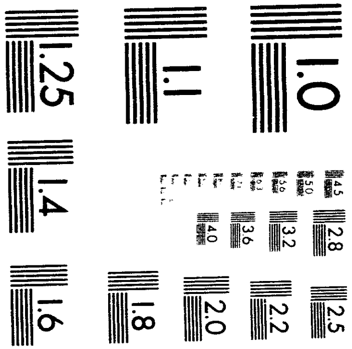
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PREPRINT

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A Correlated k-Distribution Model of the Heating Rates for Atmospheric Mixtures of H_2O, CO_2, O_3, CH_4, and N_2O in the 0-2500 cm^{-1} Wave Number Region at Altitudes Between 0 and 60 km.*

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I. INTRODUCTION

In a recent publication (Lacis and Oinas, 1991, "LO"), a method was described for treating transmission calculations in infrared radiative transfer problems for a vertically inhomogeneous atmosphere in which there is non-gray gaseous absorption. The method known as the correlated k-distribution utilizes a mapping of the opacity-frequency relation into an opacity-probility relation within a particular frequency interval. The probability variable g(k), the cumulative distribution function, is defined as

$$g(k) = \int_0^k f(k')dk', \qquad (1)$$

where f(k')dk' is the fraction of the frequency interval occupied by absorption coefficients between k' and k'+dk' (Goody *et al.*, 1989, "G2"). The limits of g(k) range between 0 and 1 within the frequency interval. The inverse of Equation 1, k(g), the k-distribution, has been shown by LO and G_2, to be a monotonic function across the frequency interval for a particular atmospheric layer. The calculation of the transmission can be expressed in the three physically equivalent forms:

$$\begin{aligned} T(u) - 1 / \Delta\upsilon\int_{\Delta\upsilon} \exp(-k_\upsilon u)d\upsilon, & \\ = \int_0^\infty f(k')\exp(k'u)dk', & \qquad (2) \\ = \int_0^1 \exp(-k(g)u)dg, & \end{aligned}$$

where u is the absorber column density. Using the k-distribution form, the calculation can be performed with far fewer k-g points than the same calculation using k-υ (frequency) points. Thus the k-distribution method has the potential of being a much more computationally efficient method of doing radiative transfer calculations within the earth's atmosphere when compared to line by line or narrow band models.

An accurate method of obtaining k-distributions has been used by G2 and Grant et al. (1992, "GGFP"). This method involves a direct line by line calculation of the opacity-frequency relation and a direct numerical sorting of this data to obtain f(k) and the k-distribution, k(g). The problem of flux and heating rate calculations for frequency intervals in which there are overlapping absorption features of different molecular species, can be addressed by the correlated k-distribution model. An overlapping technique which combines the individual k-distributions, k(g), for each species to obtain a combined k(g) function at each atmospheric level was outlined by G2. This overlapping model is compatible with the direct k-distribution formulation of GGFP.

The main purposes of this paper are to first, use the direct method of GGFP to calculate the transmission of the individual molecules H_2O, CO_2, O_3, CH_4, and N_2O, plus the transmission of a mixture of all these molecules. Second, to use the G2 model for overlapping k-distributions to calculate the transmission for the CH_4-N_2O and H_2O-CO_2 systems in the spectral regions in which there are overlapping absorption features. For the wavenumber interval 0-2500 cm^{-1} and altitude range of 0-60 km, a calculation of the atmospheric heating rates, upward fluxes, and downward fluxes will be made for each of the above cases and compared to line by line calculations.

II. THE K-DISTRIBUTION METHOD

The direct calculation of the molecular k-distributions contains the following steps. First the HITRAN91 database (Rothman et. al., 1991) is utilized to determine the line transitions and physical properties of the selected lines. Second, a modified version of the FASCODE2 code (Clough et. al., 1986) is used to calculate a finely gridded $(\Delta\upsilon(^1/_2)/4)$, set of monochromatic absorption coefficients, with full allowance for the overlap of neighboring lines, for each layer in the atmosphere. Third, a sorting code, ABSORT, is used to calculate the f(k), g(k), and k(g) functions for each homogeneous layer.

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The output from ABSORT is the 401 point k(g) relation for each layer.

At low pressures the k(g) curves can show opacity variations of up to five orders of magnitude at g values greater than ~0.9. This kind of behavior at low pressures is thought to be due to the absence of pressure broadening on the absorption lines in the wave number band; i.e. the lines are dominated by doppler broadening near line center. These variations in the k-distributions require a careful numerical integration strategy in the transmission expression, Equation 2, in order to accurately reproduce the k(g) functions. The integration strategy which was adopted after test calculations was an 85 point variable spaced trapezoidal model with g spacings of 0.0025 for g values between 0.9 and 1.0 and larger g spacings at lower g values.

III. OVERLAPPING SPECTRA K-DISTRIBUTION MODEL

Consider a spectral region over which two gases have overlapping but uncorrelated spectra. According to G_2 the opacity distribution function for the combined gas can be written as,

$$F_{12}(\tau)d\tau = f_{12}(k)dk, \qquad (3)$$

where τ is the optical depth defined by the relation, $d\tau = mdk$, k is the absorption coefficient, and m is the column density of the mixture;

$$F_{12}(\tau) = f_{12}(k)\,/\,m. \qquad (4)$$

G2 provides an expression giving the combined cumulative probability function G_{12} (t) in terms of the individual gas cumulative probability functions G_2 (t_1) and G_2 (t_2);

$$G_{12}(\tau) = \int_0^\tau G_1(\tau - \tau_2)dG_2(\tau_2), \qquad (5)$$

$$G(\tau) = \int_0^\tau F(\tau')d\tau', \qquad (6)$$

This framework allows two individual correlated k-distribution functions, k(g) or t (g), to be combined to obtain the k(g) or t (g) function for the mixture.

IV. PARAMETERS OF THE CALCULATIONS

The parameters of the calculations are;

1. McClatchey mid latitude, summer model atmosphere pressure-temperature distribution
2. Altitude resolution;
   a. 1 km, 0-20 km altitude,
   b. 2 km, 20-80 km altitude,
3. Ground temperature of 294 K,
4. Mixing ratios;
   a. CO_2 - 300 ppm, constant with altitude,
   b. CH_4 - 1.75 ppm constant with altitude,
   c. N_2O - 0.35 ppm constant with altitude,
   d. H_2O and O_3 mixing ratios as specified in the McClatchey model atmosphere, non uniform altitude distribution.
5. Wave number ranges;
   a. CH_4 and N_2O, 1100-1340 cm^{-1}, 20 and 40 cm-^{1} subintervals,
   b. O3, 500 - 900 cm^{-1}, 900-1200 cm^{-1}, 25 and 50 cm^{-1} subintervals,
   c. CO_2, 550 - 850 cm^{-1}, 840 - 1200 cm^{-1}, 2000 - 2520 cm^{-1}, 25 and 50 cm^{-1} subintervals,
   d. H_2O, 0 - 2500 cm^{-1}, 25 cm^{-1} subintervals,
   e. Molecular mixture of H_2O, CO_2, O3, CH_4, and N_2O, 0- 2500 cm^{-1}, 25 cm^{-1} subintervals.

V. RESULTS

Figure 1 shows the k(g) functions for H_2O in atmospheric layers at 1 mb (lower curve) and 945 mb (upper curve) in the wave number range 225-250 cm^{-1}. At a pressure of 1mb the spectra contains many narrow, Doppler broadened, high opacity line cores which cause the distribution function to have small but finite values at high k values. This causes the k(g) function to show a variation of approximately five orders of magnitude at g values greater than ~0.9. Note that the k(g) function for the 945 mb layer shows much less of a variation at the high g values. This is due to large pressure broadening effects on the lines. Figures 2 shows the heating rate, as a function of altitude, for the wavenumber range 0-2500 cm^{-1} for the complete mixture of gases. The correlated k-distribution is shown as a solid line. The GFDL line by line heating rates as published by Ridgeway et al. (1991) for the mid latitude summer atmosphere are shown by the dotted line. Agreement between these calculations is of the order of ten percent. Figure 3 shows the heating rate, as a function of altitude, for the wave number range 0-2500 cm^{-1} for the CO_2-H_2O overlap calculation. The solid line shows the heating rates for the overlap model and the dotted line shows the heating rates for a single gas combined mixture. Agreement between the two models is of the order of eight percent.

VI. ACKNOWLEDGEMENT

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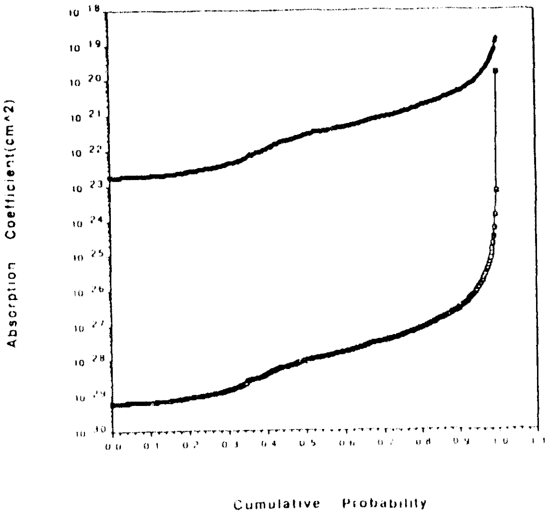

Figure 1. The H_2O k-distribution, k(g), for the wave number band 225-250 cm^{-1} at two atmospheric pressure levels P = 945 (upper curve) and1 mb (lower curve).

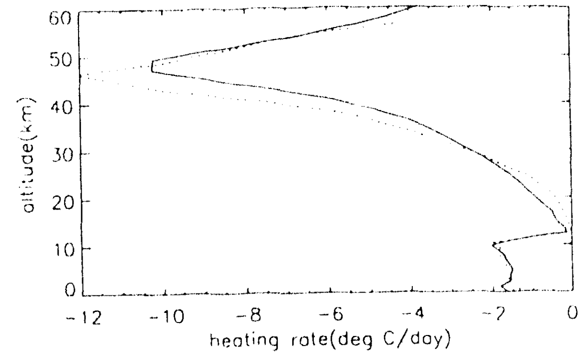

Figure 2. The altitude (km) variation of the heating rate (solid line) for the mixture in the wave number band 0-2500 cm^{-1} using a 25 cm^{-1} subinterval size. The dotted line is the GFDL line by line calculation given by Ridgway et. al. (1991).

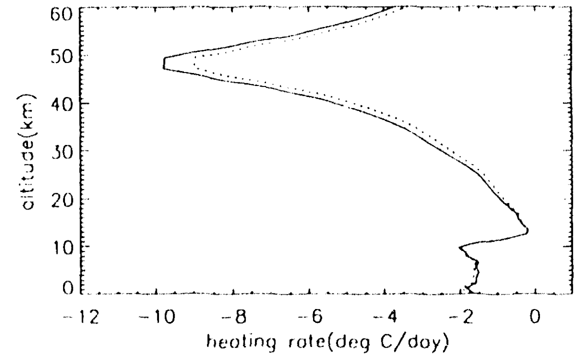

Figure 3. The altitude (km) variation of the heating rate (solid line) for the overlap model of H_2O-CO_2 in the wave number band 0-2500 cm^{-1} using a 25 cm^{-1} subinterval size. The dotted line represents the heating rate calculated using a single gas combined H_2O-CO_2 model.

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