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NON-EQUILIBRIUM MOLECULAR EMISSION AND SCATTERING INTENSITY SUBROUTINE (NEMESIS) VOLUME 1

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This interim technical report describes the initial development of the SHARC radiative transfer subroutine NEMESIS (Non-Equilibrium Molecular Emission and Scattering Intensity Subroutine). NEMESIS computes the enhancement of upper atmospheric molecular excited state populations due to radiative trapping. The physical processes considered include external illumination by the sun and upwelling earthshine, collisional excitation and de-excitation, radiative decay and multiple emission-absorption. A Monte Carlo procedure for simulating the multiple emission-absorption process is developed. The procedure is validated by comparison to exact solutions for the closely related cloud scattering problem.

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1. INTRODUCTION

The Strategic High Altitude Radiation Code (SHARC) will provide a comprehensive model for calculating atmospheric radiation for arbitrary paths within the 50 to 300 km regime. SHARC will calculate ambient radiation in the 1-30 μm spectral region with a nominal spectral resolution of 5 cm^{-1}. The code will be modular in construction so that the science incorporated in it can be modified or upgraded as additional information and/or models become available. Other features include a band-model approach for the radiation transport that will eventually include the effects of a combined Doppler-Lorentz (or Voigt) lineshape. Because of its band-model formulation, SHARC will be both relatively fast running, suitable for systems-type calculations. The code can be considered as a successor to the AFGL/Visidyne HAIRM Code (High Altitude Infrared Radiance Model.[1] The SHARC modules include chemical kinetics, radiative transport, geometry and input/output. Work is presently underway on all these models, and the initial version of SHARC is scheduled to be available in December 1988.

This report describes the development of the initial version of the SHARC radiative transfer subroutine NEMESIS (Non-Equilibrium Molecular Emission and Scattering Intensity Subroutine). NEMESIS computes the enhancement of atmospheric molecular excited state populations due to radiative trapping. Certain molecular bands, such as the 4.3 μm CO_2 band, are optically opaque in the upper atmosphere. An emitted photon in these bands may be absorbed and re-emitted many times before it is either collisionally quenched or escapes the atmosphere.

A schematic of the radiative transfer problem is shown in Fig. 1. Semi-infinite plane parallel geometry is assumed for the calculation of the enhanced excited state populations. Earth curvature effects are not important for determining the enhanced distributions; however, they must be

1. T. C. Degges and H. J. P. Smith, "A High Altitude Infrared Radiance Model," AFGL-TR-77-0271, Air Force Geophysics Laboratory, Hanscom AFB, MA (30 November 1977). ADA059242

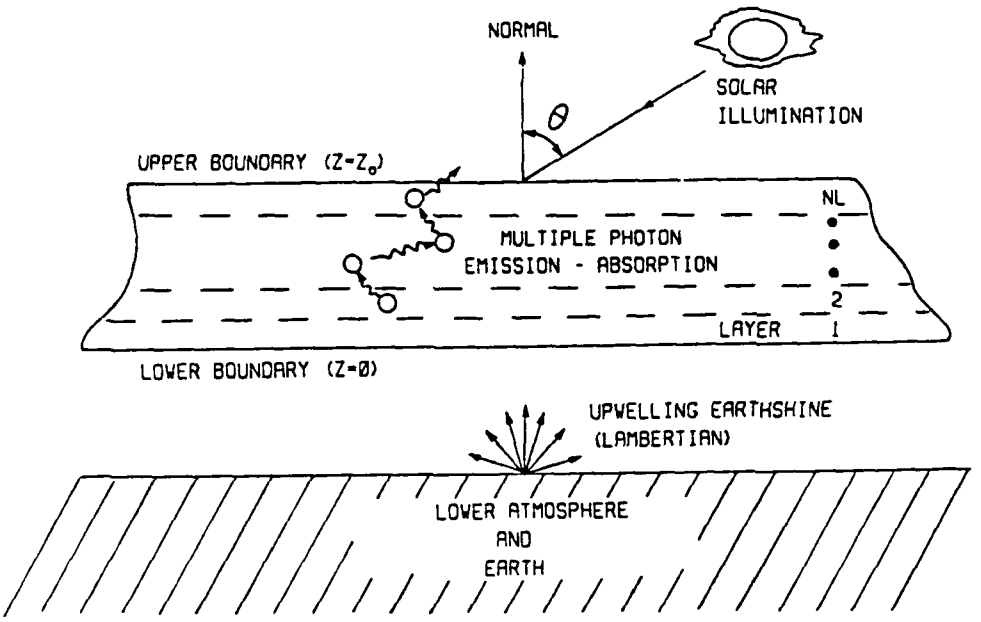

Figure 1. Radiative Transfer Schematic for High Altitude Atmospheric Emission.

included for line-of-sight emission calculations in order to determine the proper column density of emitters. The atmosphere is divided into a number of homogeneous layers. Two external sources of light are considered, upwelling earthshine from the lower atmosphere and downwelling sunshine. The earthshine is given a Lambertian angular distribution. Molecular excited states are created by absorption of external light sources and by collisional excitation and energy transfer from other excited states. Excited states are destroyed through collisional quenching, energy transfer to other states, and radiative decay.

The objective of the NEMESIS code development is to calculate the steady state atmospheric molecular excited state population distributions within the upper atmosphere (60 km and up) taking into account all of these processes. The basic approach involves two overall steps:

1. determination of the steady state excited state population distributions due to external illumination and collisional processes only, and

2. determination of the enhancement of the step (1) distributions due to internal layer emission and radiative trapping.

The separability of these steps is based on the approximation that the lower state populations are not significantly depleted due to radiative trapping in step (2).

The enhancement of the "source" excited state populations is determined using a Monte Carlo simulation of the radiative trapping. Trial photons are started out from all the sublayers and their trajectories are followed until they exit the top or bottom of the upper atmosphere. Each absorption event contributes to the enhanced excited state population of the sublayer in which it occurs. The physical approximations which are used in this initial version of NEMESIS are:

- semi-infinite plane parallel geometry,
- translation-rotation temperature equilibration,
- complete frequency redistribution across the line shape function after each absorption event,
- complete rotational level redistribution after each absorption event,
- no overlap of absorption lines,
- temperature independent radiative transfer, and
- restriction to just the Doppler line shape.

These approximations correspond to those typically assumed in developing simplified analytical solutions to the problem, and are the exact same approximations used in the Degges model.[1] All of these approximations can be relaxed in the Monte Carlo approach. In particular, the relaxation of the last two approximations will be investigated as part of the first SHARC upgrade effort.

2. MONTE CARLO SIMULATION

The Monte Carlo approach to solving the radiative transport equation involves separating the problem into a number of sequential physical processes where the outcome of each process can be chosen from an appropriate probability distribution. By following the outcome of many trial photons statistically converged values for desired quantities, such as excited state populations, can be calculated. For the problem considered here the basic steps in the Monte Carlo simulation are:

1. determine the "source" steady state population distribution due to external illumination, collisional processes, and radiative decay.
2. pick the initial location for emission of a trial photon.
3. pick the direction of photon emission.
4. pick the emission-absorption line strength.
5. pick the absorption cross section.
6. pick the length of photon travel before absorption.
7. integrate through the layers until absorption occurs or the photon escapes out the top or bottom of the upper atmosphere.
8. increment desired output distributions and return to step (3) if absorption occurs or return to step (2) to start the next trial photon.

The algorithms used for each of these steps are discussed below.

2.1 Steady State "Source" Populations

For the initial version of NEMESIS described here the following rate scheme was assumed for determining the steady state populations due to the external light sources, collisional processes, and radiative decay:

$$M + M \xrightarrow{k_1} M^* + M \quad \text{(collisional excitation)} \qquad (1)$$

$$M^* + M \xrightarrow{k_2} M + M \quad \text{(collisional quenching)} \tag{2}$$

$$M^* \xrightarrow{k_3} M + h\nu \quad \text{(radiative decay)} \tag{3}$$

$$M + h\nu \xrightarrow{k_4} M^* \quad \text{(external illumination)} \tag{4}$$

where M denotes a ground state molecular species, "k" is the rate constant, the superscript * denotes an excited molecular state, and $h\nu$ denotes a photon. The steady state solution for the excited state population is given by,

$$\frac{[M^*]}{[M_t]} = \frac{k_1[M_t] + k_4}{k_1[M_t] + k_2[M_t] + k_3 + k_4} \tag{5}$$

where $[M_t] = [M]+[M^*]$ is the total concentration of species M. This solution for the excited state population is applied to each sublayer since the molecular concentrations and the transmission of the external light sources are sublayer dependent. The initial version of NEMESIS assumes a constant molecular concentration (i.e., sublayer independent) which must be generalized to account for the real atmospheric concentration profiles.

There are two contributions to the external illumination rate constant, k_4, which are solar and earthshine excitation. Although this rate constant varies with position within each sublayer an average value is used for each sublayer.

2.1.1 Solar Excitation

The total rate of excitation for an entire absorption band is calculated from,

$$k_4 = \frac{F_0(\omega_0)}{\Delta z} \int_z^{z+\Delta z} dz \int_{-\infty}^{+\infty} d\omega \int_{S_{min}}^{S_{max}} dS g(S)\sigma(S,\omega)\exp(-\rho\sigma z) \tag{6}$$

where F_o (photons cm^{-2} per cm^{-1}) is the solar flux at the center of the band located at wavenumber ω_o (cm^{-1}), Δz (cm) is the thickness of the sublayer, S (cm) is line strength, g (cm^{-1}) is the distribution of line strengths for the band, σ (cm^2) is the absorption cross section which depends both on line strength and line shape, and ρ (cm^{-3}) is the density of absorbing molecules. The form of the line strength distribution function, g (S), will be discussed in a later section. By integrating over the sublayer thickness and by rearranging terms the rate constant can be more compactly expressed as,

$$k_4 = \frac{F_o(\omega_o)}{\Delta z \rho} \int_{S_{min}}^{S_{max}} dS g(S)\{W(S,z)-W(S,z+\Delta z)\} \qquad (7)$$

where W (cm^{-1}) is the equivalent spectral width of a line with line strength, S, and optical opacity determined by the penetration distance, z. This expression for k_4 is based on normal incidence for the sunlight. For non-normal incidence the only modification required is to replace z by z/μ where μ is the cosine of the solar zenith angle (0 deg is normal incidence).

The functional form of the equivalent width depends on the assumed line shape function.[2] The initial version of NEMESIS is based on a Doppler line shape, an upgrade to a Voigt line shape is planned for the initial SHARC code. An analytical approximation to the exact Doppler equivalent width integral is used and is given by,[2]

$$W = 1.70\gamma_d(\ln\{1+(0.589Su/\gamma_d)^2\})^{1/2} \qquad (8)$$

where γ_d (cm^{-1}) is the Doppler width and u (molecules cm^{-2}) is the column density of absorbing molecules. The Doppler width is calculated from

2. C. B. Ludwig, W. Malkmus, J. E. Reardon, and J. A. L. Thomson, "Handbook of Infrared Radiation from Combustion Gases," NASA Report SP-3080 (1973).

$$\gamma_d = 3.58 \times 10^{-7} \omega_o \sqrt{T_a/M} \quad (9)$$

where T_a (K) is atmospheric temperature and M (amu) is the absorbing species molecular weight. The molecular column density is given by,

$$u = \rho z/\mu \quad . \quad (10)$$

2.1.2 Earthshine Excitation

The expression for earthshine excitation involves an additional integration over illumination angle since it is not a collimated source. It is given by,

$$k_4 = \frac{2N(\omega_o, T_b)}{\Delta z} \int_{S_{min}}^{S_{max}} dS g(S) \int_0^1 d\mu \mu \{W(S, z/\mu) - W(S, (z + \Delta z)/\mu)\} \quad (11)$$

where N (photons cm^{-2} sr^{-1} per cm^{-1}) is the black body emission function evaluated at an effective atmospheric background temperature T_b (K), and μ is direction cosine of the Lambertian angular integration.

2.2 Initial Location for Photon Emission

The rate at which photons are emitted from any point within the upper atmosphere is proportional to the local excited state number density. If one were to pick the initial photon emission location from this distribution one would oversample the lower part of the upper atmosphere and greatly undersample the upper part of the upper atmosphere. It is more useful to uniformly sample the entire upper atmospheric region and then weight the contribution of each photon to the final result by the local excited state number density at the initial sample location. The initial location is determined from,

$$z = z_o \beta \quad (12)$$

where z_o is the total thickness of the layer and β is a uniformly distributed random number over the interval $0<\beta<1$.

2.3 Emission Direction

The direction of photon emission is isotropic and is chosen from,

$$\mu_z = 2\beta - 1 \tag{13}$$

where μ_z is the direction cosine with respect to the z axis.

2.4 Emission-Absorption Line Strength

In principle it is possible to choose lines directly from a line atlas compilation, however in practice it is much more efficient to sample the line strength from an analytical approximation to the actual line strength distribution. For the initial version of NEMESIS the following form for the line strength distribution is assumed,

$$g(S) = \frac{\alpha}{S} \tag{14}$$

where α is a normalization constant. The normalization is defined by,

$$\int_{S_{min}}^{S_{max}} dS \frac{\alpha}{S} = g_o \tag{15}$$

where g_o is the total number of lines in the absorption band between S_{min} and S_{max}. Other choices of the line strength distribution will be investigated for incorporation in the initial SHARC code. This form for the line strength distribution also assumes that there is no temperature variation. It should be feasible to incorporate the effect of temperature variation into the distribution.

The probability of emitting at a particular line is proportional to the strength of that line. Including the line degeneracy factor given by g(s), then the probability of emitting at a given line strength is,

$$P_{emis}(S) = Sg(S) = \text{constant} \tag{16}$$

where $P_{emis}(S)$ is the probability of emitting at S. Thus all line strengths are equally probable and can be sampled via,

$$S = S_{max} - \beta(S_{max} - S_{min}) \quad . \tag{17}$$

2.5 Absorption Cross Section

The form of the absorption cross section for a Doppler line is given by,

$$\sigma = \sigma_o \exp(-x^2) \tag{18}$$

where $\sigma_o = 0.4697S/\Upsilon_d$ is the cross section at the center of the line and $x = 0.8325\ (\omega-\omega_o)/\Upsilon_d$ is the relative displacement from the line center. This distribution can be sampled through the following procedure,

$$r^2 = -\ln(\beta) \quad , \tag{19}$$

$$\theta = \frac{\pi}{2}\beta \quad , \text{ and} \tag{20}$$

$$x^2 = r^2\cos(\theta)^2 \quad . \tag{21}$$

As a check on this sampling procedure, 100,000 values of x were chosen and the resulting cross section curve is compared to the exact result in Fig. 2.

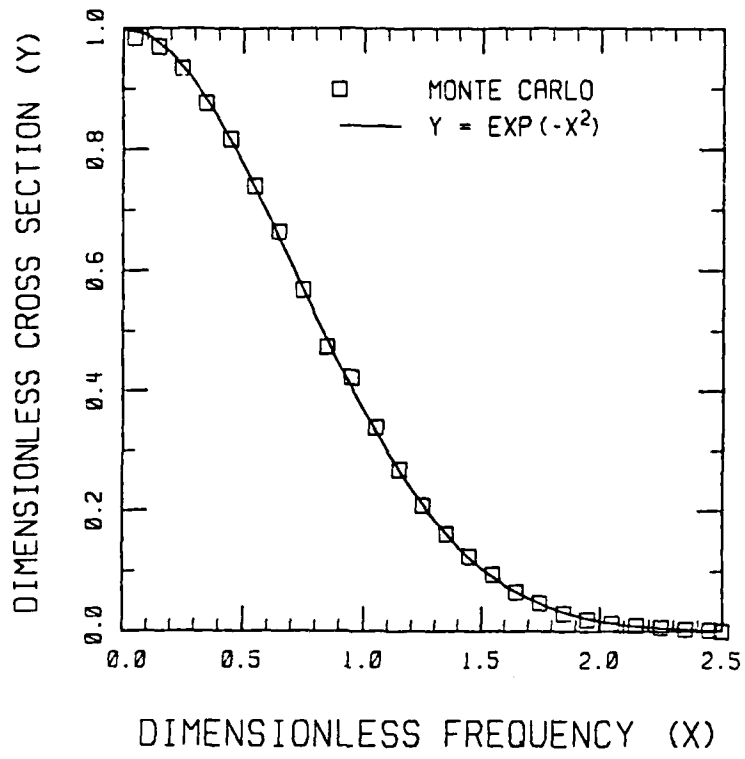

Figure 2. Comparison of Exact and Monte Carlo Sampled Doppler Profile.

2.6 Length of Photon Travel

The probability that a photon will travel an optical depth, x, is given by Beer's law,

$$P(x) = \exp(-x) \tag{22}$$

where $x = \rho\sigma z$. This distribution can be sampled through,

$$x = -\ln(\beta) \quad . \tag{23}$$

2.7 Integration Through Sublayers

For the homogeneous absorber concentration assumed in the initial version of NEMESIS the location of the photon after each emission event is given by,

$$z_f = z_i + \mu_z \frac{x}{\rho\sigma} \tag{24}$$

where z_f is the final location and z_i is the initial position. For an inhomogeneous absorber profile the final location is found from,

$$x = \int_{z_i}^{z_f} \frac{dz}{\mu_z} \rho(z)\sigma(z) \quad . \tag{25}$$

The photon is said to have escaped the upper atmosphere if either boundary, $z = 0$ or $z = z_o$, is reached before the equality is satisfied.

2.8 Event Distributions

The event distribution of most interest is the enhancement of the source excited state populations due to radiative trapping. Several weighting factors are utilized in the Monte Carlo simulation in order to compute this distribution. One is the local excited state number density, which as mentioned earlier arises because the upper atmosphere is uniformly sampled for the initial photon emission. This factor is defined by,

$$P_i^o = [M^*]_i \tag{26}$$

where $[M^*]_i$ is the source excited state concentration for the i'th sublayer given in Eq. (5). In the initial version of NEMESIS we actually use the normalized population, that is $[M^*]_i/[M_t]$, since the total concentration is assumed constant for each sublayer.

The other weighting factor is the probability of re-emission after each absorption event. This is given by,

$$w_i = \frac{k_3}{k_3 + k_2\rho_i} \tag{27}$$

and is simply the ratio of the radiative decay rate to the sum of the radiative and collisional quenching rates.

Before presenting the general formula for computing the enhanced distributions it is conceptually simpler to consider the example shown in Fig. 3. For this three sublayer atmosphere we wish to calculate the enhancement of the level 3 excited state population due to a trial photon started at level 1. Given the indicated trajectory of the photon the resulting enhancement is computed from,

$$\Delta P_3 = P_1^o(w_3 + w_3w_2w_3 + \cdots) \tag{28}$$

where it is seen that for this particular case there is no second order contribution because the photon resided in level 3 after the first and third scattering events.

The general enhancement formula is defined by,

$$w^k = w_{i(1)}w_{i(2)}\cdots w_{i(k)} \quad , \tag{29}$$

$$W_{ij} = W_{ij} + w^k \quad , \text{ and} \tag{30}$$

$$P_i = P_i^o + \sum_{j=1}^{NL} P_j^o \frac{W_{ij}}{N_j} \tag{31}$$

where NL is the number of sublayers and N_j is the total number of trial photons which originated from the j'th sublayer.

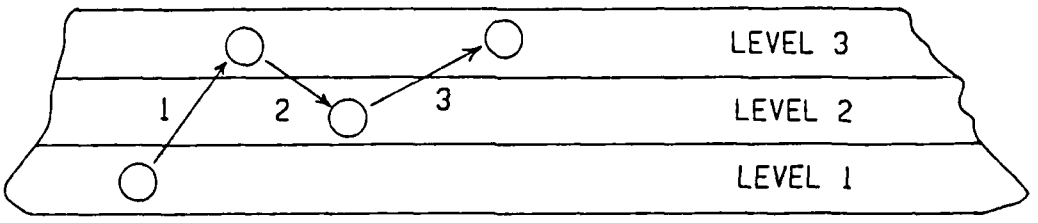

Figure 3. Sample Trajectory for a Photon Initiated in Level 1.

3. VALIDATION

The Monte Carlo simulation used in NEMESIS was validated through analogy to the problem of light scattering by clouds for which many exact and approximate solution methods have been developed. The basic assumptions used in NEMESIS, semi-infinite plane parallel geometry, homogeneous composition, finite optical thickness, characteristic single scattering albedo, and isotropic scattering, are formally equivalent to those typically made for the cloud scattering problem. A number of validation comparisons were made to different types of cloud scattering problems and include:

- 1-Dimensional scattering for which there is an exact analytical solution,[3]
- 3-Dimensional single scattering for which there is an exact analytical solution,[4]
- 3-Dimensional scattering with infinite optical thickness for which there is an exact numerical solution,[4] and
- 3-Dimensional scattering with finite optical depth for which there is an approximate solution.[5]

For each of the above comparisons the reflectance and transmittance of the cloud was determined as a function of optical thickness and single scattering albedo. In all cases the Monte Carlo results agreed with the exact or approximate solutions to within the inherent statistical uncertainty in the Monte Carlo method.

In order to simulate these various cloud scattering problems the source population distributions had to be appropriately chosen. The reflectance and transmittance results were then determined by two different methods.

---

3. D. Adamson, "The Role of Multiple Scattering in One-Dimensional Radiative Transfer," NASA TN-D-8084, NASA Langley Research Center Hampton, VA (December 1975).
4. S. Chandraskhar, "Radiative Transfer," Dover Pub., New York (1960).
5. R. E. Danielson, D. R. Moore, and H. C. van de Hulst, "Transfer of Visible Radiation Through Clouds," J. Atmos. Sci., 26, 1078 (1969).

3.1 Source Distributions

For a collimated light source both the 1-D and 3-D source functions are identical. This function is given by Beer's law,

$$P_i^o = \exp(-x_i/\mu) \tag{33}$$

where x_i is the optical depth at the center of the i'th layer determined with respect to the illuminated boundary (i.e., x = 0). The source distribution for a Lambertian light source is derived from Eq. (33) by integration over all illumination angles and weighting the integrand by "μ". The result is given by,

$$P_i^o = 2E_2(x_i) \tag{34}$$

where E_2 is the second exponential integral.

3.2 Reflectance and Transmittance Functions

The reflectance and transmittance of the external source can be determined from the Monte Carlo simulation by two methods, (1) the first method involves simply keeping track of the fraction of trial photons that are reflected and transmitted, and (2) the second method utilizes the enhanced excited state population distribution. For the first approach the reflectance is determined by,

$$R = \frac{x_o}{N_t} \sum_{N=1}^{N_t} P_{i(N)}^o \omega_o^{k(N)} \tag{35}$$

where x_0 is the total optical depth, N_t is the total number of trial photons, i(N) denotes the i'th layer for the initiation of the N'th trial photon, ω_0 is the single scattering albedo (not to be confused with the earlier use of this symbol for the band origin), and k(N) denotes the number of scattering events that occurred for the N'th photon before it

exited the cloud. Only photons which exit the cloud from the illuminated surface are included in the reflectance summation. This formula for computing the reflectance applies to all the above source functions. The transmittance is calculated in an equivalent manner by including only photons which passed through the cloud in the summation. The multiplicative factor, x_o, is included as a weighting factor to correct for the fact that photons are initiated uniformly within the cloud.

For the second approach the reflectance in the 1-D case is given by,

$$R = \frac{\omega_o}{2} \sum_{i=1}^{i_{max}} P_i \Delta x \exp(-x_i) \tag{36}$$

where P_i is the enhanced population (see Eq. (31)), and Δx is the thickness of the sublayers. The reflectance for the 3-D collimated and 3-D Lambertian sources is calculated from,

$$R = \frac{\omega_o}{2} \sum_{i=1}^{i_{max}} P_i \Delta E_2(x_i) \quad . \tag{37}$$

The transmittance for all three sources is determined simply by substitution of $x_o - x_i$ for x_i in the above equations.

3.3 Example Calculations

A comparison of the reflectance of a Lambertian source for a finite optical thickness cloud calculated by the Monte Carlo and an analytical approximation developed by Danielson, Moore and Van de Hulst[5] is shown in Fig. 4. The difference of about 1% between the two calculations is well within the accuracy of the analytical approximation. The Monte Carlo calculations were converged to better than 0.1%.

In order to get an approximate idea on the computational time required and accuracy expected for applying the Monte Carlo method to the NLTE atmospheric emission problem an appropriate test case was considered. The

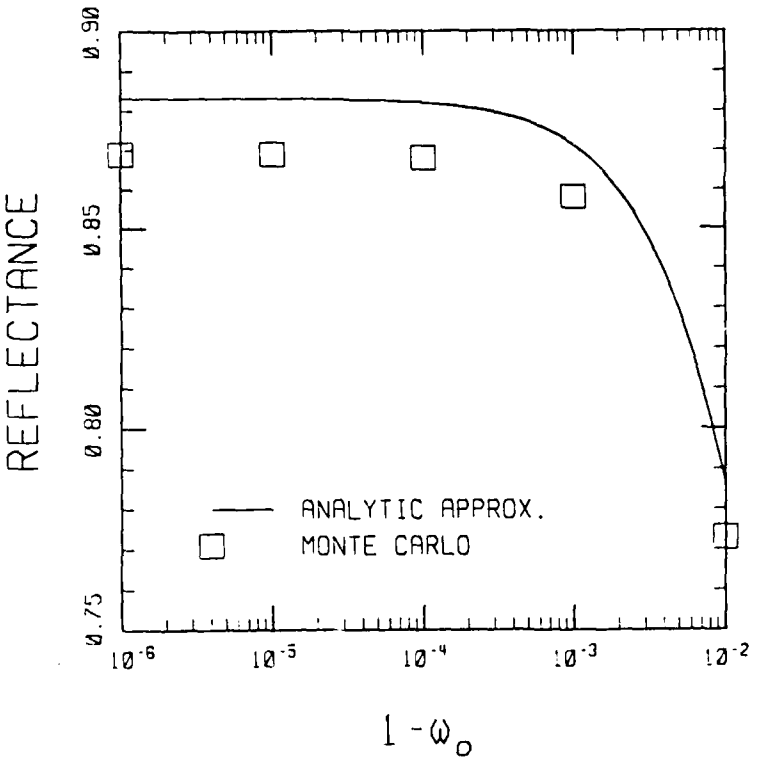

Figure 4. Comparison of Monte Carlo to Analytical Approximation for an Extended Lambertian Source.

values of the computational parameters were chosen to be representative of the 4.3 μm CO_2 band at 100 km altitude. A 10 km homogeneous layer was used and it was divided into 50 sublayers. The effective albedo for this case was 0.83. The total number of trial photons used was 10,000 and 60 orders of scattering were allowed before a given photon was terminated. The resulting excited state distribution is shown in Fig. 5. This computation required 1.43 min on an HP 9000 computer (this is comparable to a VAX 750). From the plot it can be estimated that the populations in each of the 50 sublayers are converged to better than 10%. This implies that line-of-sight emission calculations which integrate through a large number of sublayers will be even better converged, typically to around 1%. The relative statistical error in Monte Carlo simulations scales inversely with the square root of the number of trial photons. This means that one can

effectively trade CPU time for convergence. For the present example if 20% rather than 10% convergence for the sublayer populations was acceptable then 2,500 rather than 10,000 trial photons could have been used. This would result in a four fold decrease in CPU time.

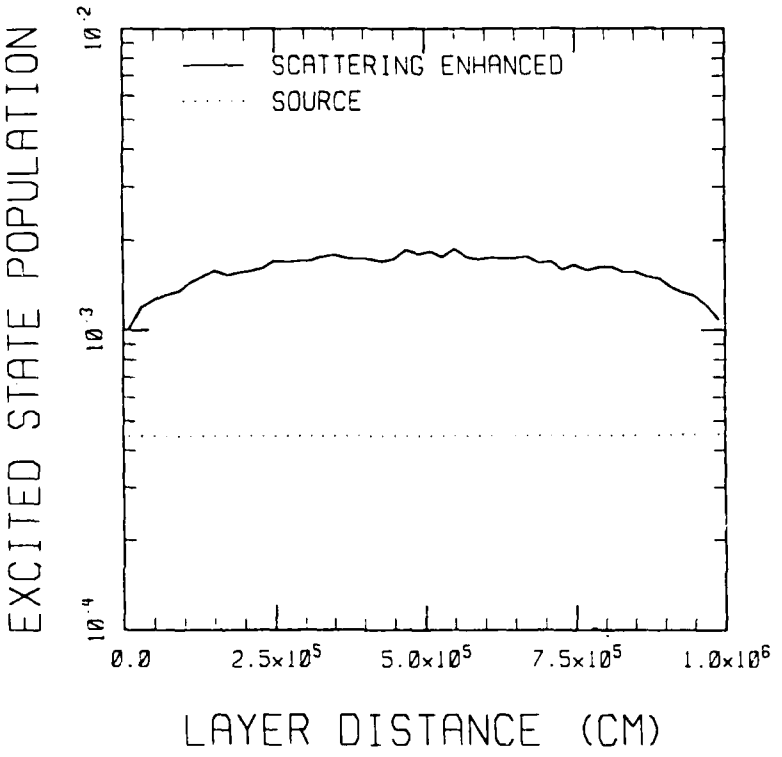

Figure 5. Enhancement of Excited State Populations for 4.3 μm CO_2 Band for 10 km Homogeneous Slab at 100 km Altitude and Day Light Conditions.

4. CODE OVERVIEW

The current, preliminary version of NEMESIS was developed to demonstrate the application of Monte Carlo simulation approach to the NLTE atmospheric emission problem. This initial version was designed as a stand alone program in order to simplify the initial development and validation. In order to fully integrate this code into the overall SHARC framework the following issues have to addressed:

- generalization from homogeneous to inhomogeneous sublayers, which involves using altitude dependent concentration profiles,
- incorporating the effects of energy transfer reactions on the radiative transfer, such as for the nearly resonant CO_2 (ν_3) and N_2 vibrational levels,
- consideration of the need, if any, to couple the kinetic and radiative codes and to run them in an iterative fashion,
- explicit inclusion of the direct solar and earthshine excitation rates into the kinetic code,
- generalization of the line strength distribution function, if required, and fitting of the distribution parameters to the AFGL Hitran compilation for each band of interest, and
- consideration of the most important upgrades, which include the Voigt line shape, and temperature dependent radiative transfer effects.

The initial version of NEMESIS utilizes five files. These include, (1) *nem.f* which is the source code and includes detailed input instructions on the first page of the listing, (2) nem.com which is the common block referred to in the "INCLUDE nem.com" statements, (3) nem.in which is the program input, (4) nem.out which is the output, and (5) nem.dat which is a data file used for plotting the enhanced and source populations. For completeness these files are included as appendices to this report.

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1. T. C. Degges and H. J. P. Smith, "A High Altitude Infrared Radiance Model," AFGL-TR-77-0271, Air Force Geophysics Laboratory, Hanscom AFB, MA, (30 November 1977) ADA059242

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