A MODEL FOR COMPUTING INFRARED TRANSMISSION

THROUGH ATMOSPHERIC WATER VAPOR AND CARBON DIOXIDE

By: Paul A. Davis and William Viezee

Prepared under Contract NAS 5-2919

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SPECIAL REPORT

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ABSTRACT

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Analytical expressions are developed for the direct computation of infrared transmission as a function of the amount, pressure, and temperature of the absorber. The parameters that are necessary for the application of the expressions are tabulated over the wave number range between 25 and 2150 per centimeter (400 to 4.65 microns in wavelength) in intervals of 25 per centimeter. Comparisons are made between the computed transmissions and corresponding transmissions that have been presented in recent literature. author

I INTRODUCTION

The distribution of atmospheric patterns of absorption and emission of long-wave radiation varies with evolving meteorological conditions and identifies sources and sinks of energy. With the advent of infrared measurements from satellites, greater urgency has been placed on the adequate description, in some spectral detail, of the concurrent radiation field between satellite altitudes and the surface of the earth. In lieu of networks for obtaining routine tropospheric radiation measurements, a convenient numerical method could provide a means for establishing relationships between infrared data and significant atmospheric properties.

In any model of infrared radiative transfer the paramount problem is that of properly specifying the transmission through different spectral regions. If the model is oversimplified, significant radiative properties may be overlooked or distorted; if the model is too sophisticated, it will not be practicable for routine application to sizable quantities of data. In general, the minimum complexity demanded of a model is related to the desired spectral resolution and the significance of any computation depends on the reliability of the basic meteorological data.

For this investigation a transmission representation was considered satisfactory if it met the following requirements:

(1) It should be reproducible and practicable for objective application without excessive empiricism or data listings.

(2) It should respond adequately to the variable pressure, temperature, and absorber conditions of the troposphere and lower stratosphere.

(3) It should be capable of representing the transmission over wave number intervals of about 50 cm^{-1} or less.

(4) It should be compatible with available experimental data, and

flexible enough to permit a simple adaptation to new data that becomes available.

Since many methods for describing transmission have been used, it is likely that different opinions exist regarding the relative merits of applied techniques. It is not likely that most models would completely satisfy all of the requirements listed above. The purpose of this report is to present a practical model for making direct computations of transmission for a variety of applications.

II EMPIRICAL REPRESENTATION

An empirical representation of the transmission must be bounded by the limits of unity and zero. As these limits are approached, uncertainty arises when absorber amounts and pressures are encountered for which transmission data do not exist. In general, extensive testing is necessary to ensure that the transmission functions behave in a proper physical sense for all variations in the conditions to which they may be applied. One type of difficulty may arise in the spectral region of transition from one transmission form to another (c.f., Wark, et al., 1964). In addition, within a given spectral interval, there are physical constraints to the derivatives of the transmission functions. For example, as a given layer is extended from a fixed level in the atmosphere toward lower pressure and temperature, even with only a very slight increase in absorber amount, the transmission should decrease. In contrast, the lower pressure and temperature may tend to increase the transmission through a fixed optical thickness. Thus the pressure and temperature must be inserted with care in the transmission expression. Unfortunately, it is difficult to accurately specify the proper effective pressures and temperatures for application to all types of non-homogeneous paths.

Since one purpose of an empirical representation is to provide the average transmission over a finite spectral interval, the nature of the representation will be strongly dependent on the width and location of the interval. Figure 1 illustrates some of the transmission variations with wave number and spectral width in a weak absorption region of a carbon dioxide band. All of the data for Fig. 1 were taken from Stull et al., (1963). The two dashed curves are based on computations for a spectral width of 50 cm^{-1}, centered at 550 cm^{-1} and 575 cm^{-1}, with a 50-percent overlap. The three solid curves refer to spectral widths of 20 cm^{-1}, centered at intervals of 10 cm^{-1} in the same spectral region. It is apparent from Fig. 1 that in certain spectral regions the shapes of the transmission curves may change significantly as the width of the spectral interval changes. Furthermore, the three solid curves show that the average of the transmissions at 570 cm^{-1} and 550 cm^{-1} differs from the actual transmission at 560 cm^{-1}. It may be inferred that, in general, it is not proper to apply a transmission which has been determined at a particular spectral width to another spectral width, or to assume that the smoothed transmission varies linearly with wave number. Finally, the absolute values of the transmission may change rapidly with wave number (note the dashed curves in Fig. 1) so that comparisons of transmissions from different sources should allow for real differences unless both the spectral width and location are identical.

In order to attach physical significance to an empirical model or to provide for a logical adjustment of the model parameters to fit new data, it is necessary to establish the basic framework upon which the model was developed. The extensive analyses leading to the model presented here are omitted, but a brief review of the framework is given below.

III TRANSMISSION THROUGH WATER VAPOR

As a focal point for the analysis of laboratory data or theoretical computations, it is convenient to extract from the data an absorber amount which is associated with a fixed moderate transmission. In this study W_h is defined as the absorber amount, variant with pressure and temperature, for which the transmission is one-half. In order to develop a representation of all transmissions, the W_h must be incorporated in a general expression. For water vapor bands, the basic expression chosen for the representation was that of Goody (1952), given by

$$-\ell n\tau = \frac{\pi\sigma\alpha W}{\delta(\pi^2\alpha^2 + \pi\sigma\alpha W)^{\frac{1}{2}}} \tag{1}$$

where τ is the transmission, W is the amount of precipitable water along the path, δ is the mean line spacing, σ is the mean line strength, and α is the mean half-width for a small spectral region. At a transmission of one-half, Eq. (1) may be solved in terms of $\sigma\alpha$ in the form

$$\sigma\alpha = \frac{1}{W_h}\left\{\frac{(\epsilon\delta)^2}{2\pi} + \left[\frac{(\epsilon\delta)^4}{4\pi^2} + (\epsilon\delta\alpha)^2\right]^{\frac{1}{2}}\right\} = \frac{g}{W_h} \tag{2}$$

where $\epsilon \equiv -\ell n\frac{1}{2}$ and the quantity in braces is denoted by g. If the subscript s is used to denote standard conditions and if the half-width is expressed in the form $\alpha = \alpha_s \frac{P}{P_s}$, presumably at standard temperature, then Eq. (1) may be rewritten as

$$-\ell n\tau = \frac{\beta W}{PW_h}\left[1 + \frac{\gamma W}{P^2 W_h}\right]^{-\frac{1}{2}} \tag{3}$$

where P is the pressure ratio $\frac{p}{p_s}$, $\beta \equiv \frac{g}{\delta \alpha_s}$, and $\gamma \equiv \frac{g}{\pi \alpha_s^2}$. Both coefficients γ and β are somewhat pressure dependent through the α term in g, but their ratio, r, is independent of pressure:

$$r \equiv \frac{\gamma}{\beta} = \frac{\delta}{\pi \alpha_s} \quad . \tag{4}$$

After inserting the definitions of g and r in the definition of β, the description of β as a function of pressure becomes

$$\beta = \frac{r\epsilon^2}{2} + \left[\frac{r^2 \epsilon^4}{4} + \epsilon^2 P^2 \right]^{\frac{1}{2}} \quad . \tag{5}$$

The P term in Eq. (5) is negligible at the lower pressures in the atmosphere. From Eqs. (3), (4), and (5) it is apparent that the key parameters in the specification of τ are W_h and r. The empirical fitting of these parameters probably constitutes some departure from the randomness of the Goody model.

The first step of the analysis in this investigation was to determine W_h as a function of wave number, pressure, and temperature. Then, with the aid of a theoretical first guess, the ratio r was selected on the basis of successive trials leading to the desired transmission. To a good approximation, the parameter r was taken as constant over an entire absorption band.

Examination of W_h data from a number of sources suggested that, although W_h changed markedly with wave number, the relationship of W_h to pressure remained nearly constant over most of the intervals of a band. The W_h representation was adopted in the convenient form

$$\frac{1}{W_h} = L_\nu \, P^n \left(\frac{T}{T}\right)^{b_\nu} \tag{6}$$

where L_ν is the value of $\frac{1}{W_h}$ at standard pressure and temperature, the exponent n is considered constant over an entire band, and the exponent b_ν of the temperature ratio is a function of wave number. The parameters L_ν, n, and b_ν were determined empirically.

IV THE 1595 cm^{-1} BAND OF WATER VAPOR

For the specification of transmission through the 1595 cm^{-1} band of water vapor, data from Cowling (1950), Daw (1956), Howard *et al.* (1956), Burch *et al.* (1962), Wark *et al.* (1962), and Wyatt *et al.* (1962) were considered. Cowling's data were used only for checking at standard conditions, and Daw's data were used only as an aid to the evaluation of the pressure dependence of W_h. The pressure exponent n [see Eq. (6)] was found to vary between 0.7 and 0.95. Although much of the variability could have been associated with experimental scatter, some variation of n can be expected with pressure itself and, to a lesser extent, with wave number. Since a slight variation in n is not a dominant factor in the water-vapor model, a mean value of 0.85 was adopted for all wave numbers. If the model was to be applied to a single pressure region only, an optimum value of n could be determined, but at the lowest pressure the uncertainty in water-vapor amount becomes the dominant factor.

The determination of L_ν as a function of wave number was based on Howard *et al.* (1956), Burch *et al.* (1962), and Wyatt *et al.* (1962). Prime emphasis was given to the laboratory data of Burch *et al.* for the general shape of the curve of L_ν versus wave number, and for the wave-number location of principal transmission features, especially near the band center. A shift of the data from Howard *et al.* with wave number was necessary, in order to bring theirs into line with the other data. From

1200 cm^{-1} to 2150 cm^{-1} L_ν was tabulated for intervals with widths of 25 cm^{-1}. Since most of the data had been smoothed over intervals as large as 50 cm^{-1} before the tabulation, the appropriate application of the transmission model should include two or more successive intervals.

The temperature effect on the transmission through the entire 1595 cm^{-1} band is of minor importance to the total atmospheric emission, and no temperature dependence was included in the transmission function. However, instead of a final tabulation of L_ν for standard temperature, an adjustment was made to a mean atmospheric temperature of -20C by making use of the detailed theoretical computations of Wyatt et al. This value of $\frac{1}{W_h}$ for an average atmospheric temperature and for standard pressure was denoted by L_ν^*. Temperature adjustments in the central portion of the band are reversed from those in the wings.

After a number of successive trials of the model against available data the value of 4.9 was assigned to the ratio r and the transmission for the 1595 cm^{-1} band was expressed by

$$\tau = \exp \left\{ -\beta P^{-0.15} L_\nu^* W \left[1 + 4.9\, \beta P^{-1.15} L_\nu^* W \right]^{-\frac{1}{2}} \right\} \qquad (7)$$

where $\beta = 1.18 + (1.38 + 0.48P^2)^{\frac{1}{2}}$ and tabulations of L_ν^* are included in Table 1. Transmissions computed from Eq. (7) for two arbitrary intervals at three pressures are illustrated in Fig. 2 with the corresponding representations of Wark et al. (1962) and Wyatt et al. Deviations of computed points from the curves of Wark et al. (1962) are probably some measure of residual uncertainty. The data of Wyatt et al. refer to a slightly narrower spectral width (20 cm^{-1}) and are centered at slightly smaller wave numbers than the other curves.

V THE ROTATIONAL BAND OF WATER VAPOR

The analysis in the rotational band was based primarily on the data of Palmer (1960) for the 200 to 500 cm^{-1} region and on Yamamoto and Onishi (1949) for the remainder of the region between 25 cm^{-1} and 800 cm^{-1}. Values of L_ν for 25 cm^{-1} intervals were obtained from smoothed W_h curves in the same manner as for the 1595 cm^{-1} band. Palmer's data were separated according to pressure, and analyzed along with presentations of Wark et al. (1962) in order to determine the pressure dependence of W_h. A mean value of 0.9 was adopted for n. The temperature exponent b_ν was determined from the data of Yamamoto and Onishi for the region between 225 and 600 cm^{-1}. Both L_ν and b_ν are tabulated in Table 1.

With the empirical estimate of 3.17 for r the transmission in the rotational band was expressed by

$$\tau = \exp\left\{ -\beta P^{-0.1} L_\nu W \left(\frac{T}{T_s}\right)^{b_\nu} \left[1 + 3.17\,\beta P^{-1.1} L_\nu W \left(\frac{T}{T_s}\right)^{b_\nu}\right]^{-\frac{1}{2}} \right\} \qquad (8)$$

where $\beta = 0.76 + (0.58 + 0.48P^2)^{\frac{1}{2}}$.

The transmissions in two spectral intervals for three pressures and a temperature of 260 K were computed from Eq. (8) and compared with the corresponding representations from Wark et al. (1962) in Fig. 3.

VI THE WINDOW REGION

Transmission data for the broad window region, taken here as the interval between 800 cm^{-1} and 1200 cm^{-1}, vary from one study to another. In this study the data of Roach and Goody (1958) were used to compute the transmission for a number of pressures and water-vapor amounts.

Results were fitted to the expression

$$\tau = \exp\left\{-(k_\nu WP)^{a_\nu}\right\} \tag{9}$$

and the parameters k_ν and a_ν are tabulated for each 25 cm^{-1} interval in Table 1. The exponent a_ν decreases from near unity in the central intervals as either absorption band is approached, while the absorption coefficient k_ν varies in the opposite sense. Both parameters were fitted for an average atmospheric pressure. A more detailed pressure dependence than that contained in Eq. (9) was devised but the differences in results were insignificant except possibly along long slant paths. Although Eq. (9) includes the effects of wing absorption from distant carbon dioxide lines, the effects of absorption from ozone or the weak 1064 cm^{-1} and 961 cm^{-1} bands of carbon dioxide have not been incorporated in this transmission model for the window region.

Figure 4 illustrates the transmission computed from Eq. (9) for the 925-950 cm^{-1} interval versus the product of water-vapor amount (W) and effective pressure (P). The open dots in Fig. 4 were determined from a comparble representation by Wark et al. (1962).

VII CARBON DIOXIDE TRANSMISSION

The basic data for modeling the carbon dioxide transmission were taken from Wark et al. (1962) and Stull et al. (1963). The presentations of Wark were based in part on data from Yamamoto and Sasamori (1962). Since the initial analyses for the ten 25 cm^{-1} intervals between 550 cm^{-1} and 800 cm^{-1} were based on Wark's data, the transmission model generally gives better agreement at standard conditions with Wark et al. than with Stull et al.

Plots of the Wark data suggested a transmission expression in the form

$$\tau = \exp - \left\{ \left[A_{P,T} W + C_P^2 \right]^{\frac{1}{2}} - C_P \right\} \tag{10}$$

where the coefficient A is a function of both pressure and temperature, parameter C is a function of pressure only, and W is the amount of carbon dioxide in atmos-cm. While Eq. (10) is not unique, it is one of the simplest forms that appears to be adequate. If W_h still denotes the optical thickness for a transmission of one-half, and $-\ell n\frac{1}{2}$ is denoted by ϵ, then Eq. (10) can be solved in the form

$$A = \frac{1}{W_h} \left(\epsilon^2 + 2\epsilon C\right)$$

which shows the relationship between A and C. Furthermore, if $\frac{1}{W_h}$ is again described in the form given by Eq. (6) and if C is described in the form $C = C_s P^m$, then Eq. (10) may be rewritten in the form

$$\tau = \exp - \left\{ \left[\epsilon L_\nu (\epsilon + 2C_s P^m) P^n \left(\frac{T}{T_s} \right)^{b_\nu} W + (C_s P^m)^2 \right]^{\frac{1}{2}} - C_s P^m \right\} \tag{11}$$

The three parameters L_ν, n, and b_ν were estimated from analyses of the W_h data; minor modifications in the parameters were introduced after an examination of the behavior of computed transmissions for arbitrary pressures. The pressure exponent n increases with decreasing pressure and this variation is significant for computations based on the adopted transmission expression. Consequently, for carbon dioxide the pressure exponent n was allowed to vary with P in the following manner:

$$n = 0.4 - 0.15 \log P, \text{ for } P \geq .00631,$$
$$= .73, \text{ for } P < .00631. \tag{12}$$

The linear variation of n with log P is equivalent to an expression of the log W_h by a second-order polynomial in log P instead of a first-order polynomial as in Eq. (6). A magnitude of 0.8 for the exponent m, taken as a constant with respect to wave number, was selected by seeking the highest value that would still yield the proper variation in transmission for the lowest optical paths to be included in application. Successive comparisons of the computed transmission to available data led to the selection of 0.4 for C_s, invariant with wave number.

Finally, with the definitions $K_\nu \equiv \frac{2\epsilon}{C_s} L_\nu$ and $a \equiv n - 1.6$, Eq. (11) becomes

$$\tau = \exp\left[-0.4P^{0.8}\left\{\left[K_\nu W\,(0.87 + P^{0.8})\,P^a\left(\frac{T}{T_s}\right)^{b_\nu} + 1\right]^{\frac{1}{2}} - 1\right\}\right] \tag{13}$$

where K_ν and b_ν have been tabulated for each spectral interval in Table 1.

Comparisons of the transmissions computed from Eq. (13) with the presentation of Wark et al. (1962) and Stull et al. (1963) are illustrated in Fig. 5 for two spectral intervals, standard temperature, and three pressures. The interval 650-675 cm^{-1} corresponds to the central portion of the band. Additional comparisons are made in Fig. 6 for a weak-absorption interval, 750 to 775 cm^{-1}, for which the representations are probably less reliable than in strong-absorption intervals. Figure 6(a) shows the pressure dependence of the transmission at standard temperature and Fig. 6(b) displays the temperature dependence at standard pressure. Although there are slight differences in the spectral widths used by Wark et al. (1962) and by Stull et al., a discrepancy between estimates of the sizable temperature effect is apparent. A comparison of Figs. 6(a) and 6(b) reveals that the pressure dependence exceeds the temperature dependence.

VIII CONCLUSIONS

A model has been devised for the direct computation of infrared transmission through atmospheric water vapor and carbon dioxide under arbitrary conditions of absorber concentration, pressure, and temperature. Sufficient detail has been presented for the application and alteration of the model. Computations of the transmission described by the model have been shown to be comparable to recent published data. In its present form the model provides a practical tool for the numerical treatment of many radiative problems.

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Table 1 - Parameters appearing in analytical expressions of transmission through water vapor and carbon dioxide (Symbols defined in text)

	ROTATIONAL H_2O	
Interval	L_ν	b_ν
cm^{-1}	$(pr.\ cm)^{-1}$	
25-50	670.0	
50-75	1350.0	
75-100	2450.0	
100-125	2500.0	
125-150	2550.0	
150-175	2100.0	
175-200	1250.0	
200-225	1050.0	
225-250	955.0	0.45
250-275	710.0	1.15
275-300	410.0	1.65
300-325	290.0	1.95
325-350	265.0	2.60
350-375	140.0	3.00
375-400	53.5	2.45
400-425	37.5	2.55

	ROTATIONAL H_2O		CO_2	
Interval	L_ν	b_ν	K_ν	b_ν
cm^{-1}	$(pr.\ cm)^{-1}$		$(atmos\text{-}cm)^{-1}$	
425-450	30.500	2.75		
450-475	20.500	1.55		
475-500	11.000	1.85		
500-525	6.050	2.30		
525-550	3.700	1.55		
550-575	2.800	1.35	0.00145	4.7
575-600	2.100	0.60	0.03850	4.1
600-625	1.550		0.18000	3.1
625-650	1.100		1.70000	2.2
650-675	0.820		6.95000	0.0
675-700	0.615		4.80000	1.0
700-725	0.470		0.53000	3.0
725-750	0.370		0.11500	3.6
750-775	0.290		0.01050	4.1
775-800	0.230		0.00096	4.7

Table 1 - continued

H_2O WINDOW

Interval cm^{-1}	k_ν $(pr.\ cm)^{-1}$	a_ν	Interval cm^{-1}	k_ν $(pr.\ cm)^{-1}$	a_ν
800-825	.170	.775	1000-1025	.091	.885
825-850	.135	.820	1025-1050	.091	.885
850-875	.115	.860	1050-1075	.091	.885
875-900	.105	.880	1075-1100	.091	.880
900-925	.095	.885	1100-1125	.095	.860
925-950	.091	.885	1125-1150	.105	.830
950-975	.091	.885	1150-1175	.115	.795
975-1000	.091	.885	1175-1200	.125	.760

VIBRATIONAL - ROTATIONAL H_2O

Interval cm^{-1}	L^*_ν $(pr.\ cm)^{-1}$	Interval cm^{-1}	L^*_ν $(pr.\ cm)^{-1}$	Interval cm^{-1}	L^*_ν $(pr.\ cm)^{-1}$
1200-1225	0.28	1525-1550	570	1850-1875	18.00
1225-1250	0.42	1550-1575	295	1875-1900	11.00
1250-1275	0.75	1575-1600	87	1900-1925	7.70
1275-1300	1.50	1600-1625	110	1925-1950	6.00
1300-1325	3.10	1625-1650	235	1950-1975	4.20
1325-1350	6.40	1650-1675	370	1975-2000	2.80
1350-1375	13.50	1675-1700	405	2000-2025	1.50
1375-1400	30.00	1700-1725	320	2025-2050	0.90
1400-1425	45.00	1725-1750	220	2050-2075	0.60
1425-1450	79.00	1750-1775	135	2075-2100	0.40
1450-1475	120.00	1775-1800	87	2100-2125	0.28
1475-1500	220.00	1800-1825	52	2125-2150	0.20
1500-1525	470.00	1825-1850	30		

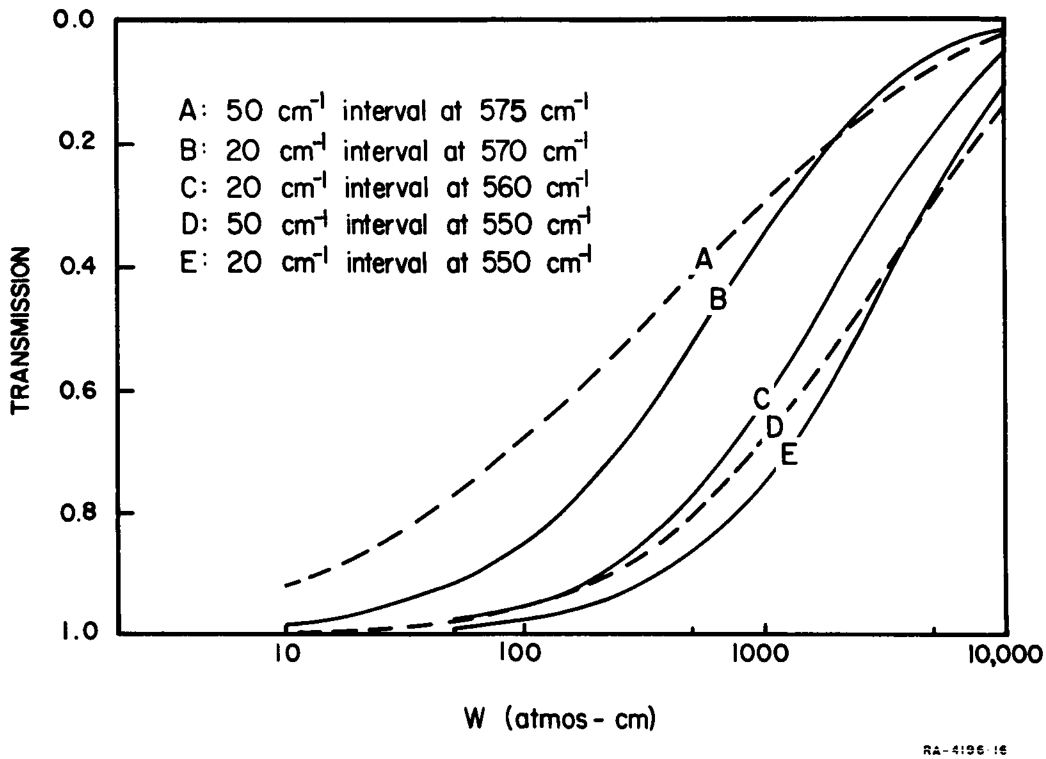

FIG. 1 CARBON DIOXIDE TRANSMISSION AT 300K AND 1-atm PRESSURE (from Stull et al., 1963)

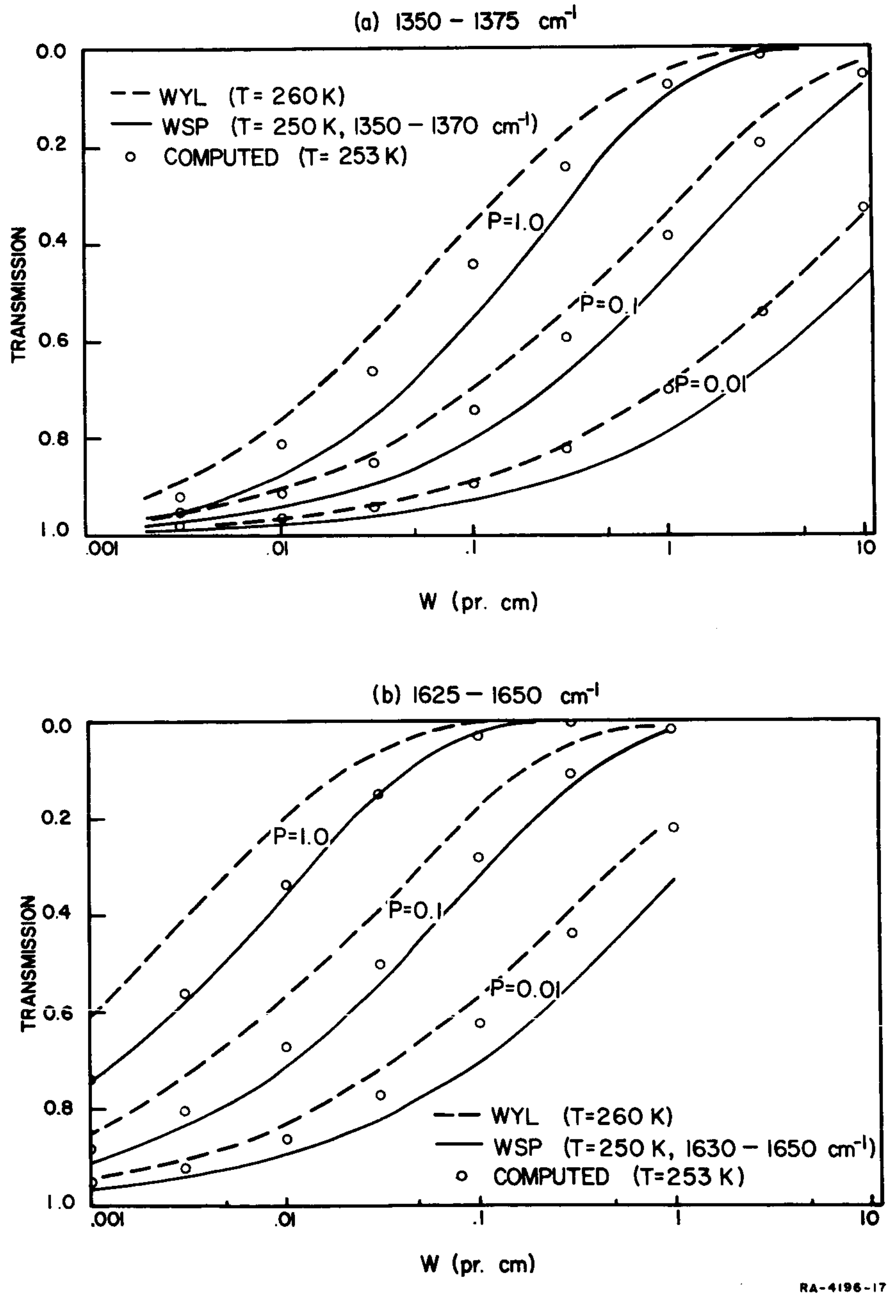

FIG. 2 TRANSMISSION THROUGH PORTIONS OF THE 1595 cm^{-1} ABSORPTION BAND OF WATER VAPOR. Note: WYL, Wark et al. (1962); WSP, Wyatt et al. (1962).

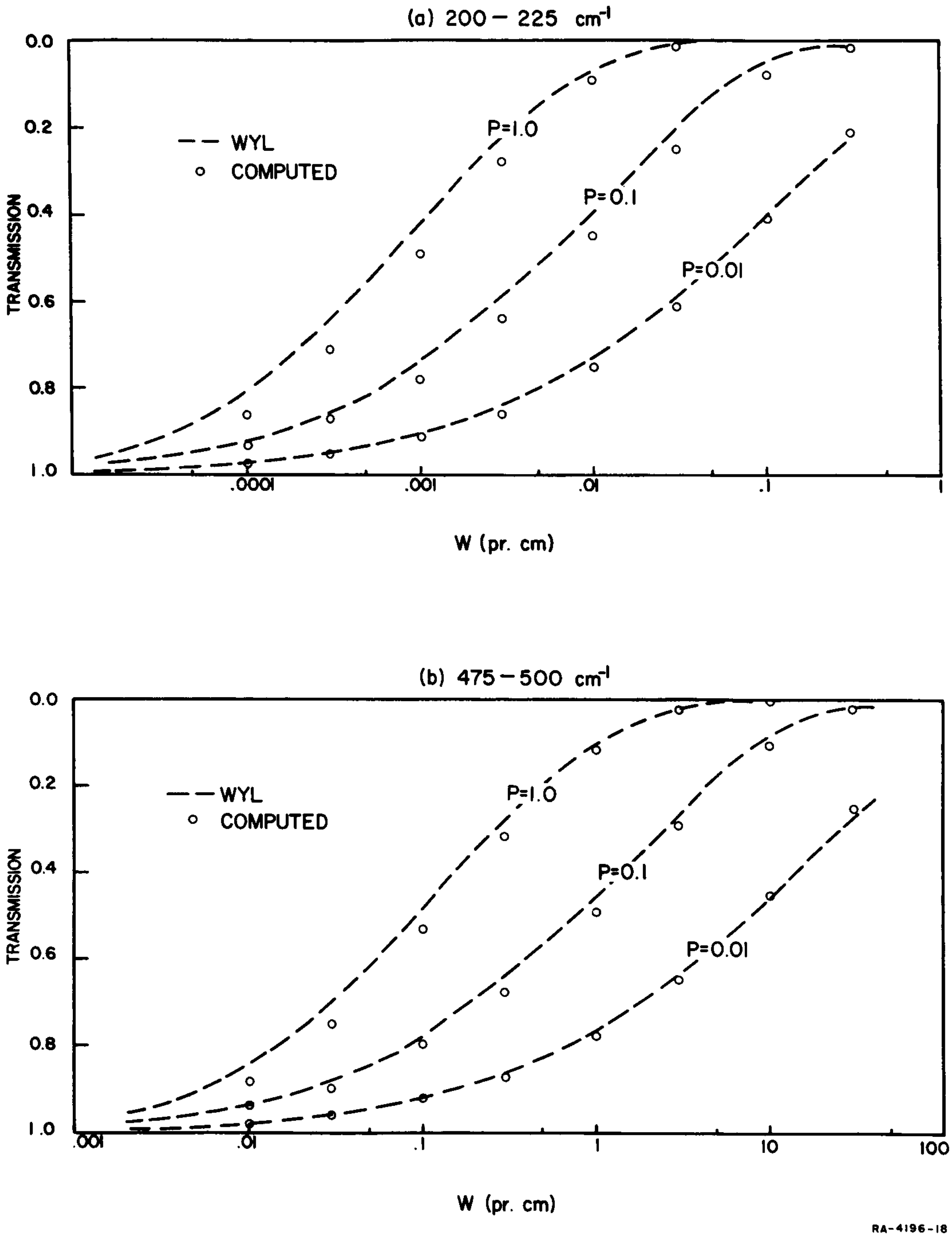

FIG. 3 TRANSMISSION THROUGH PORTIONS OF THE ROTATIONAL ABSORPTION BAND OF WATER VAPOR AT 260K. WYL: Wark et al. (1963).

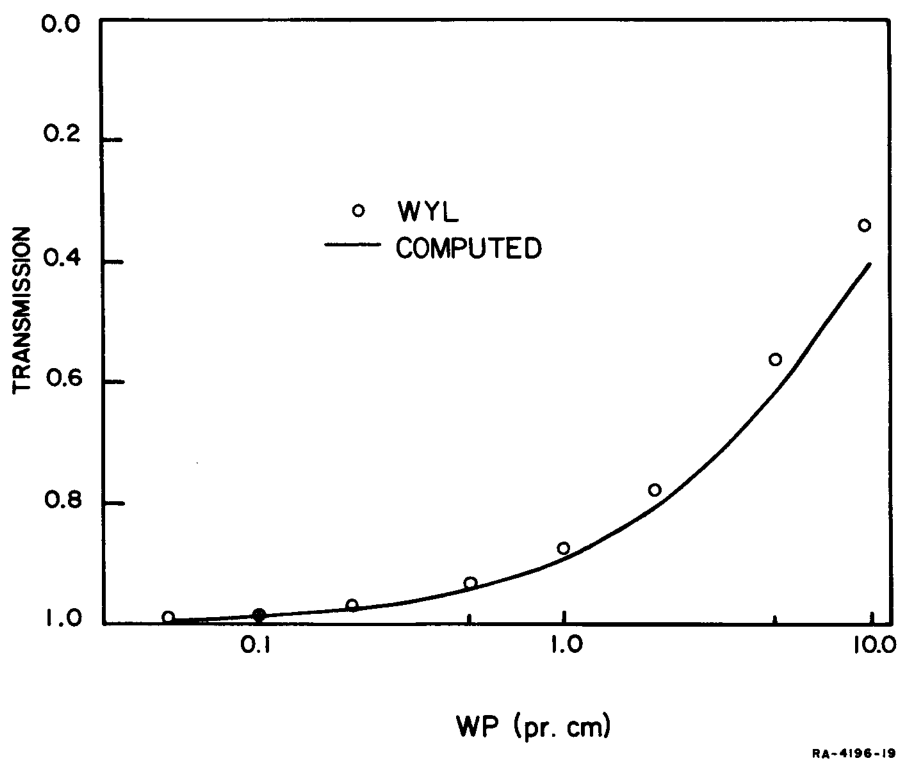

FIG. 4 TRANSMISSION THROUGH THE 925 – 950 cm^{-1} INTERVAL OF THE WINDOW REGION. WYL: Wark et al. (1962).

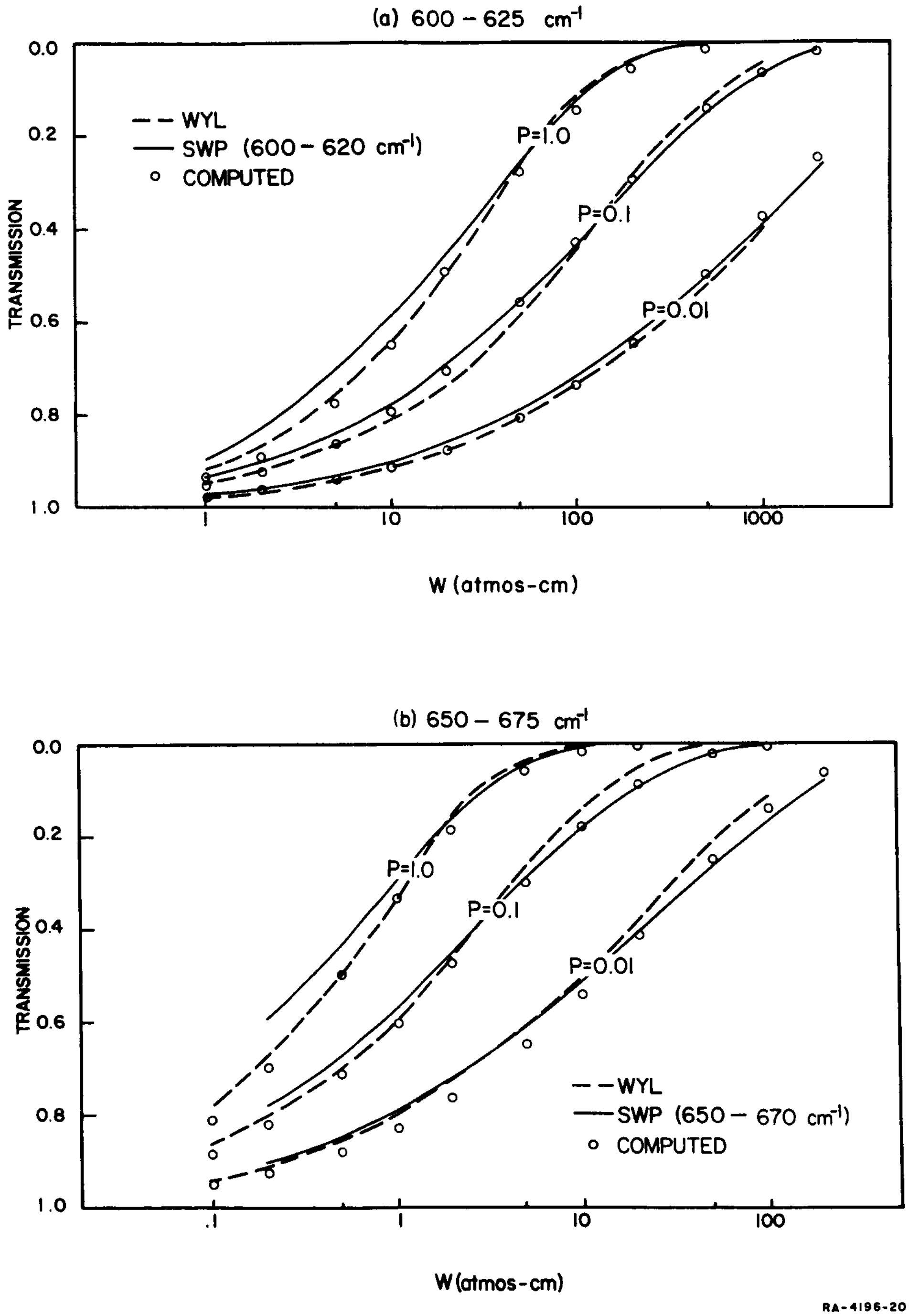

FIG. 5 TRANSMISSION THROUGH PORTIONS OF THE 667 cm^{-1} CARBON DIOXIDE BAND AT 300K. Note: WYL, Wark et al. (1962); SWP, Stull et al. (1963).

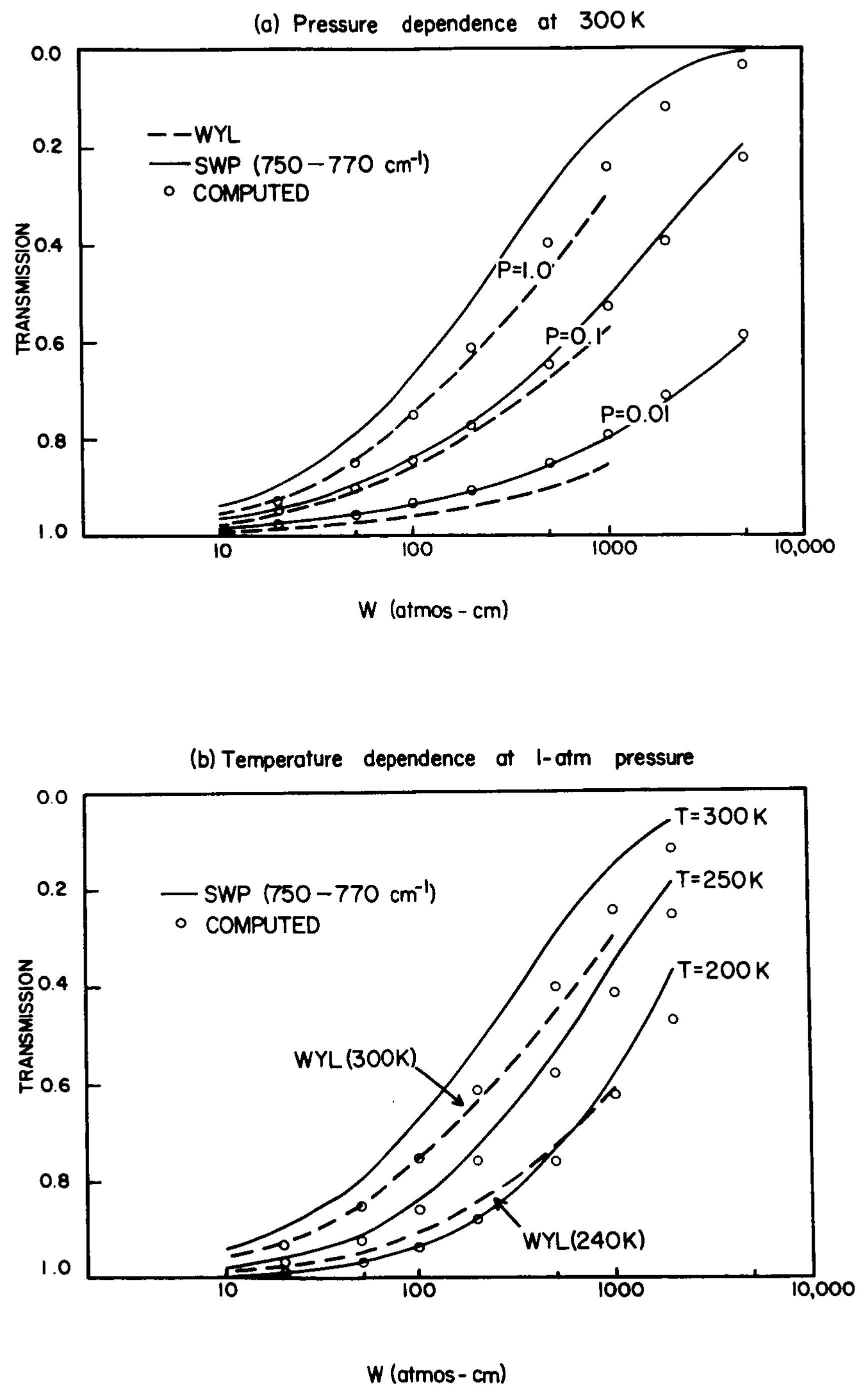

FIG. 6 TRANSMISSION THROUGH THE 750 – 775 cm^{-1} INTERVAL OF THE CARBON DIOXIDE ABSORPTION BAND. Note: WYL, Wark et al. (1962); SWP, Stull et al. (1963).