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EVALUATION OF UPWELLING INFRARED RADIANCE FROM EARTH'S ATMOSPHERE

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Prepared for the
National Aeronautics and Space Administration
Langley Research Center
Hampton, Virginia

Under
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March - October 1975

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Dr. Henry G. Reichle, Technical Monitor
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Submitted by the
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FOREWORD

This report constitutes a part of the work completed during the Summer and Fall of 1975 on the research project entitled "Radiative Transfer Models for Nonhomogeneous Atmosphere." The work was supported by the NASA-Langley Research Center through Grant No. NSG-1153. The grant was monitored by Dr. Henry G. Reichle.

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EVALUATION OF UPWELLING INFRARED RADIANCE FROM EARTH'S TROPOSPHERE

by

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SUMMARY

Basic equations for calculating the upwelling atmospheric radiation are presented which account for various sources of radiation coming out at the top of the atmosphere. The theoretical formulation of the transmittance models (line-by-line and quasi-random band model) and the computational procedures used for the evaluation of the transmittance and radiance are discussed in detail. By employing the Lorentz line-by-line and quasi-random computer programs, model calculations were made to determine the upwelling radiance and signal change in the wave number interval of CO fundamental band. These results are useful in determining the effects of different interfering molecules, water vapor profiles, ground temperatures, and ground emittances on the upwelling radiance and signal change. This information is of vital importance in establishing the feasibility of measuring the concentrations of pollutants in the atmosphere from a gas filter correlation instrument flown on an aircraft or mounted on a satellite.

I. INTRODUCTION

The present status of knowledge about the fate of the relevant pollutants in the atmosphere is limited. Determination of the concentration of various atmospheric pollutants is important because of their considerable influence on the weather and environment.

The earth's surface with its temperature in the vicinity of 300°K emits like a black body from the near to the far infrared region of the spectrum. The emission in the near infrared (between 2 and 20 microns) is particularly important because most of the minor atmospheric constituents (i.e., CO_2, N_2O, H_2O, CO, CH_4, NH_3, etc.) absorb and emit in this spectral region. The upwelling infrared radiation from the earth's atmosphere, therefore, consists of the modulated surface radiation and the radiation from the atmosphere. This radiation carries the spectral signature of all the minor atmospheric constituents amongst which gases such as CO, CH_4 and NH_3 are called the atmospheric pollutants.

Detection of the atmospheric pollutants from infrared radiation measurements requires a detailed knowledge of the atmospheric constituents which absorb and emit significantly in the spectral range of interest. A systematic representation of the absorption and emission by a gas, in the infrared, requires the identification of the major infrared bands and evaluation of the line parameters of these bands. The line parameters depend upon the temperature, pressure, and concentration of the absorbing molecules and, in general, these quantities vary continuously along a nonhomogeneous path through the atmosphere. With the availability of high resolution spectrometers, it is now possible to determine the line positions, intensities, and half-widths of spectral lines quite accurately. As a result, the

line parameters of the strong infrared bands of most minor atmospheric constituents are now known quite well [1-3].

An accurate model for the spectral absorption coefficient is of vital importance in the calculations of the transmittance of an atmospheric constituent and in the correct formulation of the radiative flux equations which are employed in the reduction of data obtained from either direct or remote measurements. High spectral resolution measurements make it necessary to employ line-by-line models for data reduction. If, however, the integrated signals over a relatively wide spectral interval are measured, then one could employ an appropriate band model. The line models usually employed in the study of atmospheric radiation are Lorentz, Doppler, and combined Lorentz-Doppler (Voigt) line profiles. A complete formulation (and comparison) of the transmittance (and absorptance) by these lines, in an infinite and finite spectral interval, is given in [4-6]. The most appropriate band model for atmospheric application is the quasi-random model which is discussed in detail in this report.

Ludwig et al. [3] have explored the possibilities of measuring the amount of atmospheric pollutants through remote sensing. An important method of measuring the pollutant concentration by remote sensing is the passive mode (also called the nadir experiment) in which the earth-oriented detector receives the upwelling atmospheric radiation. The near infrared region is particularly suitable for passive mode measurements simply because the radiation in this region is practically free from the scattering effects. Radiation in the visible and ultra-violet regions is severely affected by the scattering processes which make meaningful passive mode measurements impossible.

The purpose of this study is to present a comprehensive analysis procedure for calculating the atmospheric transmittance and upwelling radiance in the wave number interval of CO fundamental band (between 2070 and 2220 cm^{-1}). For this purpose computer programs were developed by employing the Lorentz line-by-line model as well as the quasi-random narrow band model. The basic equations for calculating the upwelling atmospheric radiance are presented in Sec. II. The theoretical formulations of the transmittance by the two spectral models is given in Sec. III. Listings of the computer programs are provided in the Appendicies. By employing the line-by-line and quasi-random computer programs, model calculations were made to study the effects of different interfering molecules, water vapor profiles, ground temperatures, and ground emittances on the upwelling radiance. These are presented in Sec. IV.

II. UPWELLING ATMOSPHERIC RADIATION

As shown in Fig. 2.1, the radiation emergent from the atmosphere, $E(\omega)$, may be given by the expression [3,5]

$$E(\omega) = E_G(\omega) + E_R(\omega) + E_\phi(\omega) + E_{R\phi}(\omega) \tag{2.1}$$

where

$E_G(\omega)$ = thermal radiation emitted by underlying surface and atmosphere

$E_R(\omega)$ = incident solar radiation reflected by the surface

$E_\phi(\omega)$ = radiation scattered by single or multiple scattering processes in the atmosphere without having been reflected from the surface

$E_{R\phi}(\omega)$ = scattered energy which has undergone a reflection from the surface.

In general, these quantities are functions of surface temperature, atmospheric temperature, surface emittance, surface reflectance, sun zenith angle, scattering characteristics of particles, and transmittance of the atmosphere.

In the spectral region of infrared measurements, the effect of scattering is negligible. The incident solar radiation reflected by the surface, however, is important especially if the surface reflectance is assumed to be high (0.2 and higher).

Upon neglecting the scattering and solar radiation, the expression for thermal radiation emerging from a plane-parallel atmosphere can be written as

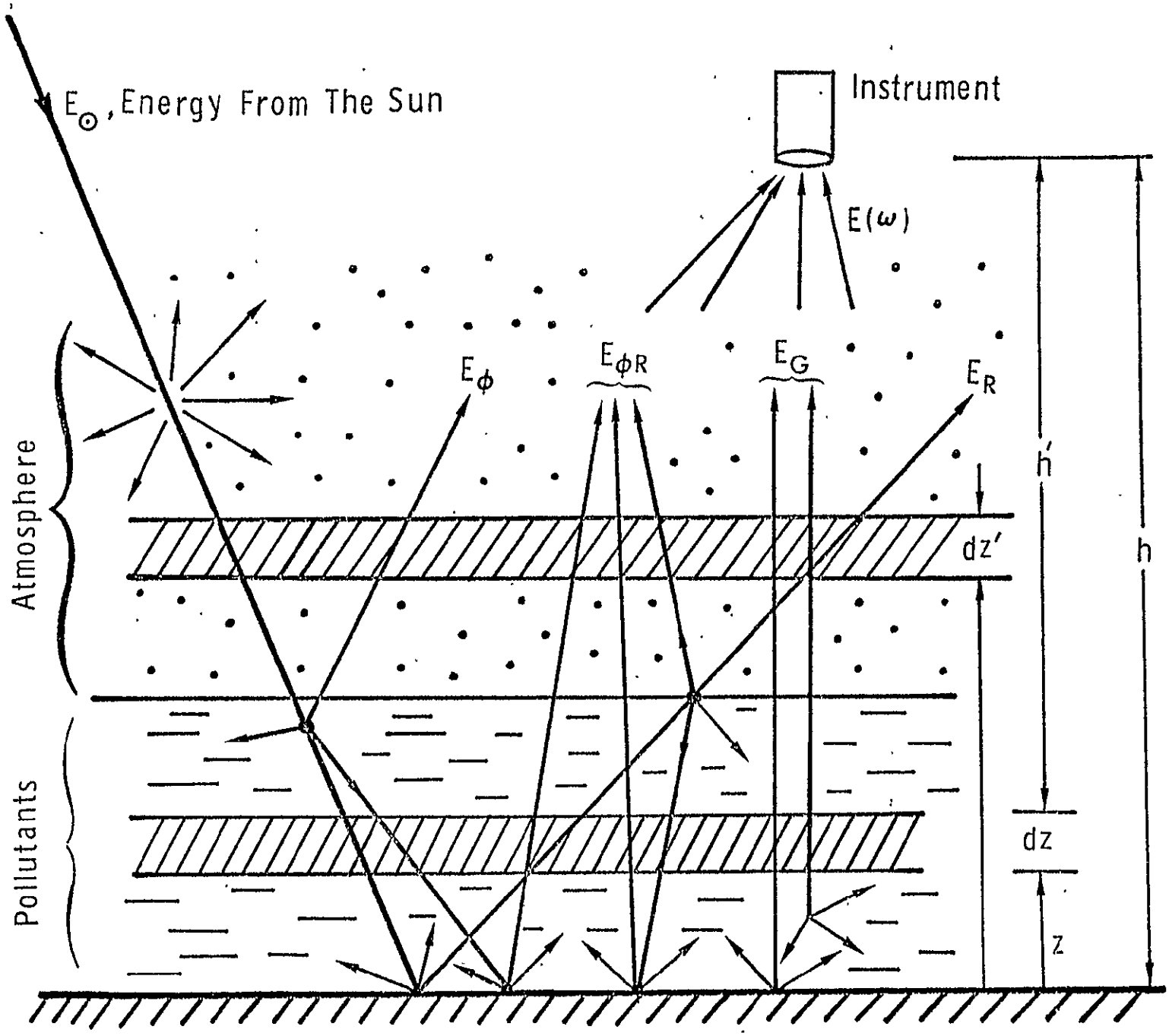

Fig. 2.1 Radiative energy received by an aircraft or satellite mounted instrument

$$E(\omega) = E_G(\omega) = \varepsilon(\omega)\ B(\omega,T_s)\ \tau(\omega,o) + \int_o^h B(\omega,T(z))\ [d\tau(\omega,z)/dz]dz \tag{2.2}$$

where $\varepsilon(\omega)$ is the surface emittance, $B(\omega,T)$ is the Plank's blackbody function, T_s is the surface temperature, $T(z)$ is the temperature at altitude z, and $\tau(\omega,z)$ is the monochromatic transmittance of the atmosphere. The first term on the right hand side of this equation represents the radiation from the surface while the second term is the radiation from the atmosphere.

The contribution from sunlight reflected from the surface becomes significant at shorter wavelengths. This contribution is given by the component $E_R(\omega)$ as

$$E_R(\omega) = (1/\pi)[1 - \varepsilon(\omega)]\ \cos\theta\ H_s(\omega)[\tau(\omega)]^{\zeta} \tag{2.3}$$

where θ is the sun zenith angle and $\zeta = 1 + f(\theta)$. Function $f(\theta) = \sec\theta$ for $o \leq \theta \leq 60°$ and equals to Ch θ for $\theta > 60°$ with Ch θ denoting the Chapman function. $H_s(\omega)$ is the sun irradiance on top of the atmosphere, and $\tau(\omega)$ is the transmission vertically through the atmosphere.

The expression for the transmittance $\tau(\omega,z)$ is obtained by employing an appropriate molecular (band or line) model, and, in general, this can be written as

$$\left.\begin{aligned} \tau(\omega,z) = \prod_i [\tau_i(\omega,z)] &= \exp[-\int_o^z \sum_i \beta_i(\omega,z')\ n_i(z')\ dz'] \\ &= \exp[-\int_o^z \sum_i \beta_i(\omega,z')\ C_i(z')\ P_t(z')\ dz']\ , \end{aligned}\right\} \tag{2.4}$$

where $\beta_i(\omega,z)$ is the extinction coefficient for species i (which is equal to the sum of absorption and scattering coefficients), $n_i(z)$ is the number density of the contributing molecules of species i in the optical path, $C_i(z)$ is the concentration of species i, and $P_t(z)$ is the total pressure. If scattering is neglected, then atmospheric transmittance can be expressed in a convenient form as

$$\tau(\omega,z) = \prod_i [\tau_i(\omega,z)] = \exp[-\int_o^x \sum_i \kappa_i^m(\omega,x') \rho_i(x') dx'] \tag{2.5}$$

where $\kappa_i^m(\omega,x')$ is the mass absorption coefficient for the ith absorbing gas, ρ_i is the mass density, and x is the depth of the level measured from the top of the atmosphere.

Upon introducing new definitions for the absorption coefficient and path length as [7,8]

$$\kappa(\omega) = \kappa^m(\omega) (\rho_r/P_g) , \tag{2.6}$$

$$du = P_g (\rho_g/\rho_r) dx , \tag{2.7}$$

Eq. (2.5) can be transformed into an alternate form as

$$\tau(\omega,z) = \exp[-\int_o^u \sum_i \kappa_i(\omega) du_i], \tag{2.8}$$

where P_g is the partial pressure and ρ_g is the mass density of the absorber, u is the optical path length in cm atm, and ρ_r is the absorber density corresponding to reference conditions (usually chosen as STP).

A combination of Eqs. (2.2) and (2.8) yields a relation for thermal radiation emerging from a plane-parallel atmosphere. This equation, with appropriate spectroscopic information, is used to obtain the concentration of

atmospheric pollutants from radiation measurements provided other governing parameters are known.

In actual calculations of atmospheric transmittance, the nonhomogeneous atmosphere is divided into a number of layers and for each layer an average value of pressure and temperature is assumed. With reference to Eq. (2.7), the pressure path length for each layer can be written as

$$du_{ij} = Q_{ij}(P_j/P_{NTP})(T_{NTP}/T_j)\ dx_j \ , \tag{2.9}$$

where Q_{ij} is the volume mixing ratio of the ith constituent in the jth layer, dx_j is the thickness of the jth layer, and P_j and T_j are the average pressure and temperature of the jth layer. Since the line intensity depends upon temperature and the line-width on temperature and pressure both, the absorption coefficient will be slightly different for different layers. Equation (2.8) can, therefore, be written as

$$\tau(\omega,z) = \exp\left[-\int_0^u \sum_j \sum_i \kappa_{ij}(\omega)\ du_{ij}\right] . \tag{2.10}$$

where $\sum_j$ indicates the summation over all the layers between the top and level z .

In general, the absorption coefficient for a single line centered at the wave number ω_n is given by

$$\kappa_{\omega n} = S_n\ f_n(\omega,\ \gamma_n) \ , \tag{2.11}$$

where S_n is the intensity of the nth spectral line and is given by

$$S_n = \int_{-\infty}^{\infty} \kappa_{\omega n}\ d(\omega-\omega_n) \ . \tag{2.12}$$

The line intensity may be described in terms of the molecular number density and Einstein coefficients, i.e., it depends upon the transition probabilities between the initial and final states and upon the populations of these states. For a perfect gas it may be shown that S_n is a function solely of temperature. The quantity $f_n(\omega, \gamma_n)$ is the line shape factor for the nth spectral line. It is a function of the wave number ω and the line half width γ_n and is normalized on $(\omega-\omega_n)$ such that

$$\int_{-\infty}^{\infty} f_n(\omega-\omega_n)\, d(\omega-\omega_n) = 1 \ . \tag{2.13}$$

Several approximate line profiles have been described in the literature. Most commonly used profiles are rectangular, triangular, Lorentz, Doppler, or Voigt (combined Lorentz and Doppler) profiles. Lorentz, Doppler, and Voigt profiles are of special interest in the atmospheric studies and these are discussed in detail in [4,6].

As indicated in Refs. [4,5,9], use of the Lorentz line profile is justified for radiative transfer analyses in earth's lower atmosphere. The shape factor, f_n, for the nth rotational Lorentz line is such that the absorption coefficient for species i can be written from Eq. (2.11) as

$$(\kappa_{ij})_n = S_n\, f_n(\omega,\gamma_n) = S_n\, \gamma_n/\{\pi[(\omega-\omega_n)^2 + \gamma_n^2]\} \ . \tag{2.14}$$

It should be emphasized here that the units for the absorption coefficient and the pressure path length, in Eqs. (2.6) and (2.7), are cm^{-1} - atm^{-1} and cm-atm respectively. In the case of water vapor, however, the path length is expressed in precipitable centimeters (pr - cm) a and the corresponding absorption coefficient in $(pr - cm)^{-1}$.

The total atmospheric transmittance is obtained by combining Eqs.(2.10) and (2.11) and integrating the resulting expression over the spectral range of interest. The exact procedure for calculating this, by employing the line-by-line and quasi-random band models, is discussed in the next section.

The total energy emergent from the atmosphere is obtained by integrating either Eq.(2.1) or (2.2) over the specified spectral interval $\Delta\omega$ as

$$E_D \approx E_{\Delta\omega} = \int_{\Delta\omega} E(\omega)\ d\omega \tag{2.15}$$

The procedure for calculating the upwelling radiance, by employing the line-by-line and quasi-random band model for the transmittance, is briefly discussed in Sec.IV.

III. EVALUATION OF ATMOSPHERIC TRANSMITTANCE

As pointed out earlier, an accurate model for the spectral absorption coefficient is essential in the calculation of atmospheric transmittance and in the correct formulation of the radiative flux equations which are used in the reduction of data obtained from either direct or remote measurements. While use of line-by-line models is essential in the data reduction of high spectral resolution measurements, an appropriate band model could be employed if integrated signals are measured over relatively wide spectral intervals. Several line-by-line and band models are available in the literature. In this section, the procedure for obtaining the atmospheric transmittance by employing the line-by-line model and the quasi-random band model is discussed.

3.1 Direct Integration (Line-By-Line Model)

A computer program has been developed to determine the atmospheric transmittance by employing the Lorentz line-by-line model. The procedure for computing the transmittance is presented here and a listing of the program is given in Appendix B. Explanation of the symbols used in the computer program is given in Appendix A. The procedure can easily be extended to incorporate other line profiles.

The direct integration method consists of calculating the absorption coefficient, and then the transmittance, at a large number of frequencies within the spectral range of interest. Since the absorption coefficient is a highly varying function of the frequency (varying by orders of magnitude over the width of a single line, which is often less than 1 cm^{-1}), it has to be evaluated at very closely spaced locations. The total absorption coefficient at any frequency location is made up of contributions from a large number of lines in the vicinity of that frequency. Some molecules

have thousands of lines in the spectral range of a particular band and the contribution from each one of these lines should be evaluated at each frequency location. It is, therefore, evident that the evaluation of the atmospheric transmittance with high accuracy is a time consuming task.

Since the absorption coefficient varies rapidly only in the vicinity of the line center, it should be evaluated at very close intervals near the line centers, while away from the line centers bigger intervals could be used without any serious loss of accuracy. Kunde and Maguire [8] and Drayson [9] have proposed a scheme for selecting the frequency locations for the calculation of absorption coefficients and transmittances. The scheme essentially consists of numerically evaluating the average transmittance over a narrow spectral interval by employing the Lengendre-Gauss quadrature formula [10]. The scheme employed in the present study is a modified form of the formulation presented in [8,9] where a different set of parameters are used. The choice of the parameters and the basic features of the computational scheme is discussed in the following subsections.

3.1.1 Spectral Divisions into Intervals and Subintervals

The entire frequency range of interest (usually the spectral interval of a particular vibration-rotation band) is first divided into a large number of rather narrow intervals $\Delta\omega$. Each of these $\Delta\omega$ intervals is then divided into a variable number k of subintervals depending upon the number of lines falling in that interval. The arrangements of spectral divisions are illustrated in Fig. 3.1. Two very narrow subintervals are created on each side of the line center and these are denoted in the computer program by ALX (see Appendix B). As shown in Fig. 3.1, an interval $\Delta\omega$ remains one subinterval if no line is present, but is divided into 6 or 11 subintervals in the presence of one or two lines respectively. For greater

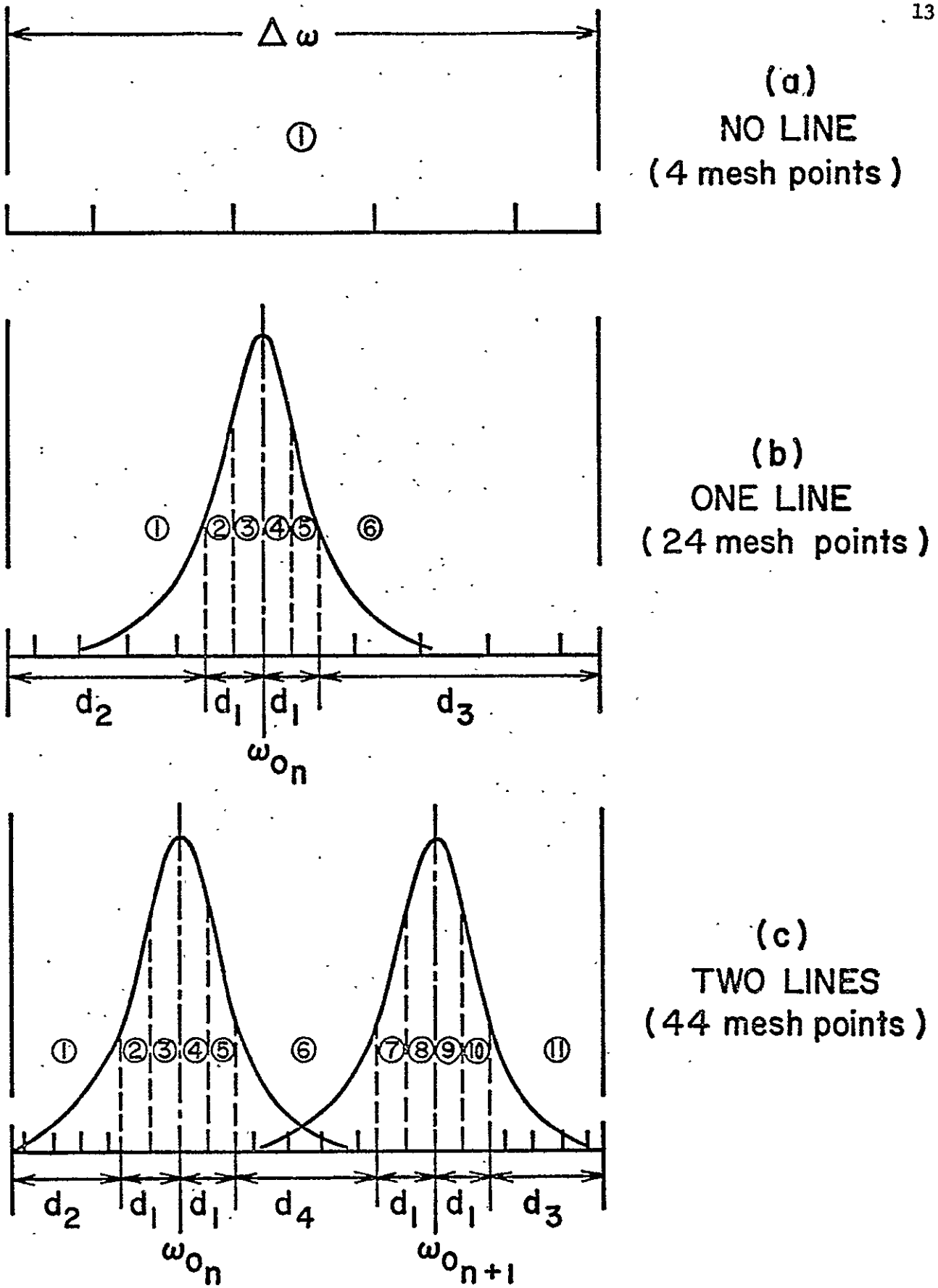

Fig. 3.1 Variable number of subintervals in a narrow interval $\Delta\omega$.

number of lines in the interval $\Delta\omega$, the number of subintervals will also be greater. Four frequency locations are then obtained within each subinterval by using the relation

$$\omega_{k\ell} = [(\omega_{Bk} - \omega_{Ak})/2]x_\ell + (\omega_{Bk} + \omega_{Ak})/2 \ , \tag{3.1}$$

where k refers to the kth subinterval ω_{BK} and ω_{AK} are the upper and lower frequency limits of the subinterval respectively, and x_ℓ are the abscissa values for the four point Gauss-Legendre quadrature formula [10].

3.1.2 Evaluation of Absorption Coefficients

The resultant magnitude of the absorption coefficient at the wave number location $\omega_{k\ell}$ is due to two separate contributions; (a) direct contribution and (b) wing contribution and is given by the equation

$$\kappa(\omega_{k\ell}) = \kappa^D(\omega_{k\ell}) + \kappa^W(\omega_{k\ell}) \ . \tag{3.2}$$

The contribution to the absorption coefficient from lines whose centers lie in close vicinity (on both sides) of the wave number under consideration is called the direct contribution and is obtained for Lorentz lines from Eq. (2.14) as

$$\kappa^D(\omega_{k\ell}) = \sum_n \kappa_n(\omega_{k\ell}) = \sum_n (S_n \gamma_n/\{\pi[(\omega-\omega_n)^2 + \gamma_n^2]\}) \tag{3.3}$$

where ω_n refers to the center of the nth contributing line. In the computer program, the range of direct contribution is denoted by DLIM. Thus, if $|(\omega-\omega_n)| \leq$ DLIM , the contribution is called the direct contribution and is evaluated by using Eq. (3.3).

The wing contribution to $\kappa(\omega_{k\ell})$ arises from lines located at wave numbers farther than DLIM from $\omega_{k\ell}$ (on both sides). The wave number range of the

wing contribution is denoted by WLIM and the absorption coefficient for this range is calculated from the equation

$$\kappa^{W}(\omega_{k\ell}) = \sum_{n} \kappa_{n}(\omega_{k\ell}) = \sum_{n} \{S_{n}\ \gamma_{n}/[\pi(\omega-\omega_{n})^{2}]\} \ , \tag{3.4}$$

only for the interval DLIM $< |(\omega-\omega_{n})| \leq$ WLIM . The contribution from the lines for which $|(\omega-\omega_{n})| >$ WLIM is found to be negligible. The range of WLIM is established by several trial calculations.

Since the number of lines between DLIM and WLIM (on each side) is very large, the wing contribution is not evaluated at each $\omega_{k\ell}$ individually. Instead, it is evaluated at the boundaries and the center of an interval. The values at all the $\omega_{k\ell}$'s within that interval is obtained by linear interpolation. As pointed out by Drayson [9], this procedure does not affect the accuracy of the results seriously.

Since S_{n} varies with temperature and γ_{n} varies with temperature as well as pressure, the nonhomogeneous atmosphere is divided into appropriate numbers of homogeneous slabs for the purpose of calculating the absorption coefficients and the atmospheric transmittances. For each slab (or layer) an average value of the temperature and pressure is assumed.

3.1.3 Optical Thickness and Transmittance

The path length of each homogeneous slab of a nonhomogeneous atmosphere is evaluated separately. For any constituent, the path length for the jth layer is found from either Eq. (2.7) or Eq. (2.9) to be

$$u_{j} = Q_{j}\ (P_{j}/P_{NTP})\ (T_{NTP}/T_{j})\ x_{j} \quad , \tag{3.5}$$

where x_{j} is the thickness of the jth layer.

The optical thickness of the jth layer at the wave number $\omega_{k\ell}$ is given by

$$\kappa(\omega_{k\ell})_j \; u_j \; , \tag{3.6}$$

and the total optical thickness for the atmosphere by

$$\sum_j [\kappa(\omega_{k\ell})_j \; u_j] \; . \tag{3.7}$$

For several absorbing species in the spectral range of interest, the total optical thickness is given by

$$\sum_j \sum_i [\kappa(\omega_{k\ell})_{ij} \; u_{ij}] \; , \tag{3.8}$$

where the summation over i constitutes the contribution of all the absorbing constituents.

The atmospheric transmittance at $\omega_{k\ell}$ can now be expressed by

$$\tau(\omega_{k\ell}) = \exp\{- \sum_j \sum_i [\kappa(\omega_{k\ell})_{ij} \; u_{ij}]\} \; , \tag{3.9}$$

where $\kappa(\omega_{k\ell})$ is given by Eq. (3.2).

The average transmittance over the interval $\Delta\omega$ is obtained from the equation

$$\bar{\tau}(\Delta\omega) = \{\sum_{k=1}^{k} [(\omega_{Bk}-\omega_{Ak})/2][\sum_{\ell=1}^{4} w_\ell \; \tau(\omega_{k\ell})]\}/\Delta\omega \; , \tag{3.10}$$

where the summation k extends over all the subintervals within the interval $\Delta\omega$, and w_ℓ's are the weight factors for the four point Gauss-Legendre quadrature formula [10].

3.1.4 Optimization of Spectral Parameters

The spectral parameters (such as $\Delta\omega$, ALX , DLIM , WLIM , etc.) entering in the numerical calculation of atmospheric transmittance are optimized for accuracy and for saving the computational time. Various

parameters are carefully chosen on the basis of considerable numerical experimentation. In a particular numerical scheme for calculation of the atmospheric transmittance, the choice of an optimized spectral parameter may slightly depend on the nature of the molecules under consideration (i.e. on the spectral distribution of the rotational lines). For the present study, spectral parameters were optimized by considering the CO spectral lines in the region 2070-2220 cm^{-1} and by assuming a uniform CO distribution of one part per million (1 ppm) by volume in the atmosphere from zero to ten kilometers.

As pointed out earlier, the entire spectral range of interest is first divided into a large number of narrow intervals $\Delta\omega$'s . In the computer program, this parameter is denoted by DEL (see Appendix B). By employing Eq. (3.10), the transmittance values were calculated for $\Delta\omega$ = DEL = 2.0, 1.0, and 0.5 cm^{-1} . These are given in Table 3.1 . It is seen that while the transmittance increases by about 0.1% when DEL decreases from 2.0 to 1.0 cm^{-1} , it decreases by about 0.03% when DEL goes from 1.0 to 0.5 cm^{-1} . This variation being significantly small, the intermediate value of $\Delta\omega$ = DEL = 1.0 cm^{-1} is chosen for the present study as opposed to the value of $\Delta\omega$ = 0.1 cm^{-1} used by Kunde and Maguire [8] .

The effect of varying the width of the subintervals near the line centers (denoted by ALX in the computer program) was also studied by numerical experimentation. Average transmittance values were calculated for ALX = 0.04, 0.02, and 0.01 cm^{-1} and these are listed in Table 3.1. Since there is no effect of changing the ALX values on the transmittance, a value of ALX = 0.03 cm^{-1} was selected simply because the subintervals on each side of the line center will cover a relatively larger portion of the important part of the line profile.

The effect of changing the value of DLIM on the average transmittance was found to be insignificant (see Table 3.1) and a value of DLIM = 5.5 cm^{-1} was selected for the present study in order to save computational time. The effect of changing the WLIM values was, however, found to be significant and a value of WLIM = 45.5 cm^{-1} was adapted. This value of WLIM maintains the general accuracy of the program and provides savings of computational time. It was not necessary to consider a WLIM value beyond 45.5 cm^{-1} in view of the expected small gain in accuracy.

TABLE 3.1

Average Atmospheric Transmittance from CO Fundamental Band as a Function of Various Spectral Parameters.

Spectral Parameter	Spectral Parameter Range (cm^{-1})	Average Transmittance (nondimensional)
	2.0	0.79605
DEL	1.0	0.79678
	0.5	0.79655
	0.04	0.79678
ALX	0.02	0.79678
	0.01	0.79678
DLIM	5.5	0.79678
	7.5	0.79679
	25.5	0.79678
WLIM	35.5	0.79655
	45.5	0.79644

In the literature [1-3], individual line widths are available for CO and H_2O lines while only the average values are available for CO_2, N_2O, and O_3 lines. For CO and H_2O, model calculations indicate that the mean transmittances obtained by using the average line widths are different than those obtained by using the individual line widths. For CO, a value of average transmittance of 0.83282 was obtained by using the average line widths while a value of 0.82834 was obtained when individual line widths were used. Similarly for H_2O, a value of $\bar{\tau}$ of 0.85563 was obtained for average line widths while a value of 0.86948 was obtained for individual line widths. In the results of model calculations (reported in the next section), individual line widths were used for CO and H_2O lines.

The computer program listed in Appendix B calculates the atmospheric transmittance in the spectral 2070-2220 cm^{-1}. This is the range of CO fundamental band. The program accounts for the contribution of the interfering molecules such as H_2O, CO_2, N_2O, and O_3. The program can easily be modified to calculate the atmospheric transmittance in any spectral range.

3.2 Quasi-Random Band Model

The use of narrow band models (such as Elsasser, statistical, random-Elsasser, and quasi-random) is justified if integrated signals are measured over relatively wide spectral intervals. The use of these models in transmittance calculations results in a considerable reduction in computational time. The results obtained from most of these models, however, usually lack the high accuracy needed in atmospheric transmittance calculations. The quasi-random model, introduced by Wyatt, Stull, and Plass [11], is probably the best model to represent the absorption of a vibration-rotation band quite accurately. Discussions on various band models are available in the literature [12-15]. The procedure for calculating the atmospheric transmittance by employing the quasi-random band model is discussed here in detail. A listing of the computer program is given in Appendix C and various symbols used in the program are explained in Appendix A.

The fundamental features of the quasi-random band model are discussed in references [7,11]. For this model, the entire band span, Δ , is divided into a number of small subintervals of equal spectral width δ . The average transmittance is first evaluated for each δ subinterval. The lines within each subinterval are assumed to be distributed randomly. The average transmittance over the entire spectral range (i.e., over the band pass) is obtained by arithmatically averaging of the transmittances of all subintervals.

The lines in a particular subinterval δ are divided into intensity subgroups. Reckoning from the intensity of the strongest line, five intensity groups (each spanning one decade) are created. Thus, lines whose intensities are within 10^{-5} times the intensity of the strongest line (in that group) are taken into consideration. It was suggested in [11] that the contribution from still weaker lines is negligible.

Since the line positions and intensities are assumed to vary within the narrow subintervals δ (rather than the entire band pass Δ), the results obtained from this model are expected to be better than other band models.

3.2.1 Evaluation of Average Transmittance

For a homogeneous path, the spectral transmittance at ω due to a line with center at ω_n is obtained by combining Eqs. (2.8) and (2.11) as

$$\tau(\omega) = \exp[-S_n \, u \, f_n(\omega,\gamma_n)] = \exp[-S_n \, u \, f(\omega,\omega_n)] \tag{3.11}$$

where the shape factor $f(\omega,\omega_n)$ for the Lorentz line profile is defined in Eq. (2.14).

For theoretical line shapes (i.e., for Lorentz, Doppler, and Voigt lines) the location of ω is symmetrical with respect to ω_n . Thus, the average transmittance of a line over δ can be evaluated in two ways: (a) keep ω_n at its fixed location and average $\tau(\omega)$ for location of ω varying over δ , (b) keep ω fixed at the center of the subinterval and average $\tau(\omega)$ for location of ω_n varying over δ . The second approach is adapted in the calculation of the average transmittance while using the quasi-random band model.

The average transmittance over δ due to a single spectral line may, therefore, be expressed by

$$\tau_n(\omega) = \frac{1}{\delta} \int_\delta \exp[-S_n \, u \, f(\omega,\omega_n)] \, d\omega_n \, , \tag{3.12}$$

where it should be noted that ω_n is the variable of integration.

If N is the number of lines in an intensity decade then the average transmittance due to all the lines in that decade, τ_d , is given by

$$\tau_d(\omega) = \{\frac{1}{\delta} \int_{\delta} \exp[-\bar{S}_n \; u \; f(\omega,\omega_n)] \; d\omega_n\}^N \; ,$$

where $\bar{S}_n$ is the average intensity of all the lines within the decade under consideration. It is assumed that the range of intensity in a decade is not large enough to cause any serious errors because of intensity averaging. A considerable saving in computational time is realized if the number of lines in each intensity decade is large.

The average transmittance due to all lines in the five intensity decades of the subinterval δ is given by

$$\tau_k(\omega) = \prod_{d=1}^{5} \tau_d(\omega) = \prod_{d=1}^{5} \{\frac{1}{\delta_k} \int_{\delta_k} \exp[-\bar{S}_n \; u \; f(\omega,\omega_n)] \; d\omega_n\} \; , \tag{3.13}$$

where subscript k represents the kth spectral subinterval (i.e., δ_k) of the total spectral interval Δ.

Equation (3.13) represents the transmittance due to the lines within δ_k. The wings of the lines in the adjacent subintervals also make a significant contribution to the absorption in δ_k. The resultant transmittance over the subinterval δ_k, therefore, is given by

$$\tau_k(\omega) = \tau_{k-k}(\omega) \prod_{\substack{j=1 \\ j \neq k}}^{K} \tau_{k-j}(\omega) \; , \tag{3.14}$$

where $\tau_{k-j}(\omega)$ represents the transmittance in δ_k due to lines in δ_j.

Large variations are observed between the transmittances of adjacent subintervals if the above procedure is employed directly. Wyatt, Stull and Plass [11] attributed this to the arbitrary locations of the subinterval boundaries and the resulting arbitrary distribution of lines between the subintervals. This spurious variation in transmittances is smoothed out by adapting the following procedure. (a) Divide the total spectral range Δ

(starting at Δ_o) into K subintervals with boundaries at Δ_o, $\Delta_o + \delta$, $\Delta_o + 2\delta$, ..., Δ_o $k\delta$ and centers at $\Delta_o + \frac{1}{2}\delta$, $\Delta_o + \frac{3}{2}\delta$, ... etc. Evaluate transmittances at the centers, i.e. at $\Delta_o + \frac{1}{2}\delta$, $\Delta_o + \frac{3}{2}\delta$, ... etc.

(b) Shift the spectral mesh of subintervals by $\delta/2$. The subinterval centers now lie at Δ_o, $\Delta_o + \delta$, $\Delta_o + 2\delta$, ..., etc. Evaluate transmittances at these shifted spectral locations. The resultant transmittances at the centers of original set of subintervals are obtained from these two sets by using the three point sliding average procedure. For subinterval between Δ_o and $\Delta_o + \delta$, the resultant transmittance at the center $\Delta_c = \Delta_o + \delta/2$ is given by

$$\bar{\tau}_k(\Delta_c) = \frac{1}{3}[\tau_k(\Delta_o) + \tau_k(\Delta_c) + \tau_k(\Delta_o + \delta)] \ . \tag{3.15}$$

The average transmittance for the entire range Δ is now expressed by

$$\bar{\tau}(\Delta) = \frac{1}{K}\sum_{k=1}^{K} \bar{\tau}_k(\omega) = \frac{1}{K}\sum_{k=1}^{K} \bar{\tau}_k(\Delta_c) \ . \tag{3.16}$$

From the above description, it is evident that the basic quantity to be evaluated is the average transmittance due to a single line over the subinterval δ. This is given by Eq. (3.12). Upon introducing the following change of variables

$$\left.\begin{aligned} y &= \omega_n - \omega_o - \delta/2 \ , && \text{(a)} \\ z &= \omega - \omega_o - \delta/2 \ , && \text{(b)} \\ \xi_n &= S_n \, u/(\pi \, \gamma_n) \ , && \text{(c)} \\ \rho &= 2\gamma_n/\delta \ , && \text{(d)} \\ \eta &= 2y/\delta \ , && \text{(e)} \\ \varepsilon &= 2z/\delta \ , && \text{(f)} \end{aligned}\right\} \tag{3.17}$$

Eq. (3.12) can be expressed for the Lorentz line shape as

$$\tau_n(\omega) = (1/2) \int_{-1}^{1} \exp\{-\rho^2 \xi_n/[(\varepsilon-\eta)^2 + \rho^2]\} \, d\eta \, . \tag{3.18}$$

For direct contribution (i.e., contribution to the transmittance due to lines in the same subinterval), $\varepsilon = o$ and the integrand in Eq. (3.18) is symmetrical about $\eta = o$. For this case, Eq. (3.18) reduces to

$$\tau_n(\omega) = \int_{o}^{1} \exp[-\rho^2 \xi_n/(\eta^2 + \rho^2)] \, d\eta \, . \tag{3.19}$$

For evaluating the wing contribution, it is assumed that $\rho^2 \ll (\varepsilon-\eta)^2$, and Eq. (3.18) reduces to

$$\tau_n(\omega) = (1/2) \int_{-1}^{1} \exp[-\rho^2 \xi_n/(\varepsilon-\eta)^2] \, d\eta \, . \tag{3.20}$$

The numerical procedures used for evaluating the integrals in Eqs. (3.19) and (3.20) are discussed in the next subsection.

3.2.2 Optimization of Integration Procedure and Parameters

The integrand in Eq. (3.19) is a strong function of η and, therefore, an accurate procedure for evaluating the integral is required. Wyatt, Stull and Plass [11] have obtained an analytical solution of Eq. (3.19). Following the procedure suggested by Young [16], Kunde [7] divided the range of integration (0-1) into seven subintervals as

$$\eta = 0.0,\ 0.001,\ 0.005,\ 0.01,\ 0.05,\ 0.1,\ 0.5,\ 1.0 \ ,$$

and used an eight point Gauss-Legendre quadrature formula for each subinterval.

In the present work, a much simpler scheme was used to evaluate Eq.(3.19). Twenty-six abscissa points were chosen in the interval (0-1) and suitable subintervals around them were created by a graphical experiment. Table 3.2 lists the abscissa values and the subintervals associated with them. The

integrand is evaluated at the twenty-six abscissa points, multiplied by the corresponding subinterval width, and the results are then summed. A comparison of results of this procedure with the results of ten subinterval ten-point Gauss-Legendre quadrature formula (for the same interval) revealed excellent agreement. It is, therefore, concluded that this procedure yields results of high accuracy.

The integrand in Eq.(3.20) is a slow varying function of η. Thus, a simple twenty-one point Simpson's rule quadrature formula was used to evaluate the integral instead of a ten-point Gauss-Legendre quadrature formula suggested by Kunde [7]. Accuracy checks were made on this quadrature scheme, and no appreciable differences were observed.

It should be emphasized here that the use of these simple quadrature schemes results in considerable reduction in computational time.

TABLE 3.2

Abscissa Points and Subintervals Selected to Evaluate the Direct Contribution.

Abscissa	Subinterval	Abscissa	Subinterval
0.0	0.0006	0.04	0.01
0.001	0.0006	0.05	0.01
0.0015	0.0006	0.06	0.015
0.002	0.0007	0.08	0.02
0.003	0.001	0.10	0.03
0.004	0.001	0.15	0.05
0.005	0.001	0.20	0.08
0.006	0.0015	0.30	0.10
0.008	0.002	0.40	0.10
0.01	0.003	0.50	0.10
0.015	0.005	0.60	0.15
0.02	0.008	0.80	0.20
0.03	0.01	1.00	0.10

The optimization of the computational parameters was carried out in a separate study by considering the CO spectral lines in the region 2070-2220 cm^{-1} and by assuming a uniform CO distribution of one part per million by volume.

Computations were made for four different values of the subinterval size δ . This is denoted in the computer program by DEL (see Appendix C). Average transmittances obtained for the entire range of CO fundamental band (between 2070-2220 cm^{-1}) are shown in Table 3.3 for the four subinterval sizes. An attempt was also made to compute the transmittance for DEL = 3 cm^{-1} but was eventually abandoned as the computational cost became too large. A value of DEL = 6 cm^{-1} was adapted for the present study simply because of the cost considerations. It was not considered necessary to go to even lower values of δ in order to gain slight accuracy at higher cost.

The number of adjacent subintervals (on each side of the main subinterval) contributing to the wing effects were also investigated. The results shown in Table 3.3 indicate that consideration of seven subintervals on each side yields sufficiently accurate results. It was not necessary to consider the influence of all neighboring subintervals in order to gain slight improvement (<0.02%) in the final result.

Since averaging of the line widths over each decade in every subinterval is unavoidable (because of the approximations in the basic formulation of the band model), no attempt was made to consider the individual line widths even for CO and H_2O lines. Average line widths for these molecules were found to have 10-15% standard deviation. The effect of using the average line widths on the overall transmittance is expected to be minimal.

TABLE 3.3

Average CO Fundamental Band Transmittance as a Function of Various Quasi-Random Band Model Computational Parameters

Parameters	Range	Average Transmittance (nondimensional)
DEL (cm^{-})	15	0.81664
	10	0.81523
	6	0.81183
	5	0.81050
Number of Intervals	4	0.81225
	7	0.81198
	8	0.81194
	10	0.81190
	all	0.81183

IV. MODEL CALCULATIONS

In order to establish the feasibility of measuring the average concentration of pollutants in the atmosphere (either from an aircraft mounted instrument or from satellites), it is essential to perform model calculations to evaluate upwelling radiance and signal change under physically realistic conditions. By using the appropriate line parameters and employing the Lorentz line-by-line model and quasi-random band model, upwelling radiance (and signal change) calculations were made in the spectral range of CO fundamental band (2070-2220 cm^{-1}). Results were obtained to study the effects of different interfering molecules, water vapor profiles, ground temperatures, and ground emittances on the upwelling radiance and the signal change. In this section, the procedure for calculating the upwelling radiance and signal change is briefly discussed, information regarding data sources is provided, and finally, the discussions of various results are presented.

4.1 Procedure for Calculating the Upwelling Radiance and Signal Change

In radiation modeling for pollution measurement in a nonhomogeneous atmosphere, the upwelling radiation is calculated by dividing the atmosphere into an appropriate number of sublayers. Each sublayer is assumed to be homogeneous in species concentration, temperature and pressure.

In a specified spectral interval in which a particular pollutant absorbs, the total energy emergent from the atmosphere is obtained from Eq.(2.15). If in this interval, n independent measurements (corresponding to the number of homogeneous layers) could be made to find E_{D1}, E_{D2},--- E_{Dn}, then the uniform concentration of the pollutant in each layer (and therefore the concentration profile in the actual atmosphere) could be determined from Eq.(2.15). Because of low concentrations of pollutants in the atmosphere, however, n such measurements are not feasible. Thus, only one independent

measurement is usually made and an average value of the particular pollutant concentration in the atmosphere is obtained. Even if only one value of the pollutant concentration can be obtained from an independent measurement, it is essential to divide the nonhomogeneous atmosphere into several homogeneous layers for the purpose of data reduction. This is because the pressure, temperature, and amount of interfering molecules vary in the atmosphere, and spectroscopic parameters and pressure path lengths are strong functions of these variables.

By employing the Lorentz line-by-line model for atmospheric transmittance, the upwelling radiance at the top of the atmosphere is obtained from Eq.(2.15) for each narrow spectral interval $\Delta\omega$. The exact procedure for doing this is to evaluate the average value of the Planck function for this interval first, then by using the mean value of the transmittance for the interval, Eq.(3.10), evaluate the upwelling radiance at the top of the atmosphere. The total upwelling radiance ($E = \Sigma E_{\Delta\omega}$) at the top of the atmosphere for the entire spectral range Δ is obtained by summing the radiances of individual intervals. As pointed out earlier, for the present study the spectral range of interest is the range of CO fundamental band. The computer program for calculating the upwelling radiance in this spectral range is given in Appendix B.

By employing the quasi-random band model, the total upwelling radiance at the top of the atmosphere can be evaluated from Eq.(2.15) in the following two ways.

(a) First calculate the integrated Planck function for the entire spectral range Δ . Then by using the value of average transmittance for the range Δ , obtain the net (integrated) radiance at the top of the atmosphere.

(b) Obtain the net (integrated) radiance at the top of the atmosphere for

each subinterval by calculating the Planck function and the average transmittance for that subinterval. Obtain the total radiance for the entire range Δ by summing the integrated radiances of each subinterval.

For the spectral range of CO fundamental band, total radiances at the top of the atmosphere were obtained by employing the above two procedures and these are 2.8102 E-05 and 2.8423 E-05 respectively. Procedure (b) was adapted for the present work because of its correctness in the formulation logic. Also, results obtained by this procedure were found to be in good agreement with the line-by-line results. A further simplification was introduced in procedure (b) in the final version of the computer program. Planck functions were calculated at the center frequency of each subinterval. This value was used as a mean for the subinterval rather than calculating it by integration over each δ . No difference in the final results was observed. This is because Planck function is a slow varying function of the frequency (especially within the spectral range of subinterval δ).

The signal change $SC = \Delta E$ (in watts/cm^2-sr) can be calculated by employing Eq.(2.15) as

$$SC = \Delta E = \int_{\Delta\omega} [E(\omega,\tau_o) - E(\omega,\tau_p)]d\omega \ , \tag{4.1}$$

where τ_o represents the transmittance of a "clean" atmosphere in which the pollutant concentration is zero, and τ_p refers to the transmittance of the atmosphere in the presence of the pollutant. The numerical procedure for evaluating Eq.(4.1) is identical to that described for calculating the upwelling atmospheric radiance.

4.2 Data and Data Sources

Upwelling radiances and signal change values were calculated in the spectral range of CO fundamental band. Contributions from the thermal

radiation and reflected sunlight terms in Eqs.(2.15) and (4.1) were taken into consideration while that from scattering terms were neglected. For the present study, the top of the atmosphere was considered to be 10 km which is approximately the top of the troposphere. For numerical calculations, this nonhomogeneous atmosphere was divided in 10 layers of equal thickness. The sun zenith angle was taken to be zero (overhead sun, $\theta = o$) for all calculations.

The data used in the present work were obtained from a number of well known sources and are considered to be highly reliable.

The atmospheric temperature and pressure profiles were adapted from the U. S. Standard Atmosphere, 1962 [17]. Distributions of infrared active species, such as H_2O, CO_2, N_2O, and O_3 were taken from McClatchey et al. [18]. Rotational and vibrational partition functions, needed to account for the temperature dependence of line strengths, were obtained from McClatchey et al. [2]. Table 4.1 shows the range of variation of some of these parameters. Values of the parameters listed in the table refer to the conditions at the boundaries of each layer. Mean values of the parameters in each layer (corresponding to the values at layer centers) were used in actual calculations. Carbon dioxide and nitrous oxide are assumed to be uniformly mixed in the atmosphere. For these gases, average values for the concentration used in the calculations are: CO_2 = 330 ppmV , and N_2O = 0.28 ppmV.

TABLE 4.1

Distribution of Pressure, Temperature, Water Vapor, and Ozone in the Earth's Troposphere

Altitude (km)	Temperature (°K) [Ref.17]	Pressure (mb) [Ref.17]	Water Vapor (ppmV) [Ref.18]	Ozone Conc. (ppmV) [Ref.18]
0	288.15	1013.25	7.756 E+3	2.663 E-2
1	281.65	898.76	6.068 E+3	2.936 E-2
2	275.15	795.01	4.637 E+3	3.239 E-2
3	268.66	701.21	3.187 E+3	3.321 E-2
4	262.17	616.60	2.162 E+3	3.391 E-2
5	255.68	540.68	1.399 E+3	3.691 E-2
6	249.19	472.18	9.268 E+2	4.118 E-2
7	242.70	411.05	5.731 E+2	4.914 E-2
8	236.22	356.52	3.676 E+2	5.973 E-2
9	229.73	308.01	1.586 E+2	9.181 E-2
10	223.25	265.00	7.008 E+1	1.315 E-1

Science Applications Incorporated (NASA-Contractor, responsible for the development of the non-dispersive correlation instrument for pollution measurement [3,19]) has compiled spectral line parameters (position, strength, width, and lower energy level) for lines of CO fundamental band and for lines of other molecules which interfere with the CO band. In the calculation of transmittances, these line parameters are directly read from a tape provided by SAI [19] to NASA-Langley.

Solar irradiances at the top of the atmosphere, at a few selected wave numbers, are also available from the SAI tape [19]. Values obtained from the tape, for the spectral range of present interest, are listed in Table 4.2. In the evaluation of contribution of the reflected solar radiation to the upwelling radiance, the solar irradiance for each spectral subinterval is obtained from a linear interpolation of values given in Table 4.2.

TABLE 4.2

Solar Irradiances at the Top of the Atmosphere
at Selected Wave Numbers

Wave Number (cm^{-1})	Solar Irradiance (watts cm^{-2} sr^{-1} $(cm^{-1})^{-1}$)
2061.86	0.307 E-6
2105.26	0.323 E-6
2150.54	0.330 E-6
2197.80	0.343 E-6
2247.19	0.359 E-6

4.3 Results of Model Calculations

By employing the Lorentz line-by-line and quasi-random band model for atmospheric transmittance, upwelling radiance and signal change were calculated for several illustrative cases. As indicated before, all calculations were made for the spectral range of CO fundamental band.

The results of integrated upwelling radiance at the top of the troposphere (i.e., at 10 km.) for different CO concentrations (uniformly distributed through the troposphere), in the presence of various interfering molecules, are illustrated in Fig. 4.1. The solid curves represent the results of the line-by-line model and broken curves for the quasi-random band model. As would be expected, the upwelling radiance E decreases with increasing CO concentration and with the inclusion of different interfering molecules. Inclusion of O_3 causes a slight decrease in radiance (not exceeding 0.5%) and it was difficult to illustrate this decrease in Fig. 4.1. The agreement between the line-by-line and the quasi-random band model results is seen to be excellent for the case of CO + H_2O. The slightly lower radiances for the next two cases is attributed to the over-estimation of absorption by the band model. The reason for this lies in the assumption of random distribution of many lines

(in the presence of interfering molecules) in the subintervals of the band model. In the actual spectra, however, the lines are more closely spaced in some regions than in others. The reason for slightly higher radiance values, with the band model for the case of pure CO atmosphere (where relatively small number of lines are present), is not clear at this time. The variation in the signal change, ΔE , with the CO concentration is illustrated in Fig. 4.2. These results follow the general trend of the results presented in Fig. 4.1.

The influence of different amounts of water vapor on the upwelling radiance and the signal change is shown in Figs. 4.3 and 4.4 respectively. Increased water vapor concentration results in increased absorption in the atmosphere. This, in turn, results in lower values for upwelling radiance and signal change. It should be noted that the effect of CO concentration on the signal change would be relatively small in the presence of larger quantity of water vapor.

Figures 4.5 and 4.6 show the upwelling radiances and signal changes for surface temperatures of 280, 290, and 300 °K and a surface emittance of 0.8. The strong dependence of the upwelling radiance and signal change on the surface temperature is obvious from these results. The relatively lower radiance values obtained with the band model are indicative of slight over-estimation of absorption by this model.

Figure 4.7 shows the variation of upwelling radiance for three different values of surface emittance and for a surface temperature of 288 °K. As explained earlier, the radiances obtained from the band model are lower than the line-by-line model because of overestimation of absorption by the band model. The relative increase of the difference for the lower ε-values is due to lower total emission from the earth for the small values of surface

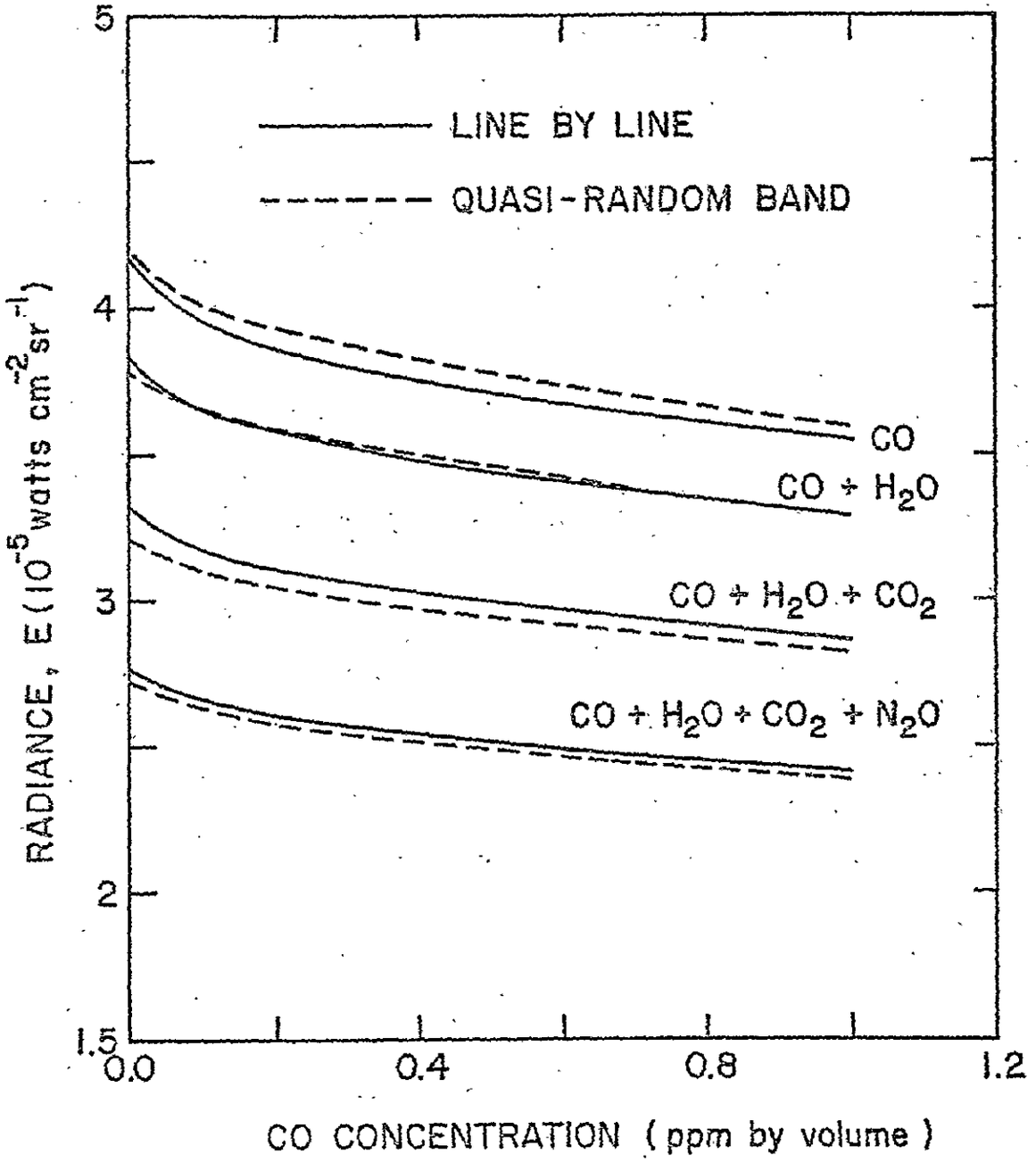

Fig. 4.1 Upwelling radiance as a function of CO concentration in the presence of interfering molecules, $T_s = 288°K$, $\varepsilon = 0.8$.

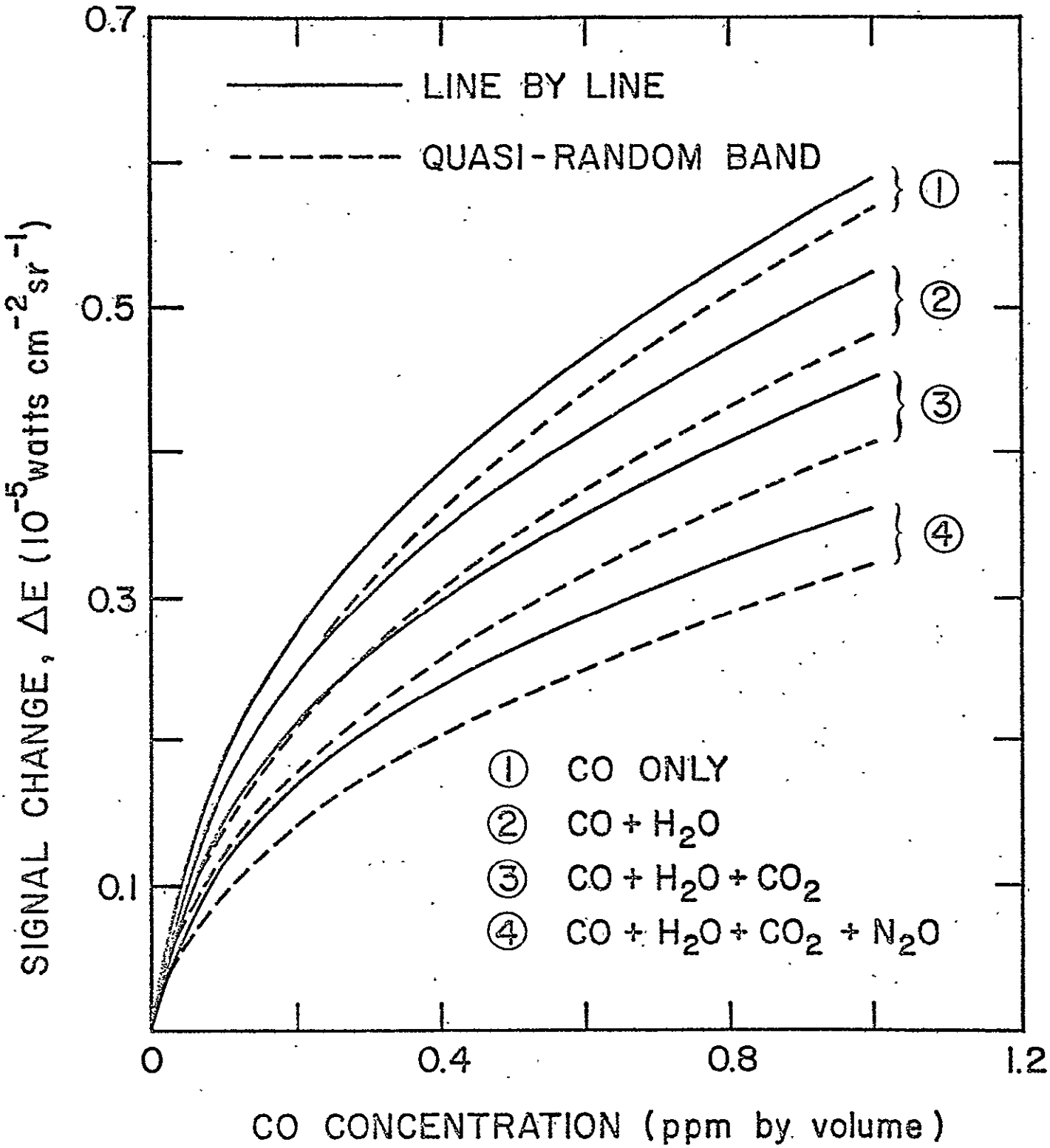

Fig. 4.2 Signal change as a function of CO concentration in the presence of different interfering molecules, $T_s = 288°K$, $\varepsilon = 0.8$.

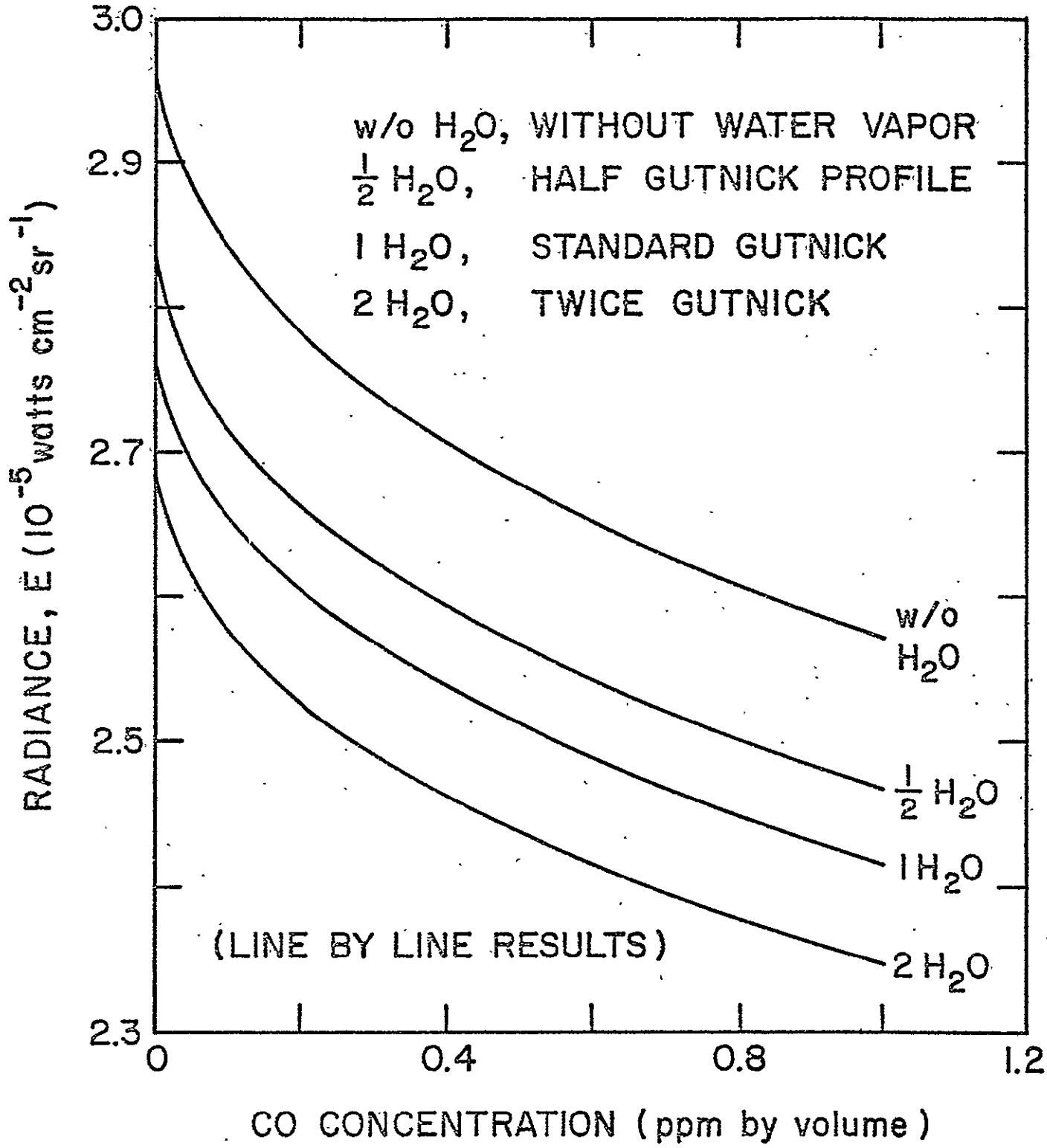

Fig. 4.3 Upwelling radiance as a function of CO concentration for different water vapor profiles, $T_s = 288°K$, $\varepsilon = 0.8$.

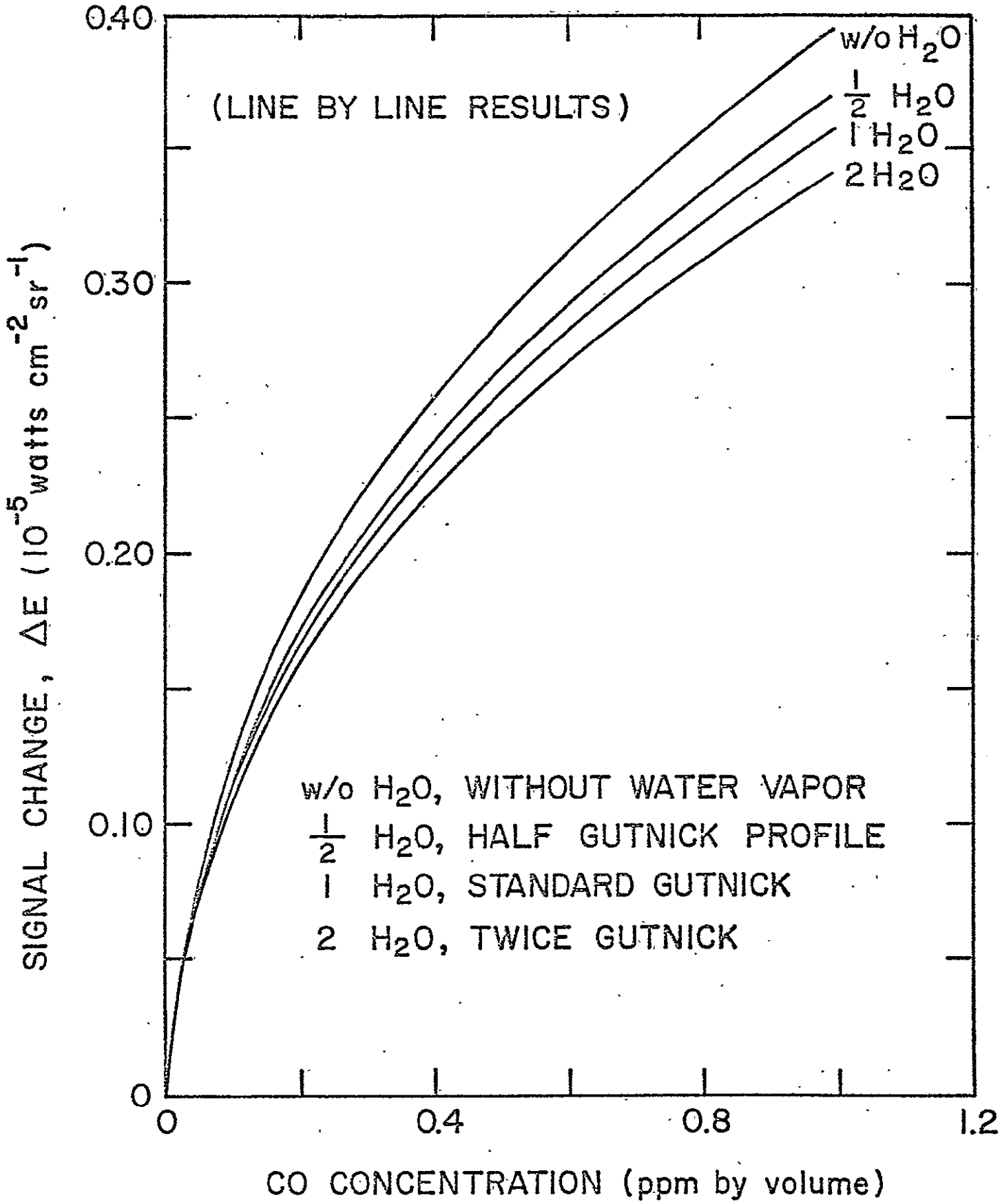

Fig. 4.4 Effects of water vapor concentration on the signal change $T_s = 288°K$, $\varepsilon = 0.8$.

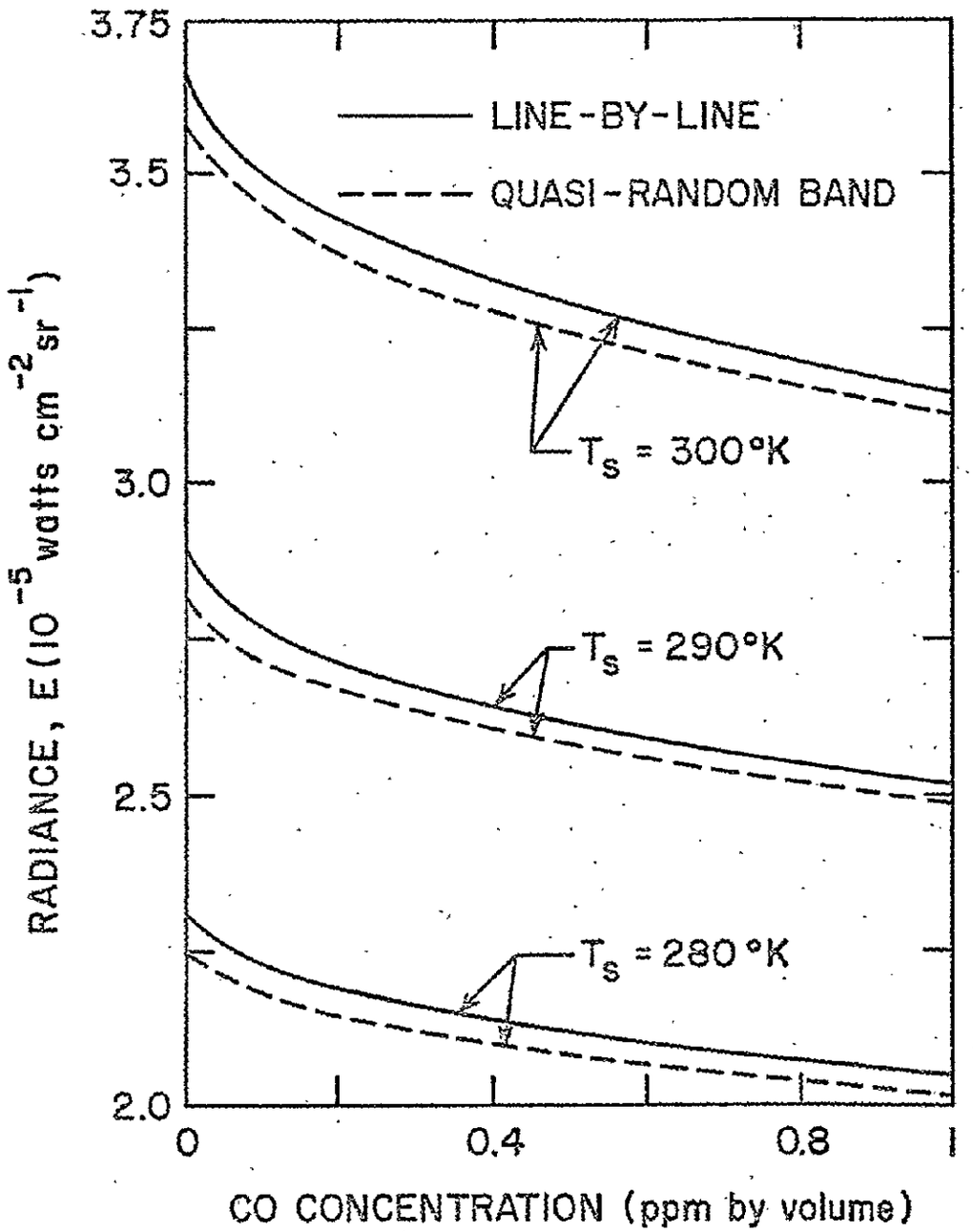

Fig. 4.5 Upwelling radiance as a function of CO concentration for three different surface temperatures (surface emittance $\varepsilon = 0.8$).

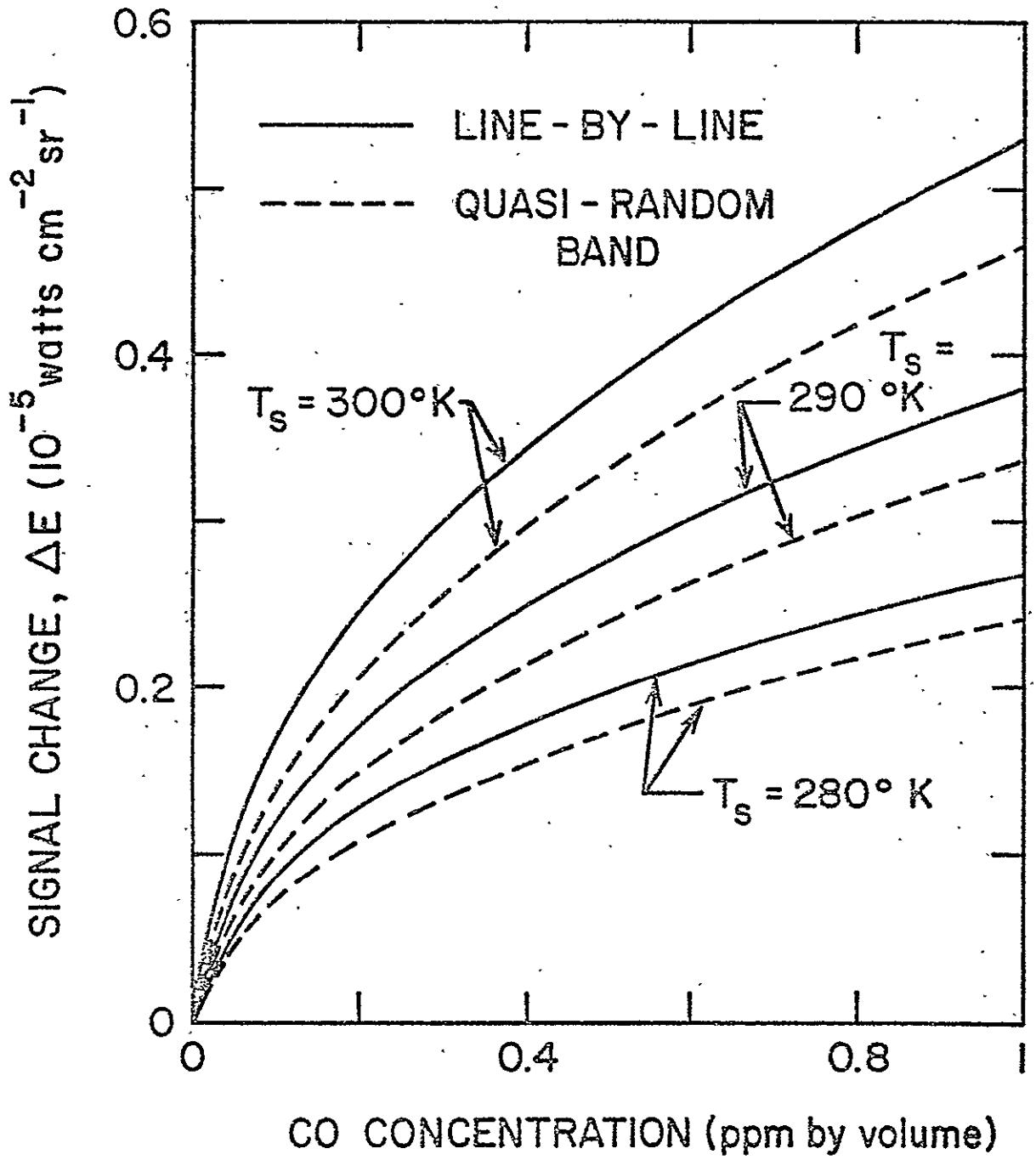

Fig. 4.6 Signal change as a function of CO concentration for three different surface temperatures (surface emittance = 0.8).

emittance. In these cases, therefore, the increased absorption by the band model has a greater relative effect on the radiance. Figure 4.8 shows the signal change for the cases considered in Fig. 4.7 and the results indicate the same general trend.

Figure 4.9 shows the variation of the upwelling radiance with the surface temperature for a fixed concentration of CO (1 ppm by volume) in the atmosphere and for $\varepsilon = 0.8$. The strong dependence of radiance on the surface temperature may be easily explained on the basis of the Stefan's law. However, because of the interference from the infrared active atmospheric molecules, the results obtained here do not exhibit an exact fourth power relationship.

Figure 4.10 shows the variation of radiance with the surface emittance for a fixed CO concentration (1 ppm by volume) and $T_s = 288$ °K. As would be expected, the results indicate the linear dependence of radiance on the surface emittance. Similar results were obtained in reference [3] for different values of the surface temperature and the sun zenith angle. In general, the ground emittance varies with the wave number. However, for the spectral range of CO fundamental band, it was shown in reference [20] that the radiance is not influenced by a significant amount when the wave number dependent ground emittance is replaced by an averaged value.

Figure 4.11 shows a comparison of the results obtained from the present line-by-line program (given the name LINBLIN) and another line-by-line program (called POLAYER) developed by the Science Applications Inc. [19]. In computing the total absorption coefficient at any wave number, the present program considers contributions from all the lines up to a fixed wave number location (on both sides) of 45.5 cm^{-1} from the wave number under consideration. This value of 45.5 cm^{-1} for the so-called wing effect was chosen after several numerical experimentations. The POLAYER, on the other hand, considers the effect of a fixed number of 20 lines on each side of the wave number under

consideration. This causes the range of wing effect to change depending upon the density of lines in the spectrum. Thus, in some cases, POLAYER will not consider the influence of lines which are only 1 cm^{-1} away from the wave number under consideration. This, of course, will result in underestimation of absorption. This, at least in part, is responsible for the higher integrated radiance obtained from the POLAYER program. The difference between the signal change curves, shown in Fig. 4.12, follows from the difference in the radiance values.

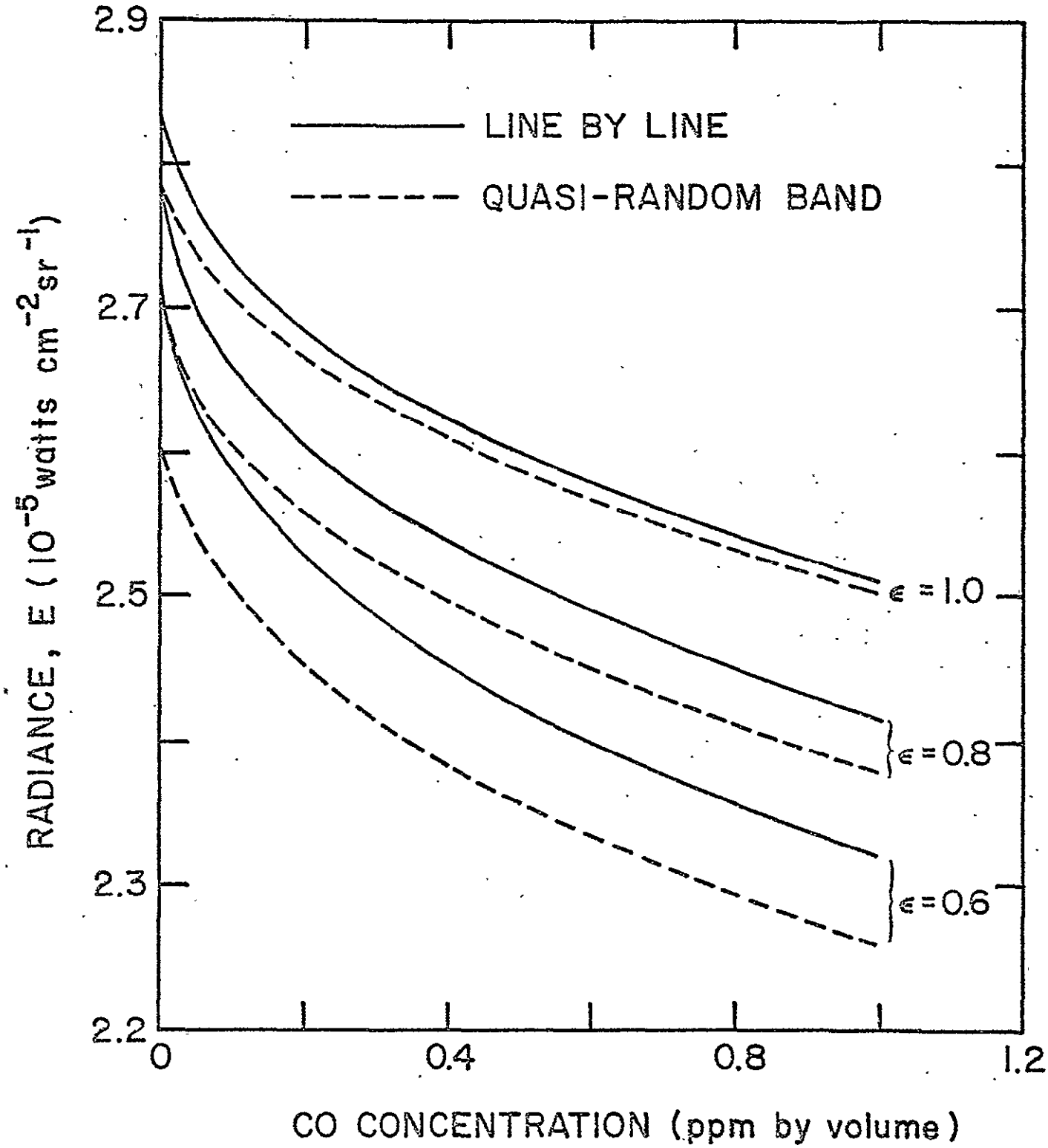

Fig. 4.7 Upwelling radiance as a function of CO concentration for three different surface emittances, $T_s = 288°K$.

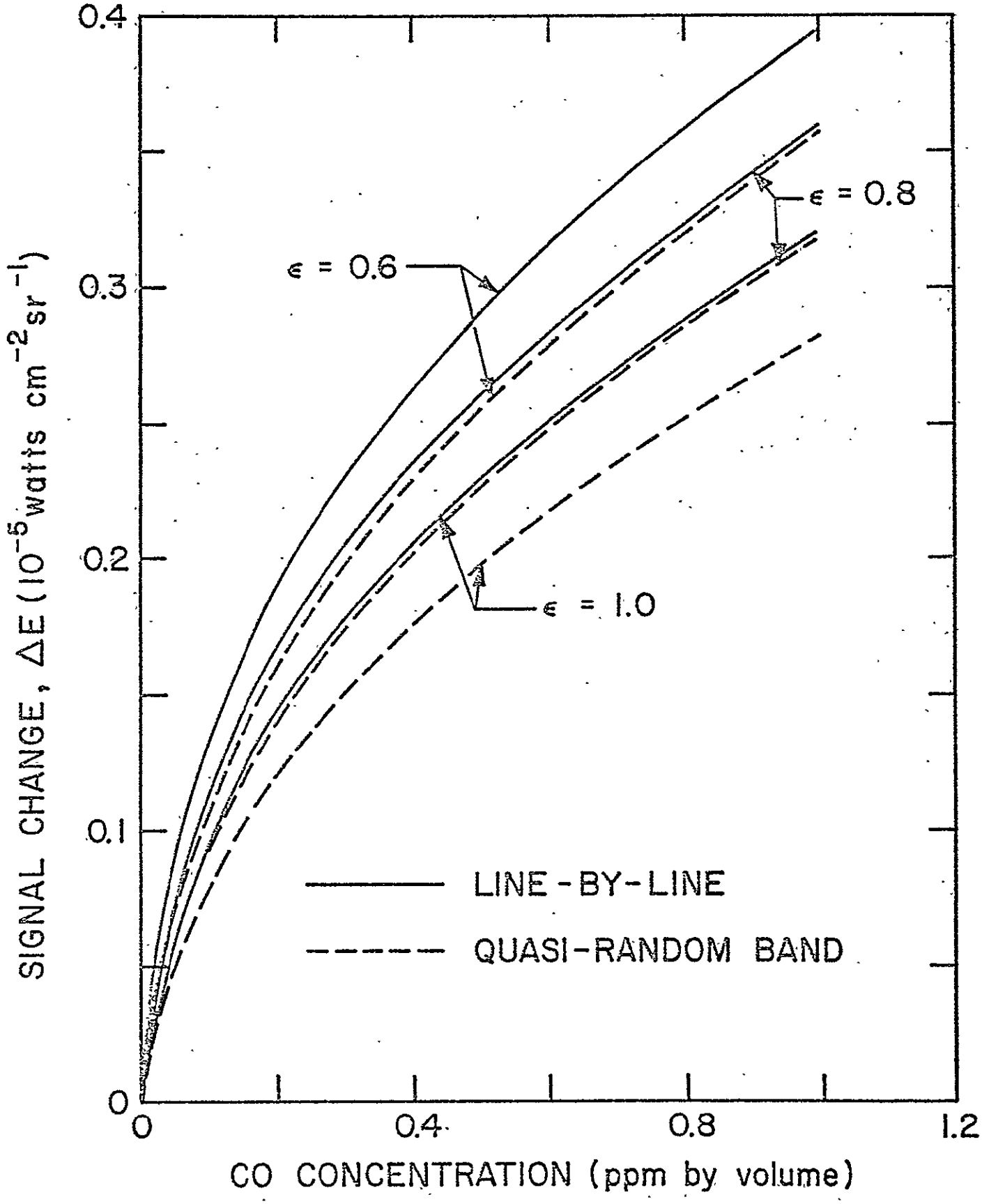

Fig. 4.8 Signal change as a function of CO concentration for three different surface emittances, $T_s = 288°K$.

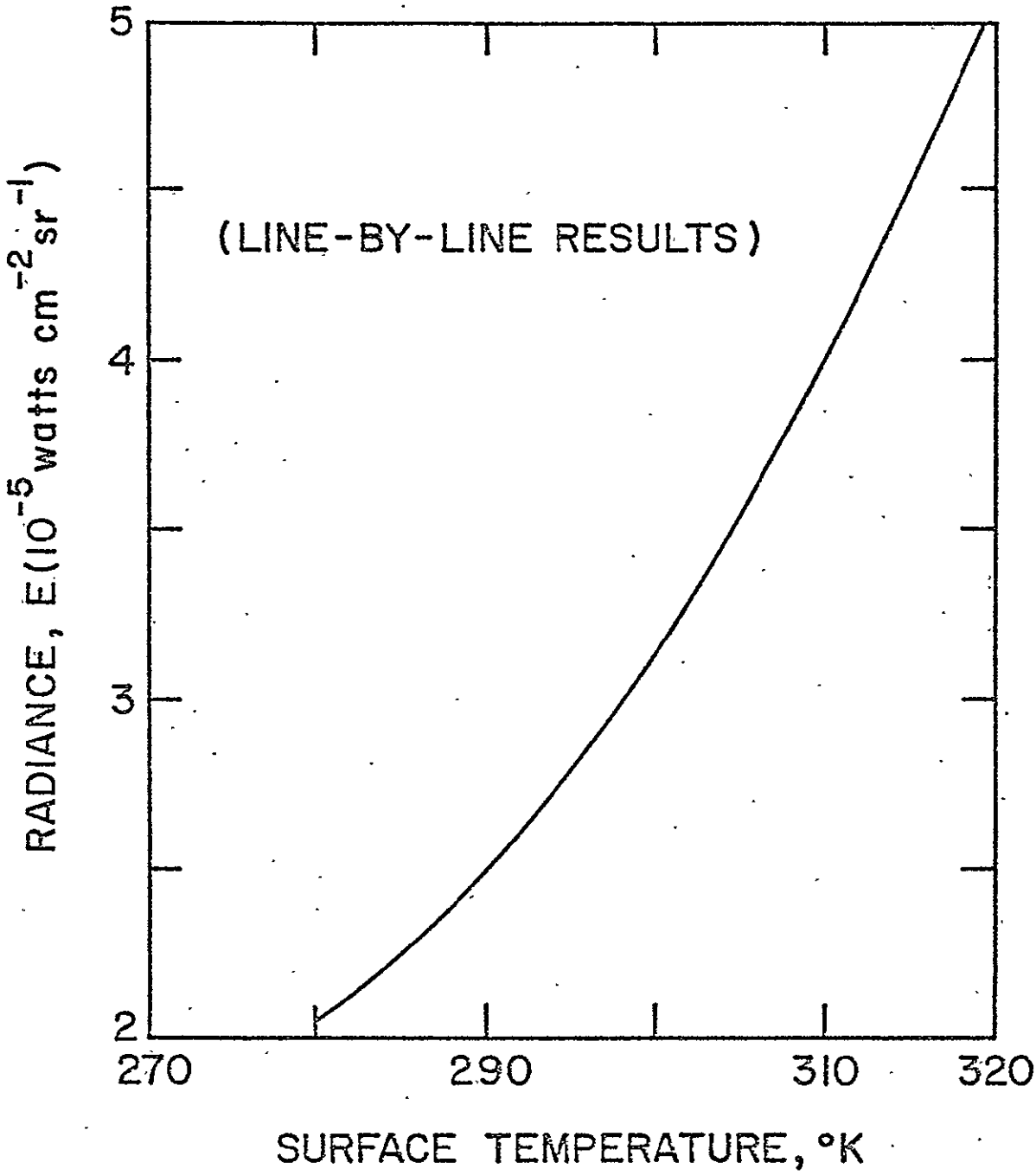

Fig. 4.9 Upwelling radiance as a function of surface temperature for a fixed CO concentration (1 ppm by volume), $\varepsilon = 0.8$.

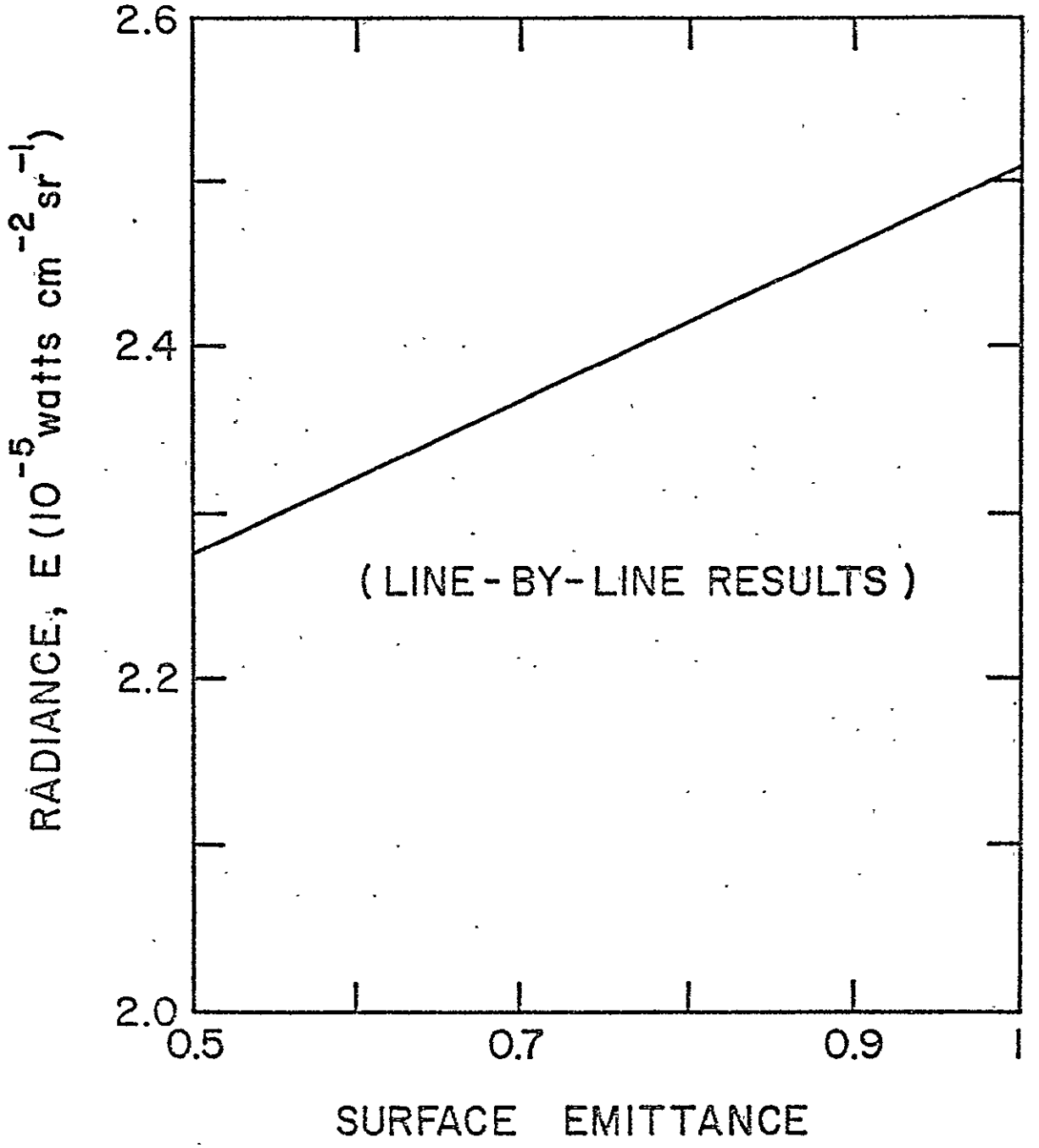

Fig. 4.10 Upwelling radiance as a function of surface emittance for a fixed CO concentration (1 ppm by volume), T_s = 288°K .

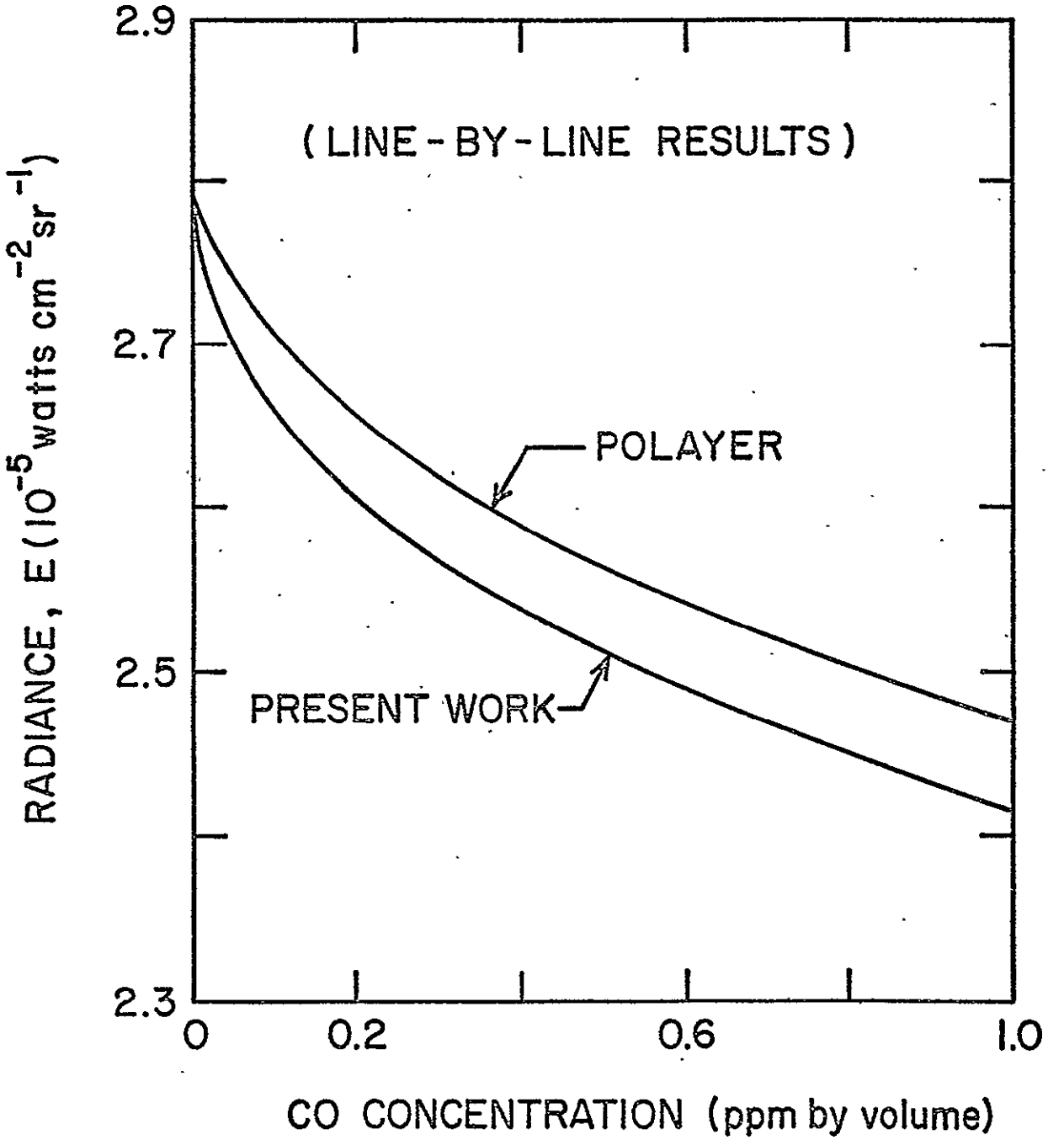

Fig. 4.11 Comparison of upwelling radiance obtained from POLAYER program and the present LINBLIN program, T_s = 288°K , ε = 0.8. On the average, LINBLIN values are 2% lower than POLAYER values.

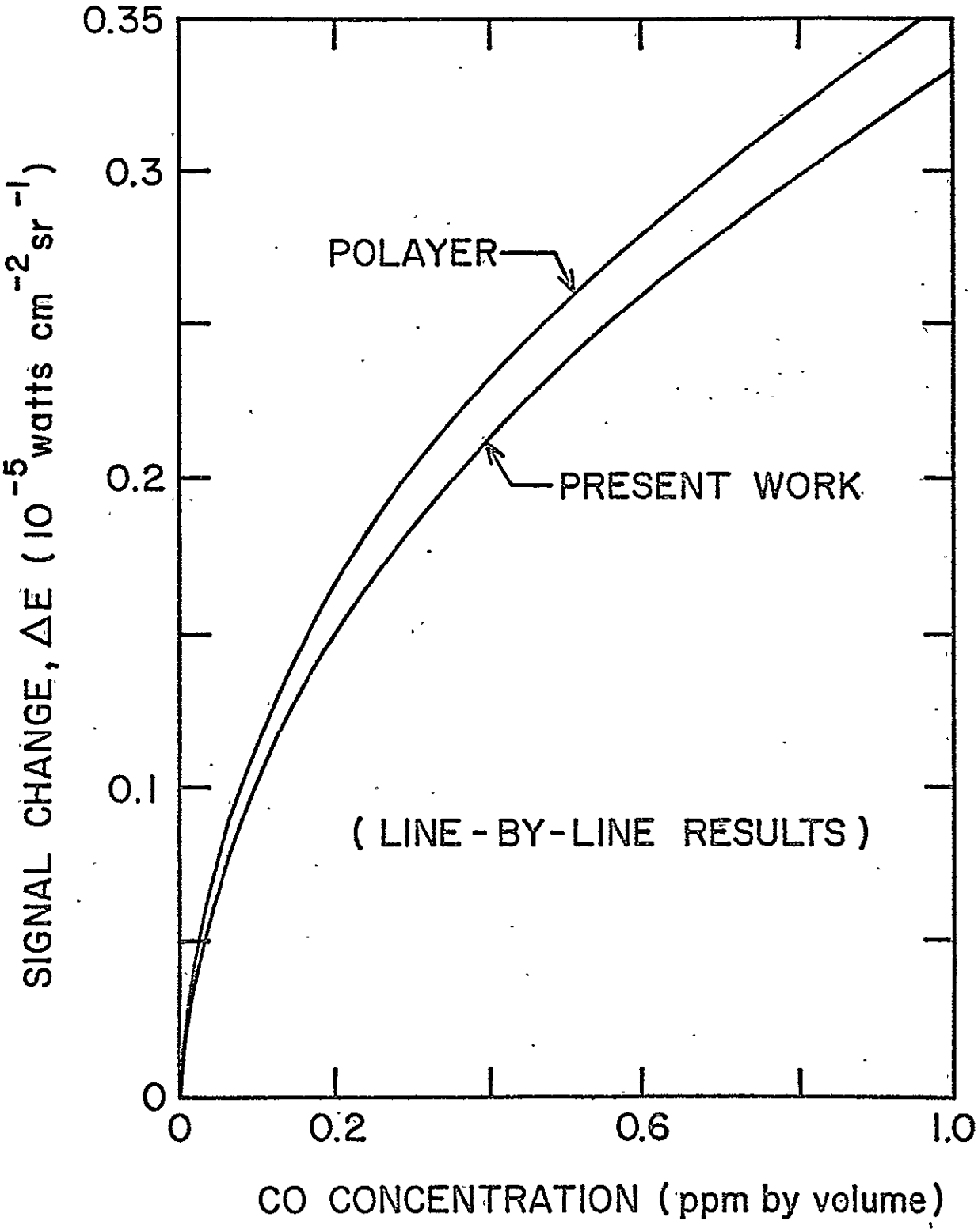

Fig. 4.12 Comparison of signal change results obtained from the program POLAYER and the present LINBLIN program, $T_s = 288°K$, $\varepsilon = 0.8$. On the average, LINBLIN values are 2% lower than POLAYER values.

V. CONCLUSIONS

A computer program has been developed for calculating the atmospheric transmittance and upwelling radiance in the spectral interval 2070-2220 cm^{-1} which employs the Lorentz line-by-line model. The spectral region selected in the region of CO fundamental band. The program allows for variation in CO concentration and accounts for the radiative contributions from the interfering gases such as H_2O, CO_2, N_2O, and O_3. The program has been optimized for accuracy and running time by varying such computation parameters as the interval width, subinterval width and the width of the region from which lines make significant contribution to the absorption at a certain frequency. Furthermore, this program has been diversified so that radiances can be computed for several values of surface temperature or surface emittance in a single run, thereby drastically reducing the computational cost. This line-by-line computer program is given the name LINBLIN. Upwelling radiance results obtained by using the present LINBLIN program are compared with the results of SAI-POLAYER program [19]. The agreement between the two results is within 2%. For homogeneous gas columns, the results obtained by LINBLIN program compare well with available experimental results. This LINBLIN program can easily be extended to any line model and for any spectral region.

A computer program similar to the line-by-line program has been developed which employs the quasi-random narrow band model. This program was given the name QRANDOM. Comparison of results obtained from LINBLIN and QRANDOM programs indicate small differences.

By employing the LINBLIN and QRANDOM programs, model calculations were made to study the effects of different interfering molecules, water vapor profiles, ground temperatures, and ground emittances on the upwelling radiance and signal change. Physically realistic values of various parameters were

used in the model calculations. This information is very useful in establishing the feasibility of measuring the concentration of pollutants in the atmosphere from a gas filter correlation instrument flown on an aircraft or mounted on a satellite.

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APPENDIX A

EXPLANATION OF SYMBOLS USED IN COMPUTER PROGRAMS

A-1. Symbols Used in Program LINBLIN

ALC, ALV	Individual line widths for CO and H_2O lines respectively, cm^{-1}.
ALX	Width of the narrow subinterval on each side of the line center, cm^{-1}.
ALY	2 x (ALX)
AL1, AL2, AL3, AL4, ALD*	Average line width for the molecules H_2O, CO_2, N_2O, O_2 and CO respectively, cm^{-1}.
DEL	Width of an interval, cm^{-1}.
DLIM	Wave number region around an interval from which the contribution to the absorption coefficient is considered direct, cm^{-1}.
EMI	Surface emittance.
EL1, EL2, EL3, EL4, ELD	Energies of the lower states for the lines of the molecules, cm^{-1}.
FRL	Lower frequency limit of the range (2070 cm^{-1}.
FRU	Upper frequency limit of the range (2220 cm^{-1}.
FRB	Wave number at the interval boundaries, cm^{-1}.
FRC	Wave number at the interval centers, cm^{-1}.
FR1, FR2, FR3, FR4, FRD	Wave numbers of the lines of the molecules, cm^{-1}.
GAM	$1 + f(\theta)$ where $f(\theta) = \sec\theta$ for $\theta \leq 60°$ and $f(\theta) = Ch(\theta)$ for $\theta > 60°$. $Ch(\theta)$ is the Chapman function.
GR	Gradients used in calculation of HL

*The same order subscripts 1,2,3,4, and D has been used for these molecules throughout the programs.

HS	Tabulated values of the solar irradiance at the top of the atmosphere, watts cm^{-2} sr^{-1} $(cm^{-1})^{-1}$.
HL	Computed solar irradiance at the top of the atmosphere in an interval, watts cm^{-2} sr^{-1}.
IN1, IN2, IN3, IN4, IND	An integer for the molecule which is 0 when average line width is used and 1 when individual line widths are used.
JQ	Number of different CO concentrations used in the computation (8).
KR	Number of spectral intervals (150).
LC	Number of layers into which the atmosphere is divided (10).
LE1, LE2, LE3, LE4, LED	Number of lines in the spectra of the molecules.
NG	Number of interfering gases.
NG1, NG2, NG3, NG4	Identifying integers for the interfering molecules H_2O, CO_2, N_2O and O_3 respectively.
PCK	Planck's function.
PNTP	Pressure at NTP, mbar
PREC	Pressure at the center of the layers, mbar
QV	Altitude distribution of the molecules H_2O, CO_2, N_2O and O_3 respectively.
QVD	Concentration of CO, ppm by volume
RADNC	Radiance in each interval, watts cm^{-2} sr^{-1}.
RADNCE	Integrated radiance, watts cm^{-2} sr^{-1}.
RCOM	Radiance component due to reflected solar radiation.
RP1, RP2, RP3, RP4, RPD	Exponent to account for the temperature dependence of the rotational partition function for the molecules.
SI1, SI2, SI3, SI4, SID	Integrated intensities for the lines of the molecules, $cm^{-2}atom^{-1}$.

TEMC	Temperatures at the layer centers, °K
TEMR	Reference temperature for line parameters, °K
TEMS	Surface temperature, °K
THC	Thickness of each layer (1 km)
TNTP	Temperature at NTP (273 °K)
TRA	Transmittances for different intervals and and altitudes for one gas.
TRF	Combined transmittances of all the interfering gases.
TRM	Average transmittance over the entire frequency range for each CO distribution.
TRT	Transmittance for each interval and CO concentration, between the top of the atmosphere and surface.
TRX	Transmittance for an interval and altitude including the contribution from CO.
VPF	Vibrational partition functions for H_2O, CO_2, N_2O and O_3 .
WLIM	Wave number range of the wing contribution, cm^{-1}.
WL1, WL2	Weight factors for the 4-point Gauss-Legendre quadrature formula.
WN	Wave numbers at which the solar irradiance at the top of the atmosphere is tabulated.
XL1, XL2	Abscissa values for the 4-point Gauss-Legendre quadrature formula.

A-2. Symbols Used in Subroutine TRANS

AC	Total absorption coefficient at the frequency specified by the subscripts.
ACD	Direct contribution to the total absorption coefficient.
ACW	Wing contribution to the total absorption coefficient.
ACB	Absorption coefficient at the lower boundary of the interval due to wing contributions.
ACE	Same as ACB, at the upper boundary of the interval.
ACM	Same as ACB, at the center of the interval.
AL	Average width for the lines of the molecule under consideration.
ALA	Altitude dependent average width of the lines of a molecule.
ALB	Altitude dependent individual widths of the lines of a molecule (for CO and H_2O).
EL	Energies of lower states of lines of the molecule under consideration.
FACT	Factor used in the computation of altitude dependence of integrated intensity.
FR	Frequencies of the lines of the molecule under consideration.
FRE	Frequencies of the lines falling with an interval.
FRG	Frequencies of all the Gauss-Legendre quadrature points within an interval.
FRS	Frequencies at the subinterval boundaries within an interval.
IG	Number of Gauss-Legendre points within an interval.
IN	An integer for each molecule which is zero if average line widths are used and 1 if individual widths are used for that molecule.
LE	Number of lines for the molecule under consideration.

NQ	Number of subintervals within an interval.
PART	An altitude dependent factor which takes into account the vibrational and rotational partition functions.
PL	Optical path length at the frequency under consideration.
RP	Exponent which accounts for the temperature dependence of the rotational partition function.
SI	Integrated intensities of the lines of the molecule under consideration.
SIA	Altitude dependent integrated intensities of lines of the molecule under consideration.
SL1	Gradient used in the calculation of the wing contribution between ACB and ACM.
SL2	Same as SL1, between ACM and ACE.
TR	Transmittance at the frequency under consideration.
WIDF	Factor which takes into account the altitude dependence of the widths of the lines.

A-3. Symbols used in PROGRAM QRANDOM*

TRA	Combined transmittance of all the interfering gases.
TRF	Combined transmittance including CO contribution for all CO distributions.
TRFM	Average transmittances for the entire frequency range for different altitudes and CO contributions.
TRG	Transmittances for a single gas returned by the subroutine.
X1, T1	Convolution parameters for integration of direct contribution.
X2, T2	Convolution parameters for the integration of wing contribution.

*As far as possible, same symbols have been used in the programs LINBLIN and QRANDOM. Only the symbols which are defined differently for QRANDOM are explained here.

A-4. Symbols Used in SUBROUTINE SMITH

AVSI	Average value of intensity for the lines in one decade in an interval
BIGI	Intensity of the strongest line in an interval, cm^{-2} atm^{-1}.
BIG	Intensity values separating the five decades in each interval.
ELE	Altitude dependent energies of the lower states for lines in an interval.
JB	Number of adjacent intervals from which the wing contribution is considered.
NSI	Number of lines in a decade within an interval.
SFE	Intensities of the lines within a decade in an interval.
SIE	Intensities of the lines within an interval.
SLE	Altitude dependent intensities of the lines within an interval.
SSI	Sum of the intensities of the lines in a decade within an interval.
SUMSI	Optical thickness between the top of the atmosphere and the altitude under consideration.

APPENDIX B

LINE-BY-LINE COMPUTER PROGRAM TO CALCULATE ATMOSPHERIC TRANSMITTANCE AND UPWELLING RADIANCE

B-1. Computer Program LINBLIN

```
      PROGRAM LINBLIN(INPUT,OUTPUT)
      DIMENSION FR1(100),SI1(100),EL1(100)
      DIMENSION FR2(400),SI2(400),EL2(400)
      DIMENSION FR3(750),SI3(750),EL3(750)
      DIMENSION FR4(1220),SI4(1220),EL4(1220)
      DIMENSION FRD(100),SID(100),ELD(100)
      DIMENSION QVD(10),QV(10,5),ALC(100),TRF(11,150),TRX(11,150),
     /TRT(150,8),PCK(11,150),GR(5),RADNC(150,8),TRM(10),RADNCE(10),
     /VPF(10,4),WN(5),HS(5),HL(150)
      INTEGER G,X
      COMMON FRC(150),FRB(151),PREC(10),TEMC(10),QG(10),TRA(11,150),
     /TEMR,XL1,XL2,WL1,WL2,ALX,LC,KR,PNTP,TNTP,DELA,DLIM,WLIM,THC,
     /ALV(100),VP(10),ALY,DEL,PART(10),FACT(10),WIDF(10)
      READ 10, FRL,FRU,DEL,THC,PNTP,TNTP,TEMR,TEMS,EMI,ZEN
      READ 11, LC,JQ,NG,LE1,LE2,LE3,LE4,LED
      READ 10, DLIM,WLIM
      READ 10, (QVD(J),J=1,JQ)
      READ 15, ((QV(L,G),L=1,LC),G=1,NG)
      READ 10, (PREC(L),L=1,LC)
      READ 10, (TEMC(L),L=1,LC)
      READ 12, XL1,XL2,WL1,WL2
      READ 13, AL1,AL2,AL3,AL4,ALD,ALX
      READ 10, RP1,RP2,RP3,RP4,RPD
      READ 17, ((VPF(L,G),L=1,LC),G=1,NG)
      READ 11, NG1,NG2,NG3,NG4
      READ 11, IN1,IN2,IN3,IN4,IND
      READ 18, (WN(N),N=1,5), (HS(N),N=1,5)
      READ 16, (FR1(X),SI1(X),EL1(X),ALV(X),X=1,LE1)
      READ 14, (FR2(X),SI2(X),EL2(X),X=1,LE2)
      READ 14, (FR3(X),SI3(X),EL3(X),X=1,LE3)
      READ 14, (FR4(X),SI4(X),EL4(X),X=1,LE4)
      READ 16, (FRD(X),SID(X),ELD(X),ALC(X),X=1,LED)
   10 FORMAT(10F8.2)
   11 FORMAT(16I5)
   12 FORMAT(8F10.6)
   13 FORMAT(10F8.3)
   14 FORMAT(2(F11.3,E13.4,F11.3,5X))
   15 FORMAT(8E10.3/2E10.3)
   16 FORMAT(2(F11.3,E13.4,F11.3,F5.3))
   17 FORMAT(10F8.4)
   18 FORMAT(5F8.2,5E8.3)
C     CALCULATES THE NUMBER OF INTERVALS-DEFINES FREQUENCIES AT THE INTERVAL
C     BOUNDARIES AND CENTERS
      LB=LC+1
```

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```
      DELA=0.5*DEL
      RK=(FRU-FRL)/DEL+0.1
      KR=RK
      FRB(1)=FRL
      DO 101 K=1,KR
      FRB(K+1)=FRB(K)+DEL
  101 FRC(K)=FRB(K)+DELA
      ALY=2.*ALX
C   INITIALIZES THE COMBINED TRANSMITTANCES OF ALL THE INTERFERING GASES
      DO 102 K=1,KR
      DO 102 L=1,LB
  102 TRF(L,K)=1.
C   DECIDE IF WATER VAPOR IS TO BE TAKEN INTO CONSIDERATION. IF SO, THE
C   WATER VAPOR TRANSMITTANCES RETURNED BY THE SUBROUTINE ARE COMBINED
C   WITH TRF
      IF (NG1-2) 118,119,118
  119 CONTINUE
      DO 107 L=1,LC
      VP(L)=VPF(L,1)
  107 QG(L)=QV(L,1)/1245.
      CALL TRANS(FR1,SI1,EL1,LE1,AL1,RP1,IN1)
      DO 103 K=1,KR
      DO 103 L=1,LB
  103 TRF(L,K)=TRF(L,K)*TRA(L,K)
C   DECIDES IF CARBON DIOXIDE IS TO BE TAKEN INTO CONSIDERATION
  118 IF (NG2-12) 165,166,165
  166 CONTINUE
      DO 108 L=1,LC
      VP(L)=VPF(L,2)
  108 QG(L)=QV(L,2)
      CALL TRANS(FR2,SI2,EL2,LE2,AL2,RP2,IN2)
      DO 104 K=1,KR
      DO 104 L=1,LB
  104 TRF(L,K)=TRF(L,K)*TRA(L,K)
C   DECIDES IF NITROUS OXIDE IS TO BE TAKEN INTO CONSIDERATION
  165 IF (NG3-7) 167,168,167
  168 CONTINUE
      DO 109 L=1,LC
      VP(L)=VPF(L,3)
  109 QG(L)=QV(L,3)
      CALL TRANS(FR3,SI3,EL3,LE3,AL3,RP3,IN3)
      DO 105 K=1,KR
      DO 105 L=1,LB
  105 TRF(L,K)=TRF(L,K)*TRA(L,K)
```

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C    DECIDES IF OZONE IS TO BE TAKEN INTO CONSIDERATION
  167 IF (NG4-19) 169,170,169
  170 CONTINUE
      DO 110 L=1,LC
      VP(L)=VPF(L,4)
  110 QG(L)=QV(L,4)
      CALL TRANS(FR4,SI4,EL4,LE4,AL4,RP4,IN4)
      DO 106 K=1,KR
      DO 106 L=1,LB
  106 TRF(L,K)=TRF(L,K)*TRA(L,K)
  169 CONTINUE
C    CALCULATES PLANCK FUNCTIONS FOR DIFFERENT ALTITUDES AND INTERVALS
      CONS=18.*6.625*1.E-07
      CNST=6.625*0.3/1.38
      DO 115 K=1,KR
      RNUM=DEL*CONS*FRC(K)**3
      EEX=CNST*FRC(K)
      PCK(1,K)=RNUM/(EXP(EEX/TEMS)-1.)
      DO 115 L=1,LC
  115 PCK(L+1,K)=RNUM/(EXP(EEX/TEMC(L))-1.)
C    CALCULATES SOLAR IRRADIANCE AT THE TOP OF THE ATMOSPHERE IN EACH INTERVA
      DO 173 N=1,4
  173 GR(N)=(HS(N+1)-HS(N))/(WN(N+1)-WN(N))
      DO 174 K=1,KR
      N=0
  177 N=N+1
      IF (FRC(K)-WN(N)) 174,175,175
  175 IF (FRC(K)-WN(N+1)) 176,177,177
  176 HL(K)=HS(N)+GR(N)*(FRC(K)-WN(N))
      HL(K)=HL(K)*DEL
  174 CONTINUE
      ZEN=ZEN/57.29578
      GAM=1.+1./COS(ZEN)
      DO 172 X=1,LED
  172 ALV(X)=ALC(X)
      DO 178 L=1,LC
  178 VP(L)=VPF(L,1)
C    CALCULATES TRANSMITTANCES FOR ALL CONCENTRATIONS OF CO ONE BY ONE-
C    COMBINES THEM WITH TRF AND CALCULATES RADIANCE AT THE TOP TAKING
C    REFLECTED SOLAR COMPONENT INTO ACCOUNT
      DO 111 J=1,JQ
      DO 112 L=1,LC
  112 QG(L)=QVD(J)
      CALL TRANS(FRD,SID,ELD,LED,ALD,RPD,IND)
```

```
      DO 113 K=1,KR
      DO 114 L=1,LB
  114 TRX(L,K)=TRF(L,K)*TRA(L,K)
  113 TRT(K,J)=TRX(1,K)
      DO 116 K=1,KR
      RCOM=(1.-EMI)*(COS(ZEN))*HL(K)*(TRT(K,J))**GAM
      RADNC(K,J)=EMI*PCK(1,K)*TRT(K,J)*1.E-07+RCOM
      DO 116 L=2,LB
      COMP=PCK(L,K)*(TRX(L,K)-TRX(L-1,K))*1.E-07
  116 RADNC(K,J)=RADNC(K,J)+COMP
      TRM(J)=0.
      RADNCE(J)=0.
      DO 117 K=1,KR
      TRM(J)=TRM(J)+TRT(K,J)/KR
  117 RADNCE(J)=RADNCE(J)+RADNC(K,J)
  111 CONTINUE
      PRINT 60, ((TRT(K,J),J=1,JQ),K=1,KR)
      PRINT 61, ((RADNC(K,J),J=1,JQ),K=1,KR)
      PRINT 62, (TRM(J),J=1,JQ),(RADNCE(J),J=1,JQ)
   60 FORMAT(1H1/(8F15.5))
   61 FORMAT(1H1/(8E15.4))
   62 FORMAT(1H1/////(8F15.5////8E15.4))
      STOP
      END
```

B-2. Subroutine TRANS for Program LINBLIN

```
      SUBROUTINE TRANS(FR,SI,EL,LE,AL,RP,IN)
      DIMENSION FR(1220),SI(1220),EL(1220),SIA(1220),FRE(40),FRS(50),
     /FRG(200),ACD(200),ACW(200),AC(200,10),TR(200,11),ALB(100)
      INTEGER X
      COMMON FRC(150),FRB(151),PREC(10),TEMC(10),QG(10),IRA(11,150),
     /TEMR,XL1,XL2,WL1,WL2,ALX,LC,KR,PNTP,TNTP,DELA,DLIM,WLIM,THC,
     /ALV(100),VP(10),ALY,DEL,PART(10),FACT(10),WIDF(10)
      CST=SQRT(TEMR)/PNTP
C   DEFINES VARIABLES WHICH ACCOUNT FOR THE VIBRATIONAL AND ROTATIONAL
C   PARTITION FUNCTIONS AND THE ALTITUDES VARIATION OF THE WIDTH OF LINES
      DO 120 L=1,LC
      PART(L)=VP(L)*(TEMR/TEMC(L))**RP
      FACT(L)=1.439*(TEMC(L)-TEMR)/(TEMC(L)*TEMR)
  120 WIDF(L)=CST*PREC(L)/SQRT(TEMC(L))
      X=0
C   ONE INTERVAL CONSIDERED AT A TIME - FINDS ALL THE LINES FALLING WITHIN
C   IT - DETERMINES SUBINTERVAL BOUNDARIES WITHIN THE INTERVAL
      DO 123 K=1,KR
      M=0
      MP=M
  126 IF (X-LE) 124,125,125
  124 X=X+1
      IF (FR(X)-FRB(K)) 126,127,127
  127 IF (FR(X)-FRB(K+1)) 128,125,125
  128 M=M+1
      FRE(M)=FR(X)
      MP=M
      GO TO 126
  125 X=X-1
      N=1
      FRS(N)3FRB(K)
      IF (MP) 129,129,130
  130 CONTINUE
      DO 131 M=1,MP
      DIF=FRE(M)-FRS(N)
      IF (DIF-ALX) 132,132,133
  133 IF (DIF-ALY) 134,134,135
  132 FRS(N+1)=FRE(M)
      N=N+1
      GO TO 136
  134 FRS(N+1)=FRE(M)-ALX
      FRS(N+2)=FRE(M)
      N=N+2
      GO TO 136
```

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```
  135 FRS(N+1)=FRE(M)-ALY
      FRS(N+2)=FRE(M)-ALX
      FRS(N+3)=FRE(M)
      N=N+3
  136 IF (M-MP) 137,138,138
  137 DIF=FRE(M+1)-FRS(N)
      IF(DIF-ALX) 139,139,140
  140 IF(DIF-ALY) 141,141,142
  139 GO TO 131
  141 FRS(N+1)=FRE(M)+ALX
      N=N+1
      GO TO 131
  142 FRS(N+1)=FRE(M)+ALX
      FRS(N+2)=FRE(M)+ALY
      N=N+2
  131 CONTINUE
  138 DIF =FRB(K+1)-FRE(M)
      IF (DIF-ALX) 143,143,144
  144 IF (DIF-ALY) 145,145,146
  143 FRS(N+1)=FRB(K+1)
      NP=N+1
      GO TO 147
  145 FRS(N+1)=FRE(M)+ALX
      FRS(N+2)=FRB(K+1)
      NP=N+2
      GO TO 147
  146 FRS(N+1)=FRE(M)+ALX
      FRS(N+2)=FRE(M)+ALY
      FRS(N+3)=FRB(K+1)
      NP=N+3
      GO TO 147
  129 FRS(N+1)=FRB(K+1)
      NP=N+1
  147 NQ=NP-1
C   DETERMINES THE FREQUENCIES OF THE GAUSS-LEGENDRE QUADRATURE POINTS
C   WITHIN A SUBINTERVAL
      DO 148 N=1,NQ
      VAR=0.5*(FRS(N+1)-FRS(N))
      CON=0.5*(FRS(N+1)+FRS(N))
      I=4*(N-1)+1
      FRG(I)=CON-VAR*XL1
      FRG(I+1)=CON-VAR*XL2
      FRG(I+2)=CON+VAR*XL2
  148 FRG(I+3)=CON+VAR*XL1
```

```
      IG=4*NQ
      PI=3.14159
C     EACH ALTITUDE CONSIDERED SEPARATELY-DIRECT CONTRIBUTION EVALUATED
C     AT EACH GRID POINT AND WING CONTRIBUTION AT THE BOUNDARIES AND
C     CENTER OF THE INTERVAL
      DO 149 L=1,LC
      ALA=AL*WIDF(L)
      ACB=0.
      ACM=0.
      ACE=0.
      DO 179 I=1,IG
      ACD(I)=0.
  179 ACW(I)=0.
      IF (IN) 167,167,168
  167 DO 150 X=1,LE
      DIF =ABS(FR(X)-FRC(K))
      IF (DIF-WLIM) 151,151,150
  151 IF (DIF-DLIM) 152,152,153
  152 SIA(X)=SI(X)*PART(L)*EXP(EL(X)*FACT(L))
      DO 154 I=1,IG
      FD=FR(X)-FRG(I)
      DEN=PI*(FD*FD+ALA*ALA)
  154 ACD(I)=ACD(I)+SIA(X)*ALA/DEN
      GO TO 150
  153 SIA(X)=SI(X)*PART(L)*EXP(EL(X)*FACT(L))
      FB=FR(X)-FRB(K)
      FM=FR(X)-FRC(K)
      FE=FR(X)-FRB(K+1)
      PNUM=SIA(X)*ALA
      ACB=ACB+PNUM/(PI*FB**2)
      ACM=ACM+PNUM/(PI*FM**2)
      ACE=ACE+PNUM/(PI*FE**2)
  150 CONTINUE
      GO TO 174
  168 DO 169 X=1,LE
      DIF=ABS(FR(X)-FRC(K))
      IF (DIF-WLIM) 170,170,169
  170 IF (DIF-DLIM) 171,171,172
  171 SIA(X)=SI(X)*PART(L)*EXP(EL(X)*FACT(L))
      ALB(X)=ALV(X)*WIDF(L)
      DO 173 I=1,IG
      FD=FR(X)-FRG(I)
      DEN=PI*(FD*FD+ALB(X)**2)
  173 ACD(I)=ACD(I)+SIA(X)*ALB(X)/DEN
```

```
      GO TO 169
  172 SIA(X)=SI(X)*PART(L)*EXP(EL(X)*FACT(L))
      ALB(X)=ALV(X)*WIDF(L)
      FB=FR(X)-FRB(K)
      FM=FR(X)-FRC(K)
      FE=FR(X)-FRB(K+1)
      PNUM=SIA(X)*ALB(X)
      ACB=ACB+PNUM/(PI*FB**2)
      ACM=ACM+PNUM/(PI*FM**2)
      ACE=ACE+PNUM/(PI*FE**2)
  169 CONTINUE
C   WING CONTRIBUTION EVALUATED AT EACH GRID POINT  BY INTERPOLATION
  174 SL1=(ACM-ACB)/(FRC(K)-FRB(K))
      SL2=(ACE-ACM)/(FRB(K+1)-FRC(K))
      DO 156 I=1,IG
      DIF=FRG(I)-FRB(K)
      IF (DIF-DELA) 157,158,158
  157 ACW(I)=ACB+SL1*DIF
      GO TO 156
  158 ACW(I)=ACM+SL2*(DIF-DELA)
  156 CONTINUE
C   TOTAL ABSORPTION COEFFICIENTS EVALUATED AT EACH GRID POINT
      DO 161 I=1,IG
  161 AC(I,L)=ACD(I)+ACW(I)
  149 CONTINUE
      LB=LC+1
      CONST=0.1*TNTP*THC/PNTP
C   TRANSMITTANCE EVALUATED AT EACH GRID POINT
      DO 163 I=1,IG
      PL=0.
      TR(I,LB)=EXP(-PL)
      DO 163 M=2,LB
      L=LB+1-M
      SPTR=PREC(L)*QG(L)*AC(I,L)/TEMC(L)
      PL=PL+CONST*SPTR
  163 TR(I,L)=EXP(-PL)
C   AVERAGE TRANSMITTANCE EVALUATED FOR EACH INTERVAL AT EACH ALTITUDE
      DO 164 L=1,LB
      TRA(L,K)=0.
      DO 164 N=1,NQ
      VAR=0.5*(FRS(N+1)-FRS(N))
      I=4*(N-1)+1
      SUM1=TR(I,L)+TR(I+3,L)
      SUM2=TR(I+1,L)+TR(I+2,L)
      SUM=WL1*SUM1+WL2*SUM2
  164 TRA(L,K)=TRA(L,K)+SUM*VAR/DEL
  123 CONTINUE
      RETURN
      END
```

APPENDIX C

QUASI-RANDOM COMPUTER PROGRAM TO CALCULATE ATMOSPHERIC TRANSMITTANCE AND UPWELLING RADIANCE

C-1. Computer Program QRANDOM

```
      PROGRAM QRANDOM(INPUT,OUTPUT)
      INTEGER X,G,W
      DIMENSION FR1(100),SI1(100),EL1(100)
      DIMENSION FR2(400),SI2(400),EL2(400)
      DIMENSION FRD(100),SID(100),ELD(100)
      DIMENSION          QVD(10),QV(10,4),VPF(10,4),WN(5),HS(5),GR(5),
     /TRA(26,11),TRF(51,11,8),HL(25),PCK(25,11),TRFM(11,8),TRT(25,8),
     /RADNC(25,8),TRM(8),RADNCE(8)
      COMMON DEL,X1(26),T1(26),X2(21),T2(21),TRG(26,11),FRB(27),FRC(26),
     /PREC(10),TEMC(10),QG(10),VP(10),PNTP,INTP,TEMR,LC,KR,JB,THC
      READ 10, FRL,FRU,DEL,THC,PNTP,INTP,TEMR,TEMS,EMI,ZEN
      READ 11, LC,JQ,NG,JB,LE1,LE2,LE3,LE4,LED
      READ 10, (QVD(J),J=1,JQ)
      READ 10, (PREC(L),L=1,LC)
      READ 10, (TEMC(L),L=1,LC)
      READ 12, ((QV(L,G),L=1,LC),G=1,NG)
      READ 14, AL1,AL2,AL3,AL4,ALD
      READ 10, RP1,RP2,RP3,RP4,RPD
      READ 11, MP1,NR1,MP2,NR2,MP3,NR3,MP4,NR4,MPD,NRD
      READ 15, (X1(W),W=1,26)
      READ 15, (T1(W),W=1,26)
      READ 15, (X2(W),W=1,21)
      READ 15, (T2(W),W=1,21)
      READ 15, ((VPF(L,G),L=1,LC),G=1,NG)
      READ 11, NG1,NG2,NG3,NG4
      READ 18, (WN(N),N=1,5),(HS(N),N=1,5)
      READ 17, (FR1(X),SI1(X),EL1(X),X=1,LE1)
      READ 17, (FR2(X),SI2(X),EL2(X),X=1,LE2)
      READ 17, (FRD(X),SID(X),ELD(X),X=1,LED)
   10 FORMAT(10F8.2)
   11 FORMAT(16I5)
   12 FORMAT(8E10.3/2E10.3)
   14 FORMAT(10F8.3)
   15 FORMAT(10F8.4)
   17 FORMAT(2(F11.3,E13.4,F11.3,5X))
   18 FORMAT(5F8.2,5E8.3)
C     CALCULATES THE FREQUENCIES AT THE INTERVAL BOUNDARIES AND CENTERS FOR
C     UNSHIFTED MESH  AND INITIALIZES  THE RESULTANT TRANSMITTANCES
      RK=(FRU-FRL)/DEL+0.1
      KR=RK
      DELA=0.5*DEL
      FRB(1)=FRL
      DO 100 K=1,KR
      FRB(K+1)=FRB(K)+DEL
```

```
  100 FRC(K)=FRB(K)+DELA
      LB=LC+1
      DO 101 L=1,LB
      DO 101 K=1,KR
  101 TRA(K,L)=1.
C   DECIDES WHICH GASES ARE TO BE TAKEN INTO CONSIDERATION IN THE ORDER
C   WATER VAPOR, CARBON DIOXIDE, NITROUS OXIDE AND OZONE AND COMBINES
C   THEIR TRANSMITTANCES OBTAINED FROM THE SUBROUTINE WITH THE RESULTANT
C   TRANSMITTANCE
      IF (NG1-2) 102,103,102
  103 CONTINUE
      DO 104 L=1,LC
      QG(L)=QV(L,1)/1245.
  104 VP(L)=VPF(L,1)
      CALL SMITH(FR1,SI1,EL1,LE1,AL1,RP1,MP1,NR1)
      DO 105 L=1,LB
      DO 105 K=1,KR
  105 TRA(K,L)=TRA(K,L)*TRG(K,L)
  102 IF (NG2-12) 106,107,106
  107 CONTINUE
      DO 108 L=1,LC
      QG(L)=QV(L,2)
  108 VP(L)=VPF(L,2)
      CALL SMITH(FR2,SI2,EL2,LE2,AL2,RP2,MP2,NR2)
      DO 109 L=1,LB
      DO 109 K=1,KR
  109 TRA(K,L)=TRA(K,L)*TRG(K,L)
  106 IF (NG3-7) 110,111,110
  111 CONTINUE
      DO 112 L=1,LC
      QG(L)=QV(L,3)
  112 VP(L)=VPF(L,3)
      CALL SMITH(FR3,SI3,EL3,LE3,AL3,RP3,MP3,NR3)
      DO 113 L=1,LB
      DO 113 K=1,KR
  113 TRA(K,L)=TRA(K,L)*TRG(K,L)
  110 IF (NG4-19) 114,115,114
  115 CONTINUE
      DO 116 L=1,LC
      QG(L)=QV(L,4)
  116 VP(L)=VPF(L,4)
      CALL SMITH(FR4,SI4,EL4,LE4,AL4,RP4,MP4,NR4)
      DO 117 L=1,LB
      DO 117 K=1,KR
```

```
  117 TRA(K,L)=TRA(K,L)*TRG(K,L)
  114 CONTINUE
      DO 154 L=1,LB
      DO 154 K=1,KR
      KK=2*K
  154 TRF(KK,L,1)=TRA(K,L)
      DO 118 J=2,JQ
      DO 119 L=1,LC
      QG(L)=QVD(J)
  119 VP(L)=VPF(L,1)
      CALL SMITH(FRD,SID,ELD,LED,ALD,RPD,MPD,NRD)
      DO 120 L=1,LB
      DO 120 K=1,KR
      KK=2*K
  120 TRF(KK,L,J)=TRA(K,L)*TRG(K,L)
  118 CONTINUE
C   CALCULATES THE FREQUENCIES AT THE  INTERVAL BOUNDARIES AND CENTERS
C   FOR SHIFTED  MESH AND INITIALIZES  RESULTANT TRANSMITTANCES
      KR=KR+1
      FRB(1)=FRL-DELA
      DO 121 K=1,KR
      FRB(K+1)=FRB(K)+DEL
  121 FRC(K)=FRB(K)+DELA
      DO 122 L=1,LB
      DO 122 K=1,KR
  122 TRA(K,L)=1.
C   CALCULATES TRANSMITTANCES AND COMBINES THEM WITH THE  RESULTANT THE
C   SAME WAY AS FOR UNSHIFTED MESH
      IF (NG1-2) 123,124,123
  124 CONTINUE
      DO 125 L=1,LC
      QG(L)=QV(L,1)/1245.
  125 VP(L)=VPF(L,1)
      CALL SMITH(FR1,SI1,EL1,LE1,AL1,RP1,MP1,NR1)
      DO 126 L=1,LB
      DO 126 K=1,KR
  126 TRA(K,L)=TRA(K,L)*TRG(K,L)
  123 IF (NG2-12) 127,128,127
  128 CONTINUE
      DO 129 L=1,LC
      QG(L)=QV(L,2)
  129 VP(L)=VPF(L,2)
      CALL SMITH(FR2,SI2,EL2,LE2,AL2,RP2,MP2,NR2)
      DO 130 L=1,LB
```

```
      DO 130 K=1,KR
  130 TRA(K,L)=TRA(K,L)*TRG(K,L)
  127 IF (NG3-7) 131,132,131
  132 CONTINUE
      DO 133 L=1,LC
      QG(L)=QV(L,3)
  133 VP(L)=VPF(L,3)
      CALL SMITH(FR3,SI3,EL3,LE3,AL3,RP3,MP3,NR3)
      DO 134 L=1,LB
      DO 134 K=1,KR
  134 TRA(K,L)=TRA(K,L)*TRG(K,L)
  131 IF (NG4-19) 135,136,135
  136 CONTINUE
      DO 137 L=1,LC
      QG(L)=QV(L,4)
  137 VP(L)=VPF(L,4)
      CALL SMITH(FR4,SI4,EL4,LE4,AL4,RP4,MP4,NR4)
      DO 138 L=1,LB
      DO 138 K=1,KR
  138 TRA(K,L)=TRA(K,L)*TRG(K,L)
  135 CONTINUE
      DO 155 L=1,LB
      DO 155 K=1,KR
      KK=2*K-1
  155 TRF(KK,L,1)=TRA(K,L)
      DO 139 J=2,JQ
      DO 140 L=1,LC
      QG(L)=QVD(J)
  140 VP(L)=VPF(L,1)
      CALL SMITH(FRD,SID,ELD,LED,ALD,RPD,MPD,NRD)
      DO 141 L=1,LB
      DO 141 K=1,KR
      KK=2*K-1
  141 TRF(KK,L,J)=TRA(K,L)*TRG(K,L)
  139 CONTINUE
      KR=KR-1
C   CALCULATES MEAN TRANSMITTANCES BY AVERAGING RESULTS FROM SHIFTED AND
C   UNSHIFTED MESH CALCULATIONS AND FINALLY OBTAINING THE AVERAGE TRANSMITTANC
C   FOR THE ENTIRE FREQUENCY RANGE
      DO 143 J=1,JQ
      DO 144 L=1,LB
      DO 145 K=1,KR
      KX=2*K-1
      KY=2*K
```

```
      KZ=2*K+1
  145 TRF(K,L,J)=(TRF(KX,L,J)+TRF(KY,L,J)+TRF(KZ,L,J))/3.
      TRFM(L,J)=0.
      DO 144 K=1,KR
  144 TRFM(L,J)=TRFM(L,J)+TRF(K,L,J)/KR
      DO 143 K=1,KR
  143 TRT(K,J)=TRF(K,1,J)
C     CALCULATES SOLAR IRRADIANCE AT THE TOP OF THE ATMOSPHERE FROM THE
C     TABULATED VALUES BY LINEAR INTERPOLATION IN EACH INTERVAL
      DO 146 N=1,4
  146 GR(N)=(HS(N+1)-HS(N))/(WN(N+1)-WN(N))
      DO 147 K=1,KR
      N=0
  150 N=N+1
      IF (FRC(K)-WN(N)) 147,148,148
  148 IF (FRC(K)-WN(N+1)) 149,150,150
  149 HL(K)=DEL*(HS(N)+GR(N)*(FRC(K)-WN(N)))
  147 CONTINUE
C     CALCULATES PLANCK FUNCTION FOR  EACH ALTITUDE AND FREQUENCY INTERVAL
      CONS=18.*6.625*1.E-07
      CNST=6.625*0.3/1.38
      DO 142 K=1,KR
      RNUM=DEL*CONS*FRC(K)**3
      EEX=CNST*FRC(K)
      PCK(K,1)=RNUM/(EXP(EEX/TEMS)-1.)
      DO 142 L=1,LC
      PCK(K,L+1)=RNUM/(EXP(EEX/TEMC(L))-1.)
  142 CONTINUE
C     CALCULATES RADIANCE AT THE TOP OF THE ATMOSPHERE INCLUDING THE
C     REFLECTED SOLAR COMPONENT
      ZEN=COS(ZEN/57.29578)
      GAM=1.+1./ZEN
      DO 151  J=1,JQ
      DO 152 K=1,KR
      RCOM=(1.-EMI)*ZEN*HL(K)*(TRT(K,J))**GAM
      RADNC(K,J)=EMI*PCK(K,1)*TRT(K,J)*1.E-07+RCOM
      DO 152 L=2,LB
      COMP=PCK(K,L)*(TRF(K,L,J)-TRF(K,L-1,J))*1.E-07
  152 RADNC(K,J)=RADNC(K,J)+COMP
      TRM(J)=0.
      RADNCE(J)=0.
      DO  153 K=1,KR
      TRM(J)=TRM(J)+TRT(K,J)/KR
  153 RADNCE(J)=RADNCE(J)+RADNC(K,J)
  151 CONTINUE
      PRINT 60, ((TRT(K,J),J=1,JQ),K=1,KR)
      PRINT 62, ((RADNC(K,J),J=1,JQ),K=1,KR)
      PRINT 60, ((TRFM(L,J),J=1,JQ),L=1,LB)
      PRINT 61, (TRM(J),J=1,JQ),(RADNCE(J),J=1,JQ)
   60 FORMAT(1H1//(8F15.5,/))
   61 FORMAT(1H1/////(8F15.5////8E15.4))
   62 FORMAT(1H1//(8E15.4,/))
      STOP
      END
```

C-2. Subroutine SMITH for Program QRANDOM

```
      SUBROUTINE SMITH(FR,SI,EL,LE,AL,RP,MP,NR)
      INTEGER X,W
      DIMENSION FR(1220),SI(1220),EL(1220),SIE(200,26),SLE(200,26),
     /ELE(200,26),SFE(100,5,26),BIGI(26),BIG(6,26),NSI(5,26),SSI(5,26),
     /AVSI(5,26),SUMSI(5,26),PART(10),FACT(10),WIDF(10)
      COMMON DEL,X1(26),T1(26),X2(21),T2(21),TRG(26,11),FRB(27),FRC(26),
     /PREC(10),TEMC(10),QG(10),VP(10),PNTP,TNTP,TEMR,LC,KR,JB,THC
C   SETS INTEGRATED INTENSITIES AND ENERGIES FOR EACH LINE TO ZERO
      DO 120 K=1,KR
      DO 120 M=1,MP
      SIE(M,K)=0.
  120 ELE(M,K)=0.
      X=0
C   DISTRIBUTES THE LINES INTO FREQUENCY INTERVALS
      DO 121 K=1,KR
      M=0
  124 IF (X-LE) 122,123,123
  122 X=X+1
      IF (FR(X)-FRB(K)) 124,125,125
  125 IF (FR(X)-FRB(K+1)) 126,127,127
  126 M=M+1
      SIE(M,K)=SI(X)
      ELE(M,K)=EL(X)
      GO TO 124
  127 IF (K-KR) 128,123,123
  128 X=X-1
  121 CONTINUE
  123 CONTINUE
C   SETS OPTICAL DEPTH  IN EACH INTERVAL AT THE TOP OF THE ATMOSPHERE TO ZER
      DO 151 K=1,KR
      DO 151 I=1,5
  151 SUMSI(I,K)=0.
      LB=LC+1
      PI=3.141592654
      DELA=0.5*DEL
      CONST=0.1*TNTP*THC/PNTP
      CST=SQRT(TEMR)/PNTP
      ULB=0.
      BSU=0.
C   EACH LAYER IS CONSIDERED  SEPARATELY FROM TOP DOWN
      DO 150 MM=1,LC
      L=LC+1-MM
      PART(L)=VP(L)*(TEMR/TEMC(L))**RP
      FACT(L)=1.439*(TEMC(L)-TEMR)/(TEMC(L)*TEMR)
```

```
      WIDF(L)=CST*PREC(L)/SQRT(TEMC(L))
      SPTR=PREC(L)*QG(L)/TEMC(L)
      ALA=AL*WIDF(L)
      ULA=CONST*SPTR/(PI*ALA)
      ULB=ULB+ULA
      BSU=BSU+ULA*ALA
      ALB=BSU/ULB
      RHO=ALB/DELA
C   CALCULATES THE ALTITUDE DEPENDENT INTENSITY
      DO 137 K=1,KR
      DO 137 M=1,MP
  137 SLE(M,K)=SIE(M,K)*PART(L)*EXP(FACT(L)*ELE(M,K))
      DO 129 K=1,KR
      DO 129 I=1,5
      DO 129 N=1,NR
  129 SFE(N,I,K)=0.
C   ASSIGNS LINES IN THE INTERVAL TO THE FIVE INTENSITY DECADES
      DO 130 K=1,KR
      BIGI(K)=SLE(1,K)
      DO 131 M=2,MP
      IF (BIGI(K)-SLE(M,K)) 132,131,131
  132 BIGI(K)=SLE(M,K)
  131 CONTINUE
      DO 133 I=1,6
      IX=-I+1
  133 BIG(I,K)=BIGI(K)*10.**IX
      DO 130 I=1,5
      N=0
      DO 130 M=1,MP
      IF (SLE(M,K)-BIG(I,K)) 134,134,130
  134 IF (SLE(M,K)-BIG(I+1,K)) 130,130,135
  135 N=N+1
      SFE(N,I,K)=SLE(M,K)
  130 CONTINUE
C   CALCULATES AVERAGE INTENSITY FOR EACH DECADE
      DO 138 K=1,KR
      DO 138 I=1,5
      NSI(I,K)=0
      SSI(I,K)=0.
      DO 139 N=1,NR
      IF (SFE(N,I,K)) 140,140,141
  141 NSI(I,K)=NSI(I,K)+1
  139 SSI(I,K)=SSI(I,K)+SFE(N,I,K)
  140 IF (NSI(I,K)) 142,142,136
```

```
  142 NSI(I,K)=1
  136 AVSI(I,K)=SSI(I,K)/NSI(I,K)
      SUMSI(I,K)=SUMSI(I,K)+AVSI(I,K)*ULA
  138 CONTINUE
C   CALCULATES TRANSMITTANCE IN EACH INTERVAL AT ALL ALTITUDES CONSIDERING
C   DIRECT AND WING CONTRIBUTION
      DO 143 K=1,KR
      FRUC=FRC(K)
      TRG(K,L)=1.
      DO 143 J=1,KR
      JA=IABS(J-K)
      IF (JA-JB) 152,152,153
  153 TRD=1.
      GO TO 143
  152 FRBI=FRB(J)
      ZI=FRUC-FRBI-DELA
      EPSI=ZI/DELA
      TRD=1.
      DO 144 I=1,5
      NSJ=NSI(I,J)
      XI=SUMSI(I,J)
      RES=0.
      IF (J-K) 145,146,145
  146 DO 147 W=1,26
      Y=EXP(-RHO*RHO*XI/(X1(W)*X1(W)+RHO*RHO))
  147 RES=RES+Y*T1(W)
      GO TO 144
  145 DO 148 W=1,21
      Y=EXP(-RHO*RHO*XI/(EPSI-X2(W))**2)
  148 RES=RES+Y*T2(W)
      RES=RES/6.
  144 TRD=TRD*RES**NSJ
  143 TRG(K,L)=TRG(K,L)*TRD
  150 CONTINUE
C   DEFINES TRANSMITTANCES AT THE TOP OF THE ATMOSPHERE AS UNITY
      DO 149 K=1,KR
  149 TRG(K,LB)=1.
      RETURN
      END
```