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DEPARTMENT OF COMMERCE ★ UNITED STATES OF AMERICA ★

DEPENDENCE OF VTPR TRANSMITTANCE PROFILES AND OBSERVED RADIANCES ON SPECTRAL LINE SHAPE PARAMETERS

Charles Braun

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July 1975

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Rogers C. B. Morton, Secretary

NATIONAL OCEANIC AND
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Robert M. White, Administrator

National Environmental
Satellite Service
David S. Johnson, Director

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DEPENDENCE OF VTPR TRANSMITTANCE PROFILES AND OBSERVED RADIANCES ON SPECTRAL LINE SHAPE PARAMETERS

Charles Braun
National Environmental Satellite Service, NOAA, Washington, D.C.

ABSTRACT. The sensitivity of transmittance profiles and radiances to spectral line shape and line strength was calculated for the spectral intervals of the Vertical Temperature Profile Radiometer (VTPR).

Computations were done for U.S. Standard Atmosphere Supplements for 15°N and 60°N. For 15°N, the change in calculated radiance became equal to the permissible design noise level of the instrument in at least one spectral channel, when the Lorentz half-width changed by 2%, the exponent of its temperature dependence by 12%, or the line strength by 1%. The same change in calculated radiance occurred for the profile of 60°N when these parameters were varied by 4, 22, and 2%, respectively.

The effects of variations in the concentration of atmospheric CO_2, which occur with changes in geographic location and season, were also studied. If these variations are ignored and a constant value is used, the error in calculated radiance exceeds the design noise level in several spectral channels in the profile of 15°N and is close to the design noise level for one channel in the profile of 60°N.

The permitted variations in spectral line strength and line shape parameters are found to be considerably less than the uncertainty of the values determined by laboratory measurement. At present, temperature profiles cannot be accurately retrieved using transmittances calculated from these parameters alone. Empirical adjustments to the radiance data and the calculated transmittances are also necessary. More accurate laboratory measurements should be made of the spectral line parameters to eliminate the need for empirical adjustments.

INTRODUCTION

A number of satellite instruments have been designed to measure radiances in various spectral channels for use in determining atmospheric temperature profiles (Fritz et al. 1972). To obtain accurate temperature profiles from radiometric data, the atmospheric transmittance profile for each spectral channel of the radiometer must be known.

Two sets of radiances are used to retrieve a temperature profile from real data: the set actually measured in the spectral channels of VTPR, and a hypothetical set computed for the VTPR channels. The hypothetical radiances are computed, for a "first guess" temperature profile, from a set of atmospheric transmittances for the VTPR spectral channels also calculated for the first guess temperature profile (Fritz et al. 1972). The accuracy of the radiances calculated for the first guess temperature profile depends on the use of known atmospheric transmittances (as functions of pressure, temperature, and wavelength) within these spectral channels. This, in turn, requires knowledge of the temperature and pressure dependence of the strength and shape of each spectral line within the bandpass of the radiometer.

The calculated first guess radiances are combined with the measured radiances to retrieve the temperature profile. Errors in the calculated set of radiances appear on the retrieved temperature profile as errors in the measured set of radiances. It is therefore necessary that the error in calculated radiances caused by uncertainty in atmospheric transmittance be less than the allowed error for observed radiance in all spectral channels of VTPR. The maximum amount by which linewidth, its temperature dependence, line strength, and CO_2 concentration can vary, and yet keep the uncertainty in atmospheric transmittance within these bounds, is computed and discussed.

Line-by-line computer programs to calculate atmospheric transmittance have been described by Drayson (1966), Kunde and McGuire (1974), and Scott (1974).

In this paper, Drayson's program is used to calculate transmittance profiles for the VTPR (McMillin et al. 1973). The VTPR senses radiation in 6 spectral channels in the 15-μm ν_2 band of CO_2, 1 atmospheric window at 12 μm, and 1 channel in the H_2O vapor rotation band near 19 μm. Transmittance profiles and radiances for CO_2 alone were calculated for the 6 CO_2 channels of VTPR. Three parameters were varied independently in these calculations:

1) spectral linewidths, 2) the functions specifying their temperature dependence, and 3) line strength.

The fourth parameter of this study, the atmospheric CO_2 concentration, although physically independent of the other three, has the same effect on calculated transmittance profiles and radiances as the line strength. Its variation was studied simultaneously with that of line strength.

The permitted uncertainties for the values of all four parameters were found in this study to be much less than the uncertainties in their values as determined by theory and laboratory experiments. Values for linewidths and their temperature dependence are particularly uncertain because of the scarcity of data on these 2 quantities for the 15-μm band of CO_2.

Computations were done for temperature profiles (U.S. Standard Atmosphere Supplements 1966) at 15°N (annual) and 60°N (winter); these were chosen to represent cases of steep and shallow lapse rates, respectively (fig. 1). As expected, the variation of spectral radiance with spectral linewidth and total CO_2 concentration is greater for the temperature profile with the steeper lapse rate.

The need for better data, and the improvement such data would make in the retrieval of atmospheric temperature soundings from satellite radiance data, are discussed under Results and Conclusions.

CALCULATION OF RADIANCES

Equations for Atmospheric Transmittance and Radiance

Atmospheric transmittances and radiances were calculated from Drayson's line-by-line program. Two spectral line shapes are used in this program: The Lorentz line shape for atmospheric pressures of $P \geq 100$ mb, and the Voigt profile for $P < 100$ mb. The absorption coefficient k for the Lorentz line shape used by Drayson is

$$k(\nu) = \frac{S(T)\ \alpha_L\ (T,P)}{\pi[(\nu - \nu_0)^2 + \alpha_L(T,P)^2]} \tag{1}$$

where T = absolute temperature, K

$S(T)$ = line strength, $atm^{-1}\ cm^{-2}$

ν = wavenumber, cm^{-1}

ν_0 = wavenumber at the center of the spectral line, cm^{-1}

$\alpha_L(T, P)$ = Lorentz half-width, cm^{-1}.

For his line-by-line program Drayson used values of S(T) obtained from Madden (1961) and Gray and Selvidge (1965). The values of $\alpha_L(T,P)$ used in his program were taken from the work of Yamamoto et al. (1969).

The Lorentz linewidth may be expressed in terms of its value at a standard temperature T_0 and pressure P_0 as follows:

$$\alpha_L(T,P) = \lambda\, \alpha_L(T_0,P_0) \cdot \left(\frac{P}{P_0}\right) \cdot \left(\frac{T_0}{T}\right)^{\gamma} \qquad (2)$$

The parameters λ and γ are arbitrary factors used to adjust the values of the Lorentz half-widths and the exponent of their temperature dependence respectively. When $\lambda = 1.0$ and $\gamma = 0.5$ the Lorentz linewidths and their temperature dependence reduce to the values used in Drayson's program to process real data.

The absorption coefficient for the Voigt line shape is a convolution of the Lorentz and Doppler shapes. It is discussed in many texts, among them Penner (1959) and Goody (1964). A convenient way of writing the Voigt absorption coefficient (Drayson 1966) is

$$K(\nu - \nu_0) = \frac{k_0 y}{\pi} \int_{-\infty}^{\infty} \frac{dt \quad e^{-t^2}}{y^2 + (x-t)^2} \qquad (3)$$

where $k_0 = [\frac{\ln 2}{\pi}]^{\frac{1}{2}} \frac{S(T)}{\alpha_D(T)}$

$y = \alpha_L(T,P) \;/\; \alpha_D(T)$

$x = (\nu - \nu_0) \cdot [\ln 2]^{\frac{1}{2}} \;/\; \alpha_D(T)$

$\alpha_D(T)$ = Doppler half-width

and t = dimensionless variable to permit integration over all possible molecular velocities occurring in the gas.

For a particular spectral line, the line strength S(T) is defined in terms of the absorption coefficient as

$$S(T) = \int_0^{\infty} d\nu \; k(\nu,T) \tag{4}$$

This function is independent of P and is the same whether $k(\nu,T)$ is for the Lorentz shape of eq (2) or the Voigt shape of eq (3).

Transmittance at a specific wavenumber and pressure is defined by

$$\tau(\nu,P) = \exp\left\{ -\frac{C_{CO_2}}{g} \int_P^0 dP' \; k[\nu,T(P'),P'] \right\} \tag{5}$$

where C_{CO_2} = mole fraction of carbon dioxide,
g = acceleration of gravity, and
$k[\nu,T,P']$ = absorption coefficient per unit mass.

The radiance observed in one spectral channel of a satellite radiometer is closely approximated by

$$I(\nu_i) = B(\nu_i,T_s) \cdot [\tau_s(\nu,P)]_\nu + \int_{x(P_s)}^0 dx \left\langle \frac{d\tau}{dx}(\nu,x) \right\rangle_\nu B[\nu_i, T(x)] \tag{6}$$

where x = monotonically increasing function of pressure,
and ν_i = central wavenumber of the spectral channel,
$B(\nu_i,T)$ = Planck radiance at the central wavenumber ν_i, for Temperature T, and
$\tau(\nu,P)$ = transmittance given by eq (5).

The brackets $\langle \; \rangle_\nu$ indicate the wavenumber average over the spectral bandpass of the channel. The subscript s indicates the surface value of a quantity.

Radiances Calculated as a Function of Linewidth and Its Temperature Dependence

Transmittances and radiances of the six CO_2 channels of VTPR were computed for the two temperature profiles of figure 1. Radiances were computed for each temperature profile for four values of γ and three values of λ [which enter the computations through eq (2)].

Radiances computed for $\gamma = 0.5$ and $\lambda = 1.0$ are listed in table 1 and are the values used in Drayson's program. When $\gamma = 0.5$, the temperature

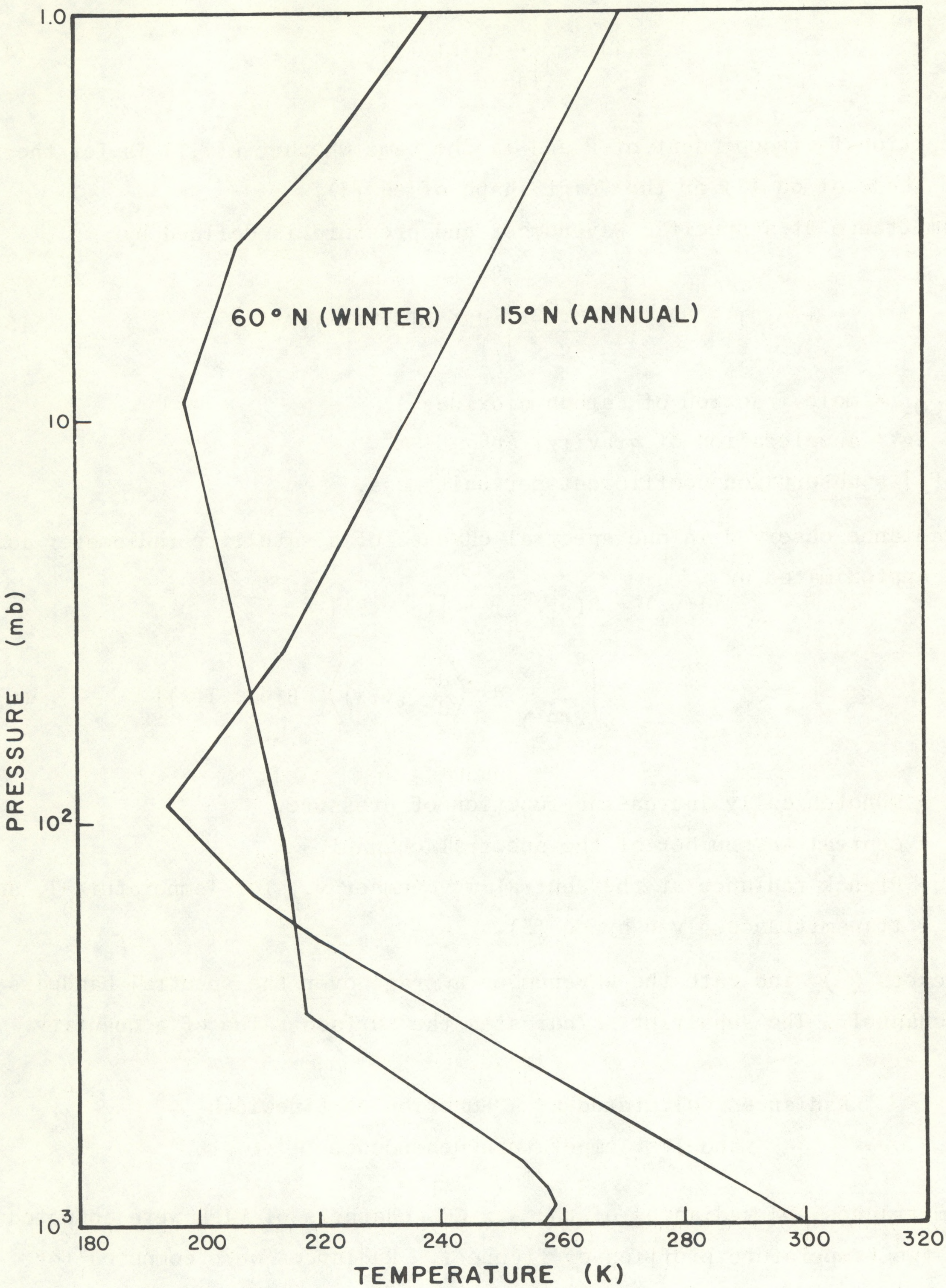


Figure 1.--U.S. Standard Atmosphere temperature profiles used for this study.

dependence of the Lorentz half-width is that predicted by the classical theory of pressure broadening, which treats colliding molecules as rigid spheres.

Table 1.--Radiances calculated for two supplementary standard atmospheres for the six CO_2 channels of VTPR

Channel no. i	Central wavenumber ν_i (cm^{-1})	Profile: 15°N (annual) $I(\nu_i)$ mw/(sr m^2 cm^{-1})	Profile: 60°N (winter) $I(\nu_i)$ mw/(sr m^2 cm^{-1})
1	668.5	54.60	38.67
2	677.5	42.70	36.20
3	695.7	44.97	38.90
4	707.2	62.53	48.29
5	724.7	85.57	58.34
6	747.5	108.87	67.67

Parameter values are: C_{CO_2} = 320 ppmv, $\gamma = 0.5$, and $\lambda = 1.0$. Nominal bandwidths are $\Delta_\nu = 3.5\ cm^{-1}$ for channel 1 and $\Delta_\nu = 10\ cm^{-1}$ for channels 2 to 6.

The changes in radiances calculated as γ is varied from 0.5 to 1.25 (for $\lambda = 1.0$) are graphed in figure 2. The changes that result as λ is varied from 1.0 to 1.8 (for $\gamma = 0.5$) are shown in figure 3.

Figures 2 and 3 indicate that calculated radiances increase in some spectral channels and decrease in others as γ or λ is increased. Increasing γ or λ broadens the spectral lines in all channels and increases their equivalent widths. This shifts the profile for the derivative of the transmittance $\langle d\tau/dx \rangle_\nu$ and its peak value $\langle d\tau/dx \rangle_\nu^{max}$ upward in each spectral channel. For spectral channels in which $\langle d\tau/dx \rangle_\nu^{max}$ occurs below the tropopause, increasing γ or λ decreases the radiance of these channels. For channels in which $\langle d\tau/dx \rangle_\nu^{max}$ occurs above the tropopause, changing either parameter has the reverse effect.* For channels 1 and 2 of the profile of 15°N and channel 1 of 60°N, $\langle d\tau/dx \rangle_\nu^{max}$ is above the tropopause, and their radiances increase if

*The only case for which this may not be true is for spectral channels in which a large amount of surface radiation reaches the satellite and when there is a strong temperature inversion near the surface.

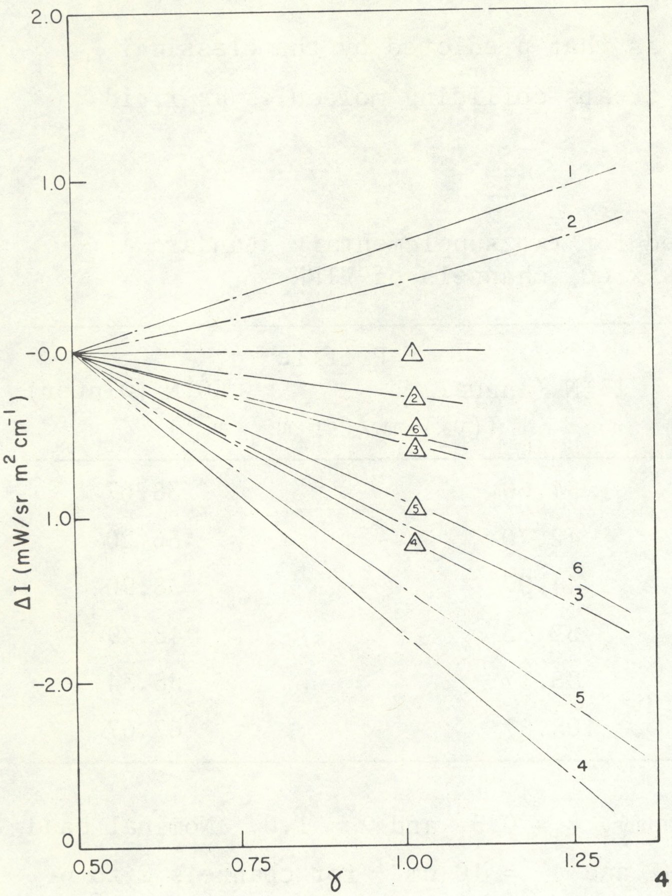
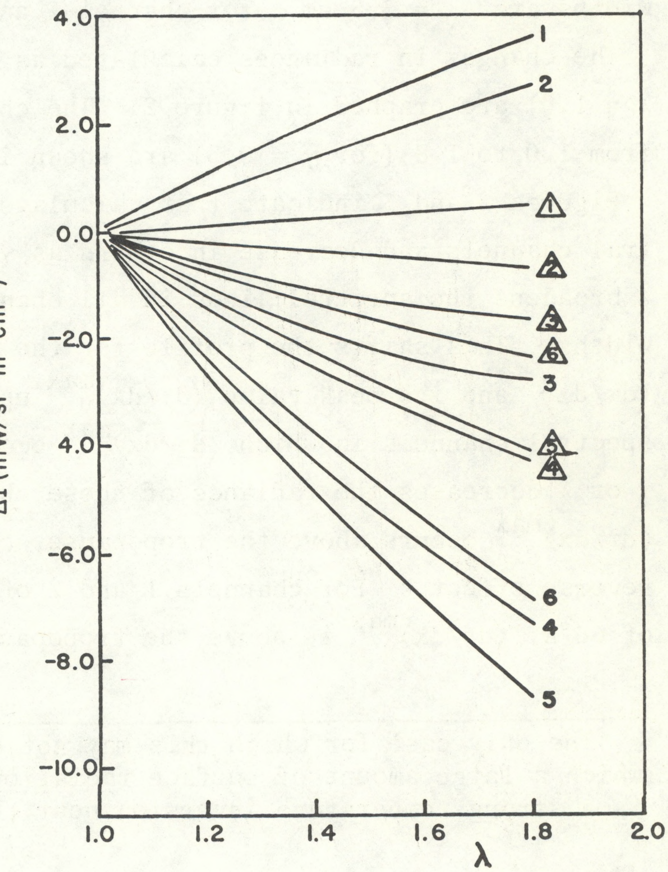


Figure 2.--Changes in spectral radiance (ΔI) for VTPR CO_2 channels calculated as a function of γ for λ = 1.0 and C_{CO_2} = 320 ppmv. Calculations for profiles of figure 1. Values for the channels at 15°N are 1, 2, ..., 6; at 60°N, 1, 2, ..., 6.

Figure 3.--Same as figure 2 except as a function of λ for γ = 0.5.



γ or λ are increased. For all remaining channels, $\langle d\tau/dx \rangle_\nu^{max}$ is below the tropopause; their radiances decrease if either quantity is increased.

The maximum permissible error in observed radiance for the spectral channels of VTPR has been set by Wark and Fleming (1966) at

$$\Delta E = 0.25 \text{ mW/(sr m}^2 \text{ cm}^{-1}\text{)}.^* \tag{7}$$

As mentioned previously, the errors in calculated radiances (from the first guess temperature profile) can be no greater than the errors allowed for observed radiances. Table 2 shows the amount by which γ and λ can be varied separately for every spectral line and still limit the change in calculated radiance to be less than ΔE in every spectral channel of VTPR.

Table 2.--Maximum variation in λ, γ, and C_{CO_2} or $S(T)$ for which the change in calculated radiance is less than ΔE of eq (7) for all spectral channels of VTPR

Parameter	Variation (absolute value) 15°N annual profile	60°N winter profile
γ	0.06	0.11
λ	0.02	0.04
C_{CO_2}	4 ppmv	7 ppmv
$S(T)$	1.3%	2.2%

The limits obtained in this study for γ and λ are considerably smaller than the uncertainties of these quantities derived from current experimental data on spectral linewidths.

Values of γ have been measured for only a few lines in the CO_2 spectrum. Measurements of the self-broadened linewidths in the ν_3 band give values of γ between 0.88 and 2.15 (Tubbs and Williams 1972). In the ν_2 band, measurements of γ for CO_2 mixed with N_2 have been made for a few lines in the "Q" branch by Aronson et al. (1974). They obtained values of γ = 0.52 to 1.05 from measurements made over a temperature range of 200 to 300 K. Values of γ have not

*The tolerance for channel 1 (the ν_2 "Q" branch) is twice this value.

been measured for other lines in the ν_2 band, but they may differ appreciably from the value $\gamma = 0.5$, assumed in Drayson's program.

Recent measurements of the linewidth $\alpha_L(T_0, P_0)$ made in the 15-m "Q" branch by Aronson et al. (1974) are consistently 10 to 20% higher than the values of Drayson's program (taken from Yamamoto et al. 1969). The only other linewidth measurements in the ν_2 band are those made by Madden (1961) for a few isolated lines. If one assumes that all linewidths in this band have been underestimated by 10 or 20%--a possible implication of Aronson's measurements--then λ should be at least 10% greater than the value now used in Drayson's program. If the current value of λ is in error by this amount, the errors in the first guess radiances calculated for these temperature profiles are well outside their permissible limits.

The spread in experimentally determined values of γ and λ, the corresponding uncertainty in radiances calculated for these parameters for the two temperature profiles of figure 1, and the spectral channel of VTPR most sensitive to variation of these parameters, are summarized in table 3. The uncertainties in calculated radiance are well outside the limits of eq (7).

It is clear that the values of γ and λ are not known with sufficient accuracy for the ν_2 band to guarantee that first guess radiances can be calculated to the accuracy required for retrieving temperature profiles from atmospheric radiances. The need for additional laboratory measurements of these parameters is apparent.

Table 3.--Range of possible values for the spectral line parameters for $CO_2\nu_2$ band and corresponding range or uncertainty of radiances calculated for VTPR

Parameter	Value used in current line-by-line program (Drayson 1966) to calculate transmittance	Range of experimentally determined value (Madden 1961, Aronson et al. 1974)	Range of calculated radiance for the most sensitive spectral channel of VTPR ($mW/sr\ m^2\ cm^{-1}$)	
			15°N profile	60°N profile
γ	0.50	0.52 to 1.05	1.8	1.2
λ	1.0	1.1 to 1.2	1.3	0.7
$S(T)/S_0(T)$	1.0	1.05 to 1.10	0.9	0.4

$S_0(T)$ is the value of line strength used in Drayson's program.

Results for Different CO_2 Concentrations

Transmittances and radiances were calculated for five values of C_{CO_2}, the mole fraction of atmospheric CO_2, for the temperature profiles described earlier. Concentration was assumed to be independent of height in each case. The mole fraction of CO_2 currently used in Drayson's program is 320 parts per million by volume (ppmv). Radiances calculated for this amount of CO_2 are listed in table 1. The changes in radiance that occurred as C_{CO_2} was varied are plotted in figures 4 and 5.

Increasing the value of C_{CO_2} also increases the total absorption, shifting the profile for $\left\langle d\tau/dx \right\rangle_{\nu}^{max}$ upward in the atmosphere. Hence, the behavior of the radiance in each spectral channel is qualitatively the same as when γ or λ is increased. This accounts for the similar behavior of the curves in figures 2, 3, 4, and 5.

The transmittance profile $\left\langle d\tau/dx \right\rangle_{\nu}$ depends on the line strength $S(T)$ in the same way it depends on C_{CO_2}. This is true because the transmittance of eq (5) contains the product of C_{CO_2} and $k(\nu,P)$, which is directly proportional to $S(T)$. Table 2 shows the maximum percentage by which C_{CO_2} or $S(T)$ can be varied for each spectral line to limit the change in calculated radiance to less than ΔE for every spectral channel of VTPR.

The limits of table 2 are considerably lower for the 15°N profile than for the 60°N profile. It can be seen in figures 2 to 5 that the sensitivity of calculated radiances to the choice of γ, λ, or C_{CO_2} is greater in each spectral channel in the profile of 15°N than for the profile of 60°N.

The simplest explanation for the greater sensitivity in the 15°N profile is that the variation of radiance calculated for a given shift in $\left\langle d\tau/dx \right\rangle_{\nu}^{max}$, by a change in either γ, λ, or C_{CO_2}, is directly proportional to the lapse rate in the region of $\left\langle d\tau/dx \right\rangle_{\nu}^{max}$. Since the lapse rates are steeper at 15°N than at 60°N, the calculated radiance changes are expected to be greater at 15°N.

Current literature (Bischof 1963, Bolin and Bischof 1970, and Woodwell et al. 1973) indicates the present global concentration of CO_2 is

$$C_{CO_2} = 325 \pm 2 \text{ ppmv},$$

with an average annual rate of increase (Machta and Telegdas 1974) of

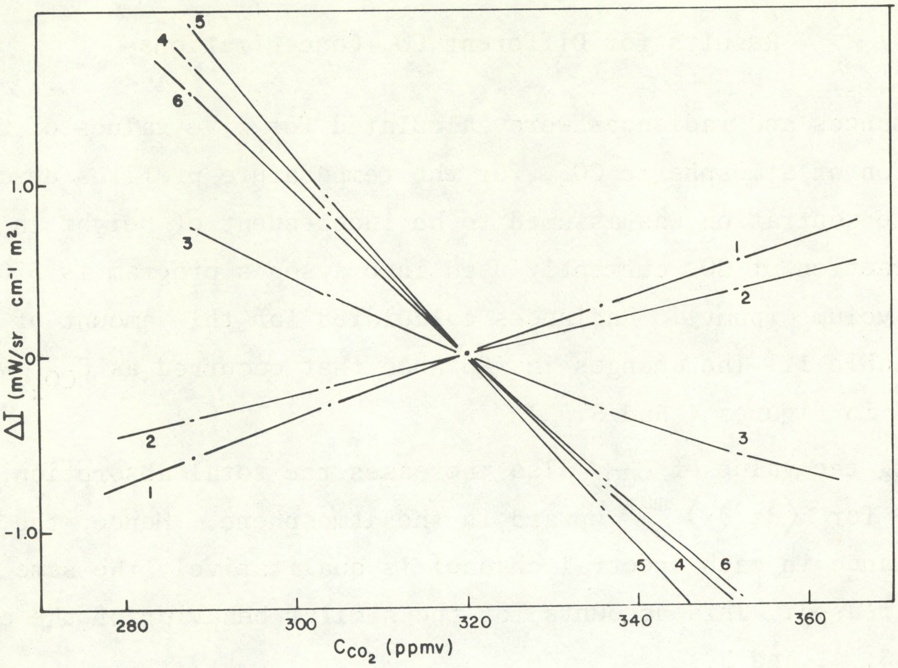


Figure 4.--Calculated shifts in spectral radiance for the 6 CO_2 channels of VTPR as a function of C_{CO_2} for λ = 1.0 and γ = 0.5, for the 15°N profile

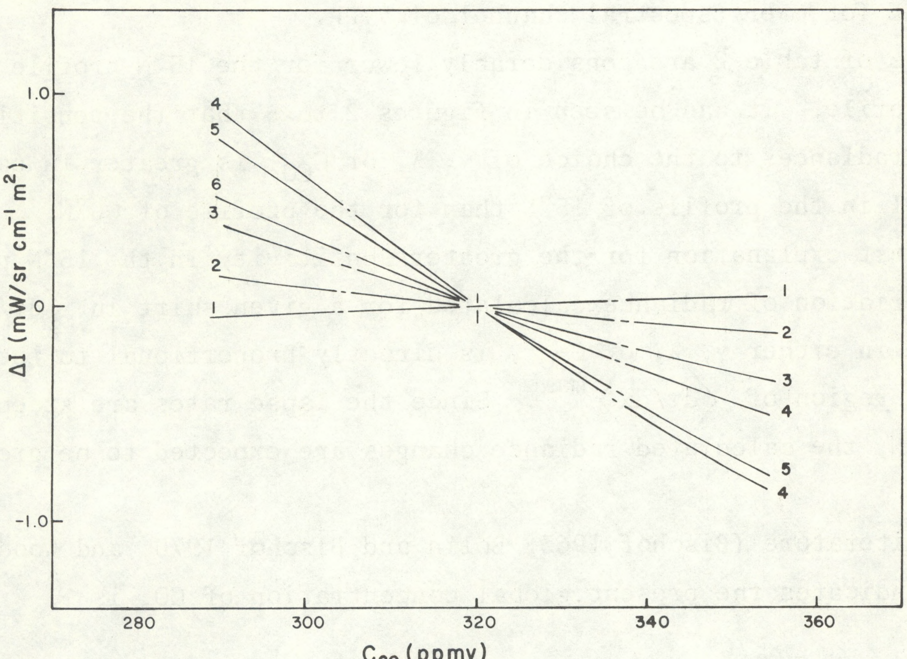


Figure 5.--Same as figure 4 except for 60°N profile

$$\frac{dC_{CO_2}}{dt} = 0.7 \pm 0.1 \text{ ppmv/yr.}$$

In addition to the secular increase of C_{CO_2}, seasonal changes of 5 ppmv occur. There are also changes with geographic location and altitude (Pales and Keeling 1965, Brown and Keeling 1965, and Bolin and Keeling 1963).

The uncertainty of 5 ppmv (1.6%) in C_{CO_2} is between the limits allowed for this quantity in table 2. A more serious source of error is the uncertainty in individual spectral line strengths.

Values for S(T) for the individual spectral lines of the VTPR CO_2 channels are determined indirectly from low-resolution measurements of the integrated absorption

$$\langle A \rangle_\nu = \int_{\nu_1}^{\nu_2} d\nu \, \{1 - \exp[-k(\nu)p\ell]\} \tag{8}$$

where p = pressure in atmospheres,

and ℓ = path length in centimeters

for CO_2 in the 14- to 16-μm spectral region. Methods for doing this have been described by Kaplan and Eggers (1956) and by Gray and Selvidge (1965).

The total strength is defined as

$$S_B = \int_{\nu_1}^{\nu_2} d\nu \, \Sigma_{\nu_i} k_{\nu_i}(\nu) \tag{9}$$

where k_{ν_i} = absorption of coefficient of spectral lines centered at wavenumber ν_i. The sum is taken over all lines of all bands that absorb in the spectral region of interest. Values for the total band strength of the 14- to 16-μm spectral region, as determined by various workers, are summarized in table 4. Only data taken since 1955, which appear to be free of experimental bias, are included in this table. The relative error estimated for the total band strength appears to be small, and is of the order of uncertainty of the value for C_{CO_2}.

The two principal difficulties in calculating individual line strengths are partitioning the total band strength between the various vibration-rotation bands in this spectral region, and then determining the strengths of the individual lines within each band from the strength assigned to that

Table 4.--Experimental values for the strengths of the CO_2 bands in the 14- to 16-μm spectral region

S (cm^{-2} atm^{-1})STP	Observer	
240 ± 5	Kaplan and Eggers	(1956)
230 ± 20	Harward and Patty	(1968)
246 ± 8	Wolk	(1967)
251 ± 11	Madden	(1961)
240 ± 36	Ludwig et al.	(1966)
241.2 ± 3.1	*	

*Mean of above measurements, and standard deviation determined from weighted variances.

band. In using these techniques for calculating individual line strengths, the assumption is that rotational and vibrational energies of the CO_2 molecule do not interact. Comparisons with the small amount of experimental data available from tunable lasers (Aronson et al. 1974) indicate that line strengths calculated in this way may be in error by 5 or 10% at temperatures and pressures encountered near and above the tropopause.

The error calculated radiance for an uncertainty of 5 to 10% in the assumed line strength is shown in table 4 for the most sensitive spectral channel of VTPR--in which the transmittance profile peaks at or above the tropopause. This error is clearly outside the limits of eq (7).

The best hope for reducing errors in calculated radiances attributable to uncertainties in S(T) is to determine k(ν) and S(T) directly for each spectral line. It will be possible to do this with tunable lasers now available for scanning the "Q" branch and those being developed for scanning the rest of the spectral region for the CO_2 ν_2 band.

RESULTS AND CONCLUSIONS

In this paper we have described the sensitivity of calculated transmittances and radiances to variation in spectral line shape and line strength or absorber concentration determined for the 6 CO_2 channels of VTPR. The changes in radiances that result as these quantities are varied are shown in figures 2 to 5 for the temperature profiles of figure 1.

As stated earlier, the error in calculated radiance (from the first guess temperature profile) can be no greater than the allowed error ΔE for observed radiances for any spectral channel of VTPR. [See eq (7).] Table 2 shows the amounts by which the line shape parameters γ or λ and the line strength S(T) or the absorber concentration C_{CO_2} can be uncertain, and still limit the errors in calculated radiances to less than ΔE for all spectral channels. The limits for both profiles are the systematic errors in these quantities for all spectral lines and the entire temperature sounding. Uncertainties in γ, λ, and S(T) for a single spectral line or for the uncertainty in C_{CO_2} at different pressure levels within a temperature sounding can probably be greater than the values of table 2.

The acceptable limits of error for γ, λ, and S(T) given in table 2 are much less than the uncertainty in our present knowledge of these quantities (as summarized in table 3). The uncertainty in C_{CO_2} is not as serious as that for the other quantities, but still gives errors in calculated radiance that are equal to the permissible noise level of VTPR for some spectral channels and for some temperature profiles.

The uncertainties in γ, λ, and S(T) appear to be too great to permit retrieval of temperature profiles from measured radiances and first guess radiances computed from calculated transmittances alone. Laboratory studies must be continued to obtain more accurate values for γ, λ, and S(T) for use in the line-by-line computer programs for calculating atmospheric transmission. Such values would lessen the need for making empirical adjustments to the radiance data to retrieve the temperature profile.

The means of obtaining the required information on these quantities is through detailed high-resolution spectroscopic measurements of the transmission of CO_2 in the 15-μm region at different pressures and temperatures. Such work is under way at the Satellite Experiment Laboratory (SEL) of the National Environmental Satellite Service (NESS). It will be carried out with the SEL high-resolution spectrometer and with tunable lasers as they become available.

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