 30.0000 H1 = 300.0000 H2 = 300.0000 HMIN = 99.9995 IERROR = -9

SUMMARY OF THE GEOMETRY CALCULATION

H1 = 300.000 KM
H2 = 300.000 KM
ANGLE = 104.065 DEG
RANGE = 3242.471 KM
BETA = 28.131 DEG
PHI = 104.065 DEG
HMIN = 100.000 KM
BENDING = .000 DEG
LONG1 = 329.339 DEG WEST OF GREENWICH
LAT1 = 61.538 DEG NORTH OF EQUATOR
PSIPO = -62.473 DEG EAST OF NORTH
LONG2 = 30.661 DEG WEST OF GREENWICH
LAT2 = 61.538 DEG NORTH OF EQUATOR
LEN = 1

OPTICAL PATH CUMULATIVE AMOUNTS TO LAYER L

LAY L	ALT (KM)	LAT (degN)	LONG (degW)	HERZBERG UV O2	TEMPERATURE DEPENDENT O2 PARAMETERS				O3 UV (ATM-CM)	TEMP DEPENDENT O3 PARAMETERS		CNTMSLF1 (	CNTMSLF2 MOL/CM2	CNTMFRN)
0	300.000	61.538	329.339											
1	290.000	61.697	329.990	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00
2	280.000	61.858	330.665	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00
3	270.000	62.020	331.368	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00

* * *

82	280.000	61.858	29.335	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00
83	290.000	61.697	30.010	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00
84	300.000	61.538	30.660	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00

OPTICAL PATH CUMULATIVE AMOUNTS TO LAYER L

LAY L	ALT (KM)	LAT (degN)	LONG (degW)	N2 CONT (ATM-CM)	MOLEC SCAT	AER 1 0-2km	AER 2 2-10km	AER 3 10-30km	AER 4 30-100km	CIRRUS CLOUDS	TEMPERATURE DEPENDENT RAIN PARAMETERS			
0	300.000	61.538	329.339											
1	290.000	61.697	329.990	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00
2	280.000	61.858	330.665	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00
3	270.000	62.020	331.368	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00

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82	280.000	61.858	29.335	2.078E-11	7.174E-05	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00
83	290.000	61.697	30.010	2.078E-11	7.174E-05	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00
84	300.000	61.538	30.660	2.078E-11	7.174E-05	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00

OPTICAL PATH INCREMENTAL AMOUNTS FROM LAYER L-1 TO LAYER L (ATM-CM)

LAY L	ALT (KM)	LAT (degN)	LONG (degW)	TBAR (K)	H2O(161)	H2O(181)	H2O(171)	H2O(162)	CO2(626)	CO2(636)	CO2(628)	O3	N2O
0	300.000	61.538	329.339										
1	290.000	61.697	329.990	972.885	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00
2	280.000	61.858	330.665	966.630	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00
3	270.000	62.020	331.368	960.370	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00
* * *													
82	280.000	61.858	29.335	960.370	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00
83	290.000	61.697	30.010	966.630	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00
84	300.000	61.538	30.660	972.885	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00
TOTAL ABSORBER AMOUNT					.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00

OPTICAL PATH INCREMENTAL AMOUNTS FROM LAYER L-1 TO LAYER L (ATM-CM)

LAY L	ALT (KM)	LAT (degN)	LONG (degW)	CO	CH4	O2	NO	SO2	NO2	NH3	HNO3	OH	NO+
0	300.000	61.538	329.339										
1	290.000	61.697	329.990	.000E+00	.000E+00	.000E+00	7.821E-10	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00
2	280.000	61.858	330.665	.000E+00	.000E+00	.000E+00	1.222E-09	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00
3	270.000	62.020	331.368	.000E+00	.000E+00	.000E+00	1.909E-09	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00
* * *													
82	280.000	61.858	29.335	.000E+00	.000E+00	.000E+00	1.909E-09	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00
83	290.000	61.697	30.010	.000E+00	.000E+00	.000E+00	1.222E-09	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00
84	300.000	61.538	30.660	.000E+00	.000E+00	.000E+00	7.821E-10	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00
TOTAL ABSORBER AMOUNT				.000E+00	.000E+00	.000E+00	5.196E-04	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	7.386E-06

RADIANCE(WATTS/CM2-STER-XXX)

FREQ	WAVLEN	ATMOS RADIANCE		INTEGRAL	TOTAL
(CM-1)	(MICRN)	(CM-1)	(MICRN)	(CM-1)	TRANS
1500.	6.667	2.37E-12	5.34E-10	1.19E-12	1.0000
1501.	6.662	4.57E-13	1.03E-10	1.64E-12	1.0000
1502.	6.658	1.71E-12	3.85E-10	3.35E-12	1.0000
1503.	6.653	3.51E-18	7.92E-16	3.35E-12	1.0000
1504.	6.649	3.28E-12	7.42E-10	6.63E-12	1.0000
1505.	6.645	2.62E-12	5.93E-10	9.25E-12	1.0000

* * *

3995.	2.503	6.02E-35	9.61E-32	5.92E-07	1.0000
3996.	2.503	5.88E-35	9.38E-32	5.92E-07	1.0000
3997.	2.502	5.73E-35	9.16E-32	5.92E-07	1.0000
3998.	2.501	5.60E-35	8.95E-32	5.92E-07	1.0000
3999.	2.501	4.37E-35	6.98E-32	5.92E-07	1.0000
4000.	2.500	4.26E-35	6.82E-32	5.92E-07	1.0000

INTEGRATED ABSORPTION FROM 1500 TO 4000 CM-1 = .07 CM-1
 AVERAGE TRANSMITTANCE =1.0000

INTEGRATED RADIANCE = 5.921E-07 WATTS CM-2 STER-1
 MINIMUM RADIANCE = .000E+00 WATTS CM-2 STER-1 (CM-1)-1 AT 3174.0 CM-1
 MAXIMUM RADIANCE = 5.873E-09 WATTS CM-2 STER-1 (CM-1)-1 AT 1847.0 CM-1

CARD 5 ***** 0

APPENDIX H
COLUMN DENSITY CALCULATION UPGRADE

APPENDIX H

COLUMN DENSITY CALCULATION UPGRADE

H.1 Introduction

The Air Force atmospheric radiative transport codes FASCODE, MODTRAN, and MOSART use the same general approach to calculate column densities and path averages over refractive path segments. The atmosphere is defined by specifying densities at a series of boundary altitudes, and densities are modeled as varying exponentially with altitude between boundaries. For this stratified atmosphere, layer column densities must be calculated for paths at various zenith angles. Unless the path is strictly vertical, densities do not vary exponentially with path length due to the curvature of the earth and refraction.

Accurate column densities are calculated by sub-dividing the path within a layer into short sub-segments. For each sub-segment, the density at the end points is determined by exponentially interpolating over altitude, and the column density is calculated assuming density varies exponentially with path length for the short segment. In MODTRAN, the sub-segments have a maximum length of 5 km. A half-tangent path of this length has a change in altitude of less than 2 meters. MODTRAN species densities do not vary significantly over such small changes in altitude.

The above prescription for calculating column densities, although accurate, can be quite clumsy. Typically, the calculation of sub-segment column densities is embedded in the refractive geometry module; this is necessary for determination of intermediate altitudes and path lengths. Paths for which column densities are being calculated are distinguished from paths being used simply to define a complete set of line-of-sight parameters. For each species, the layer scale heights are pre-calculated to expedite calculation of end point densities. The final module is quite complex.

A problem can also arise from the sub-segment approach when path averages are calculated. Occasionally the range within a layer can approach zero. Since the range cannot easily be factored from the column density expression if the sub-segment approach used, a zero divide error can result.

In this appendix, an accurate approach is presented for calculating the column densities through a single layer without sub-dividing the layer into short sub-segments. The upgraded column density expression is

$$C_{\text{upgrade}} = \frac{\rho_1 S}{2} \int_0^1 e^{-x(2a_1 + b_1^2 x)} dx + \frac{\rho_2 S}{2} \int_0^1 e^{-x(2a_2 + b_2^2 x)} dx, \quad (\text{H-1})$$

where

$$a_1 = \frac{S \cos \theta_1}{4 \Delta R} \ln \frac{\rho_1}{\rho_2} \quad b_1^2 = \frac{(R_1 + R_2 + S \cos \theta_1)(\Delta R - S \cos \theta_1)}{8 R_1 \Delta R} \ln \frac{\rho_1}{\rho_2} \quad (\text{H-2})$$

$$a_2 = -\frac{S \cos \theta_2}{4 \Delta R} \ln \frac{\rho_1}{\rho_2} \quad b_2^2 = \frac{(R_1 + R_2 - S \cos \theta_2)(S \cos \theta_2 - \Delta R)}{8 R_2 \Delta R} \ln \frac{\rho_1}{\rho_2} \quad (\text{H-3})$$

Inputs are (Figure H-1) the path length S and the earth center distances R_1 and R_2 , the zenith angles θ_1 and θ_2 , and the densities ρ_1 and ρ_2 at the beginning and end of the path; ΔR is the change in altitude, $R_2 - R_1$. The derivation of these equations is presented in Sections H.2 and H.3. Special cases are examined in Section H.4. An algorithm for numerically evaluating the integrals appearing in Equation (H-1) is presented in Section H.5. General properties of C_{upgrade} are discussed in Section H.6. Section H.7 contains a sample calculation and conclusions. The upgraded approach is found to be at least as accurate as MODTRAN's implementation of the sub-segment approach for path segments encountered using MODTRAN model atmospheres.

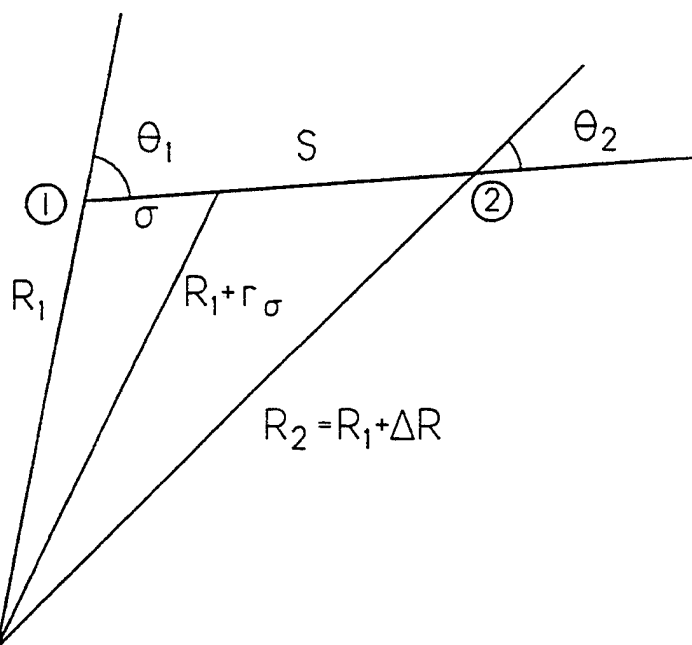


Figure H-1. Straight Layer Segment From Point 1 to Point 2.

H.2 Curved Earth Column Density Upgrade

For the flat earth with no refraction and constant scale height, density varies exponentially with path length. Under these conditions, column density is readily calculated:

$$C_{\text{flat-earth}} = \rho_1 \int_0^S (\rho_2/\rho_1)^{\sigma/S} d\sigma \quad (\text{H-4})$$

$$= S \frac{\rho_1 - \rho_2}{\ln(\rho_1/\rho_2)} \quad (\text{H-5})$$

Introduction of the curved earth and refraction complicates the problem. The exact expression for column density assuming exponential variation of density with altitude is

$$C_{\text{exact}} = \rho_1 \int_0^S (\rho_2/\rho_1)^{r_\sigma/\Delta R} d\sigma \quad (\text{H-6})$$

where ΔR is the increase in altitude from point 1 to point 2 and r_σ is the increase a distance σ along the segment, Figure H-1. For vertical paths $r_\sigma/\Delta R$ equals σ/S , but not in general. The goal here is to find a better approximation for $r_\sigma/\Delta R$ so that column densities can be calculated more accurately.

With simple manipulations, the exact column density expression can be put in the form

$$C_{\text{exact}} = \rho_1 \int_0^{S/2} (\rho_2/\rho_1)^{r_\sigma/\Delta R} d\sigma + \rho_2 \int_0^{S/2} (\rho_1/\rho_2)^{(\Delta R - r_{S-\sigma})/\Delta R} d\sigma \quad (\text{H-7})$$

If there was no refraction and the flat-earth approximation was assumed, r_σ would simply equal $\sigma \cos\theta_1$, where θ_1 is the zenith angle illustrated in Figure H-1, and Equation (H-4) would result. Throughout the IR to UV spectral range, the curvature of the earth affects atmospheric path lengths more than refraction. Therefore, as a first level of improvement, r_σ and $\Delta R - r_{S-\sigma}$ can be replaced by their curved earth forms:

$$r_\sigma = \sqrt{R_1^2 + 2\sigma R_1 \cos\theta_1 + \sigma^2} - R_1 \quad (\text{H-8})$$

CURVED EARTH

$$\Delta R - r_{S-\sigma} = R_2 - \sqrt{R_2^2 - 2\sigma R_2 \cos\theta_2 + \sigma^2} \quad (\text{H-9})$$

where R_1 and R_2 are the distance from points 1 and 2 to the earth center, respectively.

With MODTRAN standard layering structure, the longest single layer half-tangent path is the path tangent to 70 km and extending up to 100 km. Above 70 km refraction is negligible, and this longest single layer path is less than a tenth of the earth center distance. Thus, for path segments encountered in MODTRAN, r_σ and $\Delta R - r_{S-\sigma}$ can be expanded in powers of σ/R as

$$r_\sigma = \sigma \left[\cos\theta_1 + \frac{1}{2} \frac{\sigma}{R_1} \sin^2\theta_1 + O\left(\frac{\sigma^2}{R_1^2}\right) \right] \quad (H-10)$$

$$\Delta R - r_{S-\sigma} = \sigma \left[\cos\theta_2 - \frac{1}{2} \frac{\sigma}{R_2} \sin^2\theta_2 + O\left(\frac{\sigma^2}{R_2^2}\right) \right] \quad (H-11)$$

Here, $O(x)$ is used to denote terms of order x .

Defining the constants

$$a_1 = \frac{S \cos\theta_1}{4 \Delta R} \ln \frac{\rho_1}{\rho_2} \quad b_1^2 = \frac{S^2 \sin^2\theta_1}{8 R_1 \Delta R} \ln \frac{\rho_1}{\rho_2} \quad (H-12)$$

CURVED EARTH

$$a_2 = -\frac{S \cos\theta_2}{4 \Delta R} \ln \frac{\rho_1}{\rho_2} \quad b_2^2 = \frac{S^2 \sin^2\theta_2}{8 R_2 \Delta R} \ln \frac{\rho_1}{\rho_2} \quad (H-13)$$

and dropping second order terms from Equations (H-10) and (H-11), the curved earth column density has the form

$$C_{\text{upgrade}} = \frac{\rho_1 S}{2} \int_0^1 e^{-x(2a_1 + b_1^2 x)} dx + \frac{\rho_2 S}{2} \int_0^1 e^{-x(2a_2 + b_2^2 x)} dx \quad (H-14)$$

Whenever b_1^2 and b_2^2 are both positive, the column density can be expressed in terms of error functions of real arguments:

$$C_{\text{upgrade}} = \sqrt{\pi} \frac{S}{4} \left\{ \frac{\rho_1}{b_1} \exp\left(\frac{a_1^2}{b_1^2}\right) \left[\operatorname{erf}\left(\frac{a_1}{b_1} + b_1\right) - \operatorname{erf}\left(\frac{a_1}{b_1}\right) \right] \right. \\ \left. + \frac{\rho_2}{b_2} \exp\left(\frac{a_2^2}{b_2^2}\right) \left[\operatorname{erf}\left(\frac{a_2}{b_2} + b_2\right) - \operatorname{erf}\left(\frac{a_2}{b_2}\right) \right] \right\} \quad , \quad b_1^2, b_2^2 > 0 \quad (H-15)$$

where $\operatorname{erf}(x)$ is the error function of x . When the b^2 parameters are zero, the integrals reduce to simple exponentials, and when these parameters are negative, the lesser known Dawson integrals (Table 7.5 of Reference 1) result. Note that b_1^2 and b_2^2 will generally both be

non-negative; however, they will be negative if there is a density inversion (i.e. if R_2 exceeds R_1 but ρ_2 is greater than ρ_1 , then $\Delta R = R_2 - R_1$ is positive and $\ln(\rho_1/\rho_2)$ is negative).

H.3 Curved Earth and Path Column Density Upgrade

In the previous section, expressions were derived for r_σ and $\Delta R - r_{S-\sigma}$ for the curved earth assuming refractive affects could be ignored as a first level of approximation. In this section, the expressions are re-derived with refraction taken into account in an approximate way. This is accomplished by replacing the straight line path from point 1 to 2, Figure H-1, with a curved path, Figure H-2. For approximating r_σ , the curved path is taken to be the

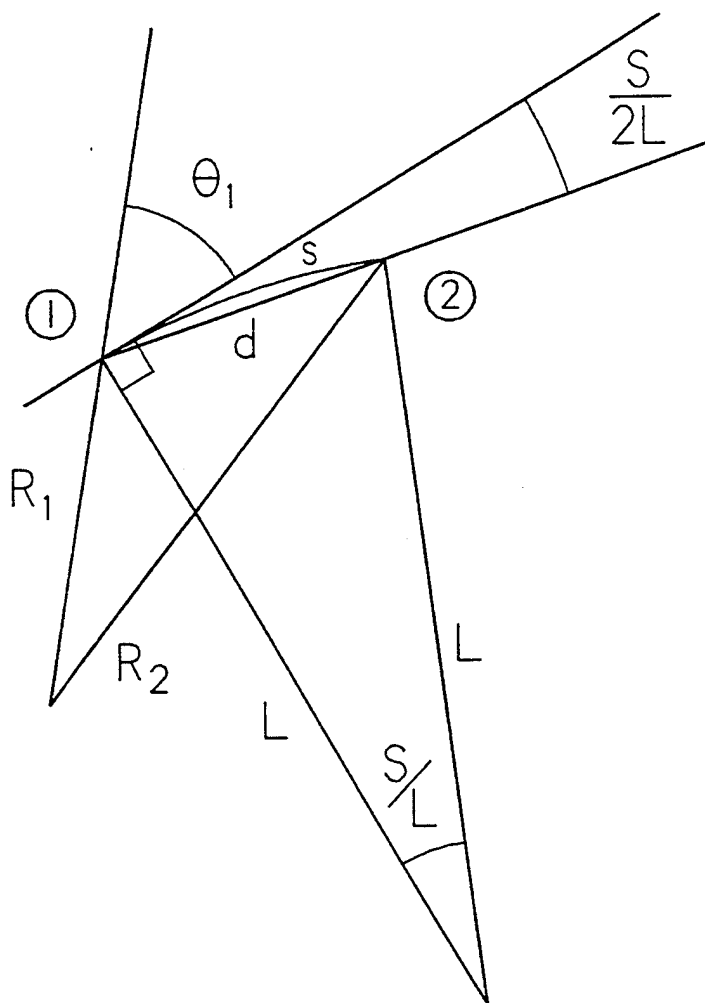


Figure H-2. Curved Layer Segment From Point 1 to Point 2.

circular arc of length S , tangent to the line-of-sight at point 1 and a distance R_2 from the earth center at point 2. The roles of point 1 and point 2 are reversed for approximating $\Delta R - r_{S-\sigma}$.

Let d be the straight line distance from point 1 to point 2 in Figure H-2. Then the equation for L_1 , the radius of curvature at point 1, as a function of R_1 , R_2 , θ_1 , and S can be derived from the relationships

$$R_2^2 = R_1^2 + d^2 + 2 R_1 d \cos(\theta_1 + \frac{S}{2 L_1}) \quad , \quad \text{and} \quad (\text{H-16})$$

$$\frac{d}{2} = L_1 \sin \frac{S}{2 L_1} \quad . \quad (\text{H-17})$$

Switching subscripts 1 and 2, expressions for L_2 , the radius of curvature about point 2, result. Expanding in powers of S/L_1 and S/L_2 , the first order expressions for the radii of curvature are

$$\frac{R_1 \sin \theta_1}{L_1} = \frac{R_1^2 + S^2 + 2 R_1 S \cos \theta_1 - R_2^2}{S^2} + O\left[\frac{S(S + 4 R_1 \cos \theta_1)}{L_1^2}\right] \quad (\text{H-18})$$

$$\frac{R_2 \sin \theta_2}{L_2} = \frac{R_2^2 + S^2 + 2 R_2 S \cos \theta_2 - R_1^2}{S^2} + O\left[\frac{S(S + 4 R_2 \cos \theta_2)}{L_2^2}\right] \quad . \quad (\text{H-19})$$

As should be expected, the radii of curvature go to infinity for straight paths. The upgraded expressions for r_σ and $\Delta R - r_{S-\sigma}$ are

$$\begin{aligned} r_\sigma &= \sqrt{R_1^2 + 2\sigma R_1 \cos \theta_1 + \sigma^2 - \sigma^2 R_1 \sin \theta_1 / L_1 + \sigma(\sigma + 4 R_1 \cos \theta_1) O(\sigma^2 / L_1^2) - R_1} \\ &= \sigma \left[\cos \theta_1 + \frac{1}{2} \left(\frac{\sigma}{R_1} \right) \frac{(R_1 + R_2 + S \cos \theta_1) (\Delta R - S \cos \theta_1)}{S^2} \right] \\ &\quad + \sigma \left[O\left(\frac{\sigma^2}{R_1^2}\right) + O\left(\frac{\sigma^3}{R_1 L_1^2}\right) \right] \end{aligned} \quad (\text{H-20})$$

$$\begin{aligned} \Delta R - r_{S-\sigma} &= \sigma \left[\cos \theta_2 - \frac{1}{2} \left(\frac{\sigma}{R_2} \right) \frac{(R_1 + R_2 - S \cos \theta_2) (S \cos \theta_2 - \Delta R)}{S^2} \right] \\ &\quad + \sigma \left[O\left(\frac{\sigma^2}{R_2^2}\right) + O\left(\frac{\sigma^3}{R_2 L_1^2}\right) \right] \quad . \end{aligned} \quad (\text{H-21})$$

For the curved earth and path, a and b constants have the values

$$a_1 = \frac{S \cos \theta_1}{4 \Delta R} \ln \frac{\rho_1}{\rho_2} \quad b_1^2 = \frac{(R_1 + R_2 + S \cos \theta_1) (\Delta R - S \cos \theta_1)}{8 R_1 \Delta R} \ln \frac{\rho_1}{\rho_2} \quad (\text{H-22})$$

$$a_2 = - \frac{S \cos \theta_2}{4 \Delta R} \ln \frac{\rho_1}{\rho_2} \quad b_2^2 = \frac{(R_1 + R_2 - S \cos \theta_2) (S \cos \theta_2 - \Delta R)}{8 R_2 \Delta R} \ln \frac{\rho_1}{\rho_2} \quad (\text{H-23})$$

The expressions for column density, Equations (H-14) and (H-15), remain the same; only the values of the b_1^2 and b_2^2 parameters change.

For the straight path, b_1^2 and b_2^2 are non-negative as long as there is no density inversion. This remains true for the curved path only if $S \cos \theta_2 \geq R_2 - R_1 \geq S \cos \theta_1$. For the flat earth, the three terms are equal. Due to the curvature of the earth, $S \cos \theta_2 > R_2 - R_1 > S \cos \theta_1$ for straight paths. As long as earth curvature affects dominate refractive affects, the inequalities remain valid.

H.4 Special Cases

The upgraded column density expression is evaluated for three special cases: vertical paths, short half-limb paths, and paths to space with a constant scale height atmosphere (total column densities). Refraction is ignored for the special cases 2 and 3, and there is assumed to be no density inversions. For this section only, the subscript "upgrade" is dropped from C_{upgrade} .

H.4.1 CASE 1: Vertical Paths

For vertical paths, $\sin \theta_1 = \sin \theta_2 = 0$, $\cos \theta_1 = \cos \theta_2 = \pm 1$, and $\Delta R = \pm S$. Substituting into Equations (H-12) and (H-13) or Equations (H-22) and (H-23), both b parameters are zero, and $a_1 = \frac{1}{4} \ln(\rho_1/\rho_2) = -a_2$. With the b parameters equal to zero, C is most easily evaluated directly from Equation (H-14). The result,

$$C_{\text{vertical}} = S \frac{\rho_1 - \rho_2}{\ln(\rho_1/\rho_2)} \quad (\text{H-24})$$

is identical to the flat-earth approximation, Equation (H-3), as it should be for a vertical path.

H.4.2 CASE 2: No Refraction, No Density Inversion, Short Half-Limb Path

For a half-limb path tangent at point 1, $\cos\theta_1 = 0$, $\sin\theta_1 = 1$, $\cos\theta_2 = S/R_2$, and $\sin\theta_2 = R_1/R_2$. If the path length is small compared to R_1 , then $R_1 \approx R_2$ and $2\Delta R \approx S^2/R_1$. With this level of approximation, the half-tangent a and b parameters equal

$$a_1 = 0, \quad a_2 = -\frac{1}{2} \ln \frac{\rho_1}{\rho_2}, \quad b_1^2 = b_2^2 = \frac{1}{4} \ln \frac{\rho_1}{\rho_2}, \quad \text{short half-limb} \quad (H-25)$$

Remembering that $\text{erf}(x) = -\text{erf}(-x)$, Equation (H-15) reduces to

$$C_{\text{short half-limb}} = \sqrt{\pi} \frac{\rho_1 S}{4} \text{erf} \left[\frac{\sqrt{\ln(\rho_1/\rho_2)}}{\sqrt{\ln(\rho_1/\rho_2)}} \right] / \sqrt{\ln(\rho_1/\rho_2)} \quad (H-26)$$

$$= \rho_1 S \left\{ 1 - \frac{1}{3} \left(\ln \frac{\rho_1}{\rho_2} \right) + \frac{1}{10} \left(\ln \frac{\rho_1}{\rho_2} \right)^2 + O \left[\left(\ln \frac{\rho_1}{\rho_2} \right)^3 \right] \right\} \quad (H-27)$$

The leading order correction to $\rho_1 S$ for $C_{\text{short half-limb}}$ is different from the leading order correction for $C_{\text{flat-earth}}$. Setting ρ_2 to $\rho_1 (1 - \epsilon)$, $C_{\text{flat-earth}}$ equals

$$C_{\text{flat-earth}} = \rho_1 S \left[1 - \frac{\epsilon}{2} + O(\epsilon^2) \right], \quad (H-28)$$

while $C_{\text{short half-limb}}$ equals

$$C_{\text{short half-limb}} = \rho_1 S \left[1 - \frac{\epsilon}{3} + O(\epsilon^2) \right], \quad (H-29)$$

The deviation from $\rho_1 S$ is less for the short half-limb expression.

H.4.3 CASE 3: Total Column Density with Constant (>0) Scale Height and No Refraction

In this case, the total column density is calculated as a function of zenith angle for $0^\circ \leq \theta_1 \leq 90^\circ$. Since r_σ and $\Delta R - r_{S-\sigma}$ were both expanded assuming S/R_1 and S/R_2 were small, it might seem inappropriate to consider the $S \rightarrow \infty$ limit. However, if the scale height D is small compared to the earth center distance R_1 , then the major contribution to the column density comes from that part of the line-of-sight for which S/R_1 is small.

The scale height is defined by the relationship

$$D = \Delta R / \ln\left(\frac{\rho_1}{\rho_2}\right) . \quad (H-30)$$

The law of sines bounds the sine of θ_2 ;

$$\sin\theta_2 = \frac{R_1}{R_2} \sin\theta_1 \leq \frac{R_1}{R_2} . \quad (H-31)$$

Noting that $R_2 \approx \Delta R \approx S$ as $S \rightarrow \infty$, the a and b parameters equal

$$a_1 = \frac{S \cos\theta_1}{4 D} \quad b_1^2 = \frac{S^2 \sin^2\theta_1}{8 R_1 D} \quad (H-32)$$

S LARGE

$$a_2 = -\frac{S}{4 D} \quad b_2^2 = \frac{S \sin^2\theta_2}{8 D} \leq \frac{R_1^2}{8 D S} \rightarrow 0 . \quad (H-33)$$

Since b_2 goes to zero as S approaches infinity, the column density integral about distant point 2 can be evaluated directly from Equation (H-14):

$$\begin{aligned} \lim_{S \rightarrow \infty} \frac{\rho_2 S}{2} \int_0^1 e^{-x(2a_2 + b_2^2 x)} dx \\ = \lim_{S \rightarrow \infty} D \rho_1 [e^{-S/(2D)} - e^{-S/D}] = 0 . \end{aligned} \quad (H-34)$$

The contribution from the far side of the line-of-sight is zero, consistent with the density falling off exponentially. The integral about point 1 is evaluated using Equation (H-15). Since $\lim_{S \rightarrow \infty} (a_1/b_1 + b_1)$ approaches infinity for any θ_1 between 0 and 90 degrees inclusive, the first error function in Equation (H-15) goes to 1. The total column density expression reduces to

$$\lim_{S \rightarrow \infty} C(\theta_1) = \sqrt{\pi} \frac{x D \rho_1}{\sin\theta_1} \exp(x^2 \cot^2\theta_1) \operatorname{erfc}(x \cot\theta_1) , \quad (H-35)$$

where $2x^2 = R_1 / D$ and erfc is the complementary error function. The normalized total column density is plotted as a function of zenith angle in Figure H-3; the scale height was set equal to $R_1/1000$, a reasonable value for total density above the earth's surface. The flat-earth approximation is recovered for θ_1 equal to zero degrees:

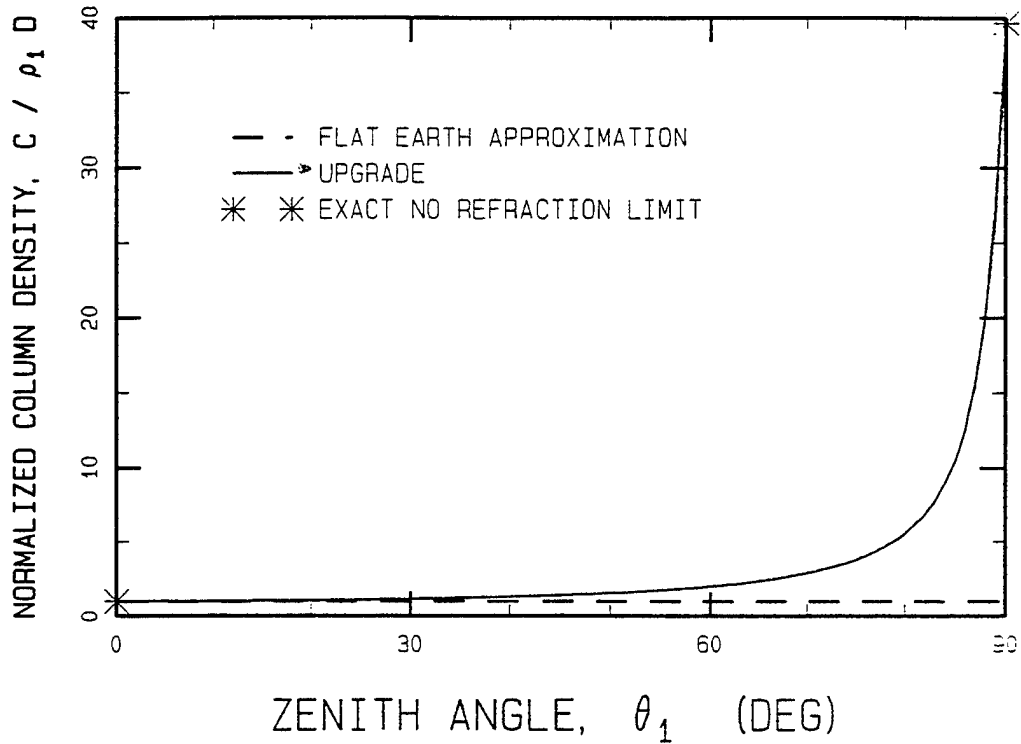


Figure H-3. Variation in Total Column Density With Zenith Angle. Scale Height was Chosen Equal to the Earth's Radius Over 1000.

$$\lim_{S \rightarrow \infty} C(\theta_1 = 0^\circ) = D \rho_1 \quad . \quad (H-36)$$

At θ_1 equal 60° , Equation (H-36) gives twice the flat-earth approximation, and for the half-limb calculation ($\theta_1 = 90^\circ$) almost 40 times the flat-earth value results:

$$\lim_{S \rightarrow \infty} C(\theta_1 = 90^\circ) = \sqrt{\pi R_1 D / 2} \rho_1 \quad . \quad (H-37)$$

To demonstrate that Equation (H-37) is reasonable, the no refraction half-limb integral can be evaluated exactly. Combining Equations (H-6), (H-8), and (H-30) with $\theta_1 = 90^\circ$ and letting the path length S approach infinity, the no refraction total column density equals

$$C_{\text{straight half-limb}} = \rho_1 e^{R_1/D} \int_0^\infty \exp\left(-\frac{1}{D} \sqrt{R_1^2 + \sigma^2}\right) d\sigma \quad . \quad (H-38)$$

Substituting $\sigma = R_1 \sinh(t)$, the integral representation of a modified Bessel function, Equation 9.6.24 of Reference 1, results

$$C_{\text{straight half-limb}} = R_1 \rho_1 e^{R_1/D} K_1\left(\frac{R}{D}\right) . \quad (\text{H-39})$$

The asymptotic expansion (Equation 9.7.2 of Reference 1) gives

$$C_{\text{straight half-limb}} = \sqrt{\pi R_1 D / 2} \rho_1 \left\{ 1 - \frac{3}{8} \frac{D}{R_1} + \dots \right\} , \quad (\text{H-40})$$

in agreement with Equation (H-37).

H.5 Numerical Evaluation of the Column Density

Calculation of the upgraded expression for column density requires evaluation of the integral

$$I(a, b^2) \equiv \int_0^1 e^{-x(2a + b^2 x)} dx \quad (\text{H-41})$$

for arbitrary real a and b^2 . In terms of $I(a, b^2)$, the column density equals

$$C_{\text{upgrade}} = \frac{\rho_1 S}{2} I(a_1, b_1^2) + \frac{\rho_2 S}{2} I(a_2, b_2^2) . \quad (\text{H-42})$$

Evaluation is performed by dividing the b^2 domain of $I(a, b^2)$ into three regions.

H.5.1 Region 1: $b^2 > 0.0001$

Throughout this subsection, b is defined as the positive square root of b^2 . For positive b^2 , $I(a, b^2)$ can be expressed in terms of error functions of real arguments:

$$I(a, b^2) = \sqrt{\pi} \frac{1}{2b} \exp\left(\frac{a^2}{b^2}\right) \left[\operatorname{erf}\left(\frac{a}{b} + b\right) - \operatorname{erf}\left(\frac{a}{b}\right) \right] . \quad (\text{H-43})$$

Evaluation is facilitated by working with the complementary error function of non-negative arguments. Three sub-cases arise:

$$I(a,b^2) = \sqrt{\pi} \frac{1}{2b} e^{a^2/b^2} \left[\operatorname{erfc}\left(\frac{a}{b}\right) - \operatorname{erfc}\left(\frac{a+b^2}{b}\right) \right], \quad \text{for } a \geq 0, \quad (\text{H-44a})$$

$$I(a,b^2) = \sqrt{\pi} \frac{1}{2b} e^{a^2/b^2} \left[\operatorname{erfc}\left(-\frac{a+b^2}{b}\right) - \operatorname{erfc}\left(-\frac{a}{b}\right) \right], \quad \text{for } a+b^2 \leq 0, \quad (\text{H-44b})$$

$$I(a,b^2) = \sqrt{\pi} \frac{1}{2b} e^{a^2/b^2} \left[2 - \operatorname{erfc}\left(\frac{a+b^2}{b}\right) - \operatorname{erfc}\left(-\frac{a}{b}\right) \right], \quad \text{otherwise} \quad (\text{H-44c})$$

Defining $J(z,b)$ by

$$J(z,b) \equiv \sqrt{\pi} \frac{1}{2b} \exp\left(\frac{z^2}{b^2}\right) \operatorname{erfc}\left(\frac{z}{b}\right), \quad (\text{H-45})$$

Equations (H-44a) through (H-44c) become

$$I(a,b^2) = J(a,b) - e^{-b^2-2a} J(a+b^2,b), \quad \text{for } a \geq 0, \quad (\text{H-46a})$$

$$I(a,b^2) = e^{-b^2-2a} J(-a-b^2,b) - J(-a,b), \quad \text{for } a+b^2 \leq 0, \quad (\text{H-46b})$$

$$I(a,b^2) = \sqrt{\pi} \frac{1}{b} e^{a^2/b^2} - e^{-b^2-2a} J(a+b^2,b) - J(-a,b), \quad \text{otherwise}, \quad (\text{H-46c})$$

For $0 \leq z < 1.883 b$, $J(z,b)$ is evaluated using a rational approximation, Equation 7.1.26 of Reference 1:

$$J(z,b) = \frac{\alpha_1 + \alpha_2 t + \alpha_3 t^2 + \alpha_4 t^3 + \alpha_5 t^4}{b + p z} \quad (\text{H-47})$$

where

$$t = \frac{b}{b + p z} \quad p = +0.3275911$$

$$\alpha_1 = +0.225836846 \quad \alpha_2 = -0.252128668$$

$$\alpha_3 = +1.259695129 \quad \alpha_4 = -1.287822453 \quad \alpha_5 = +0.940646070$$

For $z \geq 1.883 b$, $J(z,b)$ can be calculated from a truncated continued fraction, Equation 7.1.14 of Reference 1 (the continued fraction notation from Reference 1 has been adopted):

$$J(z,b) = \frac{1/(2b)}{z/b+} \frac{1/2}{z/b+} \frac{1}{z/b+} \frac{3/2}{z/b+} \frac{2}{z/b+} \frac{5/2}{z/b+} \frac{3}{z/b+} \frac{7/2}{z/b+} \frac{4}{z/b} \quad (\text{H-48a})$$

$$= \frac{8 + 140 u + 690 u^2 + 975 u^3 + 192 u^4}{z (16 + 288 u + 1512 u^2 + 2520 u^3 + 945 u^4)} , \quad (\text{H-48b})$$

where $u \equiv b^2/z^2$. The cutoff between the two expressions was set to $z/b = 1.883$ because the rational approximation and continued fraction cross at that value. Reference 1 indicates that the maximum absolute error in the rational approximation for $\text{erfc}(x)$ is 1.5×10^{-7} . With $b \geq 0.01$, the maximum possible absolute error for Equation (H-47) is 4.6×10^{-4} $[= 0.5 \sqrt{\pi} \exp(1.883^2) (1.5 \times 10^{-7}) / 0.01]$. At this maximum ($b=0.01$, $z=0.01883$), $J(b,z)$ equals 23.8 corresponding to a relative error of 1.9×10^{-5} . The actual calculation at $b=0.01$, $z=0.01883$ using Equation (H-47) results in a relative error of 1.14×10^{-5} .

H.5.2 Region 2: $|b^2| \leq 0.0001$

For $|b^2| \leq 0.0001$, $I(a,b^2)$ can be evaluated by expanding $e^{-b^2 x^2}$ from Equation (H-33) in a power series. If $2|a| \leq .01$, the full exponential $e^{-b^2 x^2 - 2ax}$ can be expanded. The results are

$$I(a,b^2) = \frac{1}{2a} \left\{ (1 - e^{-2a}) - \frac{b^2}{2a^2} [1 - e^{-2a} (1 + 2a + 2a^2)] \right\} + O(b^4) \quad (\text{H-49})$$

$$I(a,b^2) = 1 - a + \frac{2a^2 - b^2}{3} - \frac{2a^3 - 3ab^2}{6} + O[(2a)^4] + O[(2a)^2 b^2] + O[b^4] . \quad (\text{H-50})$$

H.5.3 Region 3: $b^2 < -0.0001$

Let β be defined equal to $\sqrt{-b^2} > 0$. Substituting $y = \beta x - a/\beta$ in Equation (H-41), $I(a,-\beta^2)$ equals

$$I(a,-\beta^2) = \frac{1}{\beta} e^{-a^2/\beta^2} \int_{-a/\beta}^{\beta - a/\beta} e^{y^2} dy . \quad (\text{H-51})$$

Defining $F(x)$ as the Dawson integral

$$F(x) \equiv e^{-x^2} \int_0^x e^{y^2} dy, \quad (H-52)$$

$I(a, -\beta^2)$ can be written

$$I(a, -\beta^2) = \frac{1}{\beta} [e^{\beta^2 - 2a} F(\beta - \frac{a}{\beta}) - F(-\frac{a}{\beta})], \quad \text{for } a \leq 0, \quad (H-53a)$$

$$I(a, -\beta^2) = \frac{1}{\beta} [F(\frac{a}{\beta}) - e^{\beta^2 - 2a} F(\frac{a}{\beta} - \beta)], \quad \text{for } a \geq \beta^2, \quad (H-53b)$$

$$I(a, -\beta^2) = \frac{1}{\beta} [e^{\beta^2 - 2a} F(\beta - \frac{a}{\beta}) + F(\frac{a}{\beta})], \quad \text{otherwise} \quad (H-53c)$$

The Dawson integral can be evaluated by linearly interpolating the tabulated values from Reference 1 (Table 7.5).

H.6 General Properties

Calculating the column density between two points in space should give the same answer in either direction. Also, adding a layer boundary at an altitude R between R_1 and R_2 should not change the column density if the intermediate density ρ is defined by exponentially interpolating ρ_1 and ρ_2 over altitude.

For both $C_{\text{flat-earth}}$ and C_{upgrade} , the column density is indeed independent of direction

$$C_{\text{flat-earth}}(\rho_1, \rho_2) = C_{\text{flat-earth}}(\rho_2, \rho_1) \quad (H-54)$$

$$C_{\text{upgrade}}(\rho_1, \rho_2; R_1, R_2; \theta_1, \theta_2) = C_{\text{upgrade}}(\rho_2, \rho_1; R_2, R_1; \pi - \theta_2, \pi - \theta_1) \quad (H-55)$$

For C_{upgrade} , switching direction switches the values of a_1 and a_2 and the values of b_1^2 and b_2^2 (when direction is switched, the sign of ΔR and $\ln(\rho_1/\rho_2)$ changes but S is always positive). Equation (H-55) follows from the defining expression for C_{upgrade} , Equation (H-14).

Adding an intermediate layer only approximately conserves column density

$$\begin{aligned} & C_{\text{upgrade}}(\rho_1, \rho; R_1, R; \theta_1, \theta) + C_{\text{upgrade}}(\rho, \rho_2; R, R_2; \theta, \theta_2) \\ & \approx C_{\text{upgrade}}(\rho_1, \rho_2; R_1, R_2; \theta_1, \theta_2), \end{aligned} \quad (H-56)$$

where

$$R_1 < R < R_2, \text{ and}$$

$$\rho \equiv \rho_1 (\rho_2/\rho_1)^{(R-R_1)/(R_2-R_1)}$$

The relationship is not exact, because the exponents in Equation (H-8) were approximated using truncated power series. The deviation from conservation will be less for the column density upgrade than for the flat earth expression since improved approximations for the exponents were used.

H.7 Conclusions

The goal of this effort was to demonstrate that atmospheric column densities for refractive path segments with constant scale heights could be calculated without having to sub-divide each segment into short sub-segments. The prescription laid out requires input of the path length and the density, earth center distance and zenith angle at the beginning and end of each path segment (for spherically symmetric atmospheres, the product of the earth center angle, the sine of the zenith angle and the index of refraction is a path constant, implying that the zenith angle need not be an independent input). Using Equations (H-2) and (H-3), the constants a_1 , a_2 , b_1^2 and b_2^2 are calculated. Column density is then determined from Equation (H-42). Section H.4 describes the routine used to calculate the $I(a, b^2)$ integrals.

An example illustrates the accuracy of the above prescription. MODTRAN column densities were calculated for a line-of-sight from the ground ($R_1 = 6371.23$ km) to 1 km altitude ($R_2 = 6372.23$ km) with an initial zenith angle of 90° and using the US Standard Atmosphere. The calculations were run at $0.55 \mu\text{m}$. Water's density changed most drastically over this altitude range, dropping from 733.29 atm cm/km to 521.76 atm cm/km. Path range was determined to be 123.749 km and the zenith angle at H_2 is 89.071° . The flat earth approximation predicts a column density for water of

$$C_{\text{flat earth}} = 76914. \text{ atm cm} \quad [5.6\%]$$

(the absolute percent error is in brackets). In MODTRAN, the 123.749 km path is sub-divided into 27 sub-segments and the flat earth approximation is applied to each of them:

$$C_{\text{modtran}} = 81425. \text{ atm cm} \quad [-0.008\%]$$

If the a and b parameters for a straight path and curved earth, Equations (H-12) and (H-13), are used to calculate the column density, considerable improvement over the flat-earth approximation results,

$$C_{\text{upgrade}}(\text{straight path}) = 80971. \text{ atm cm} \quad [0.57\%] \quad ;$$

however, refraction is significant at $0.55 \mu\text{m}$ for this path. Using the parameters defined by Equations (H-2) and (H-3), the column density was recalculated

$$C_{\text{upgrade}}(\text{curved path}) = 81435. \text{ atm cm} \quad [0.004\%] \quad .$$

A benchmark value was determined by calculating the curved path, curved earth column density for each of MODTRAN's 27 sub-segments. The result is

$$C_{\text{benchmark}} = 81431.5 \text{ atm cm.}$$

For long paths like the one just discussed, the upgraded expression for column density requires less computational time than required to exponentially interpolate densities at each of 26 intermediate boundaries. However, the processing time for the geometry calculation in radiative transport codes is usually small. The true advantage of the approach presented here is that it eliminates the necessity of sub-dividing each path segment into sub-segments for calculation of column densities.

H-8. References

1. M. Abramowitz and I. A. Stegun, "Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables," (New York, Dover Publications, Inc., 1964).