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COMPUTERIZED METHOD FOR THE GENERATION OF MOLECULAR TRANSMITTAN--ETC(U)

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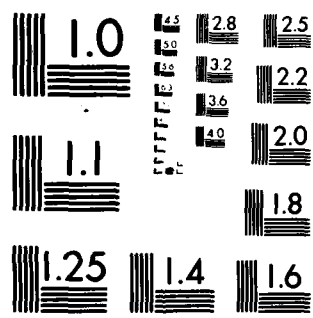
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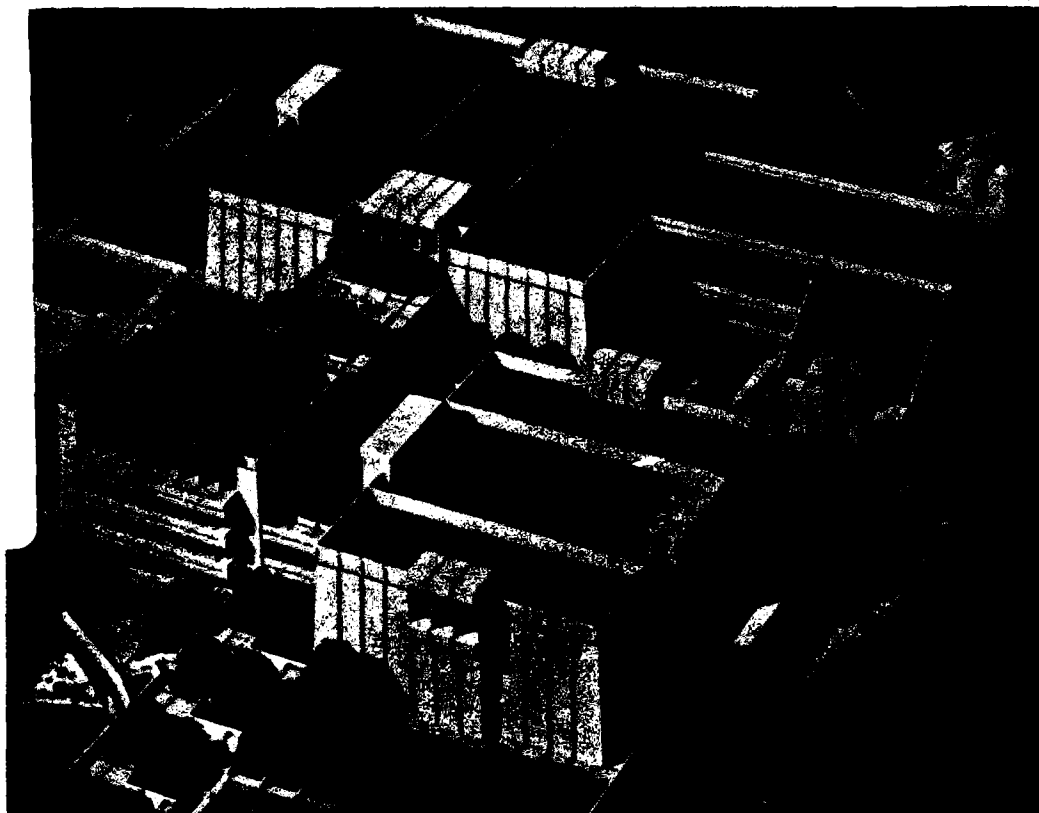
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COMPUTERIZED METHOD FOR THE GENERATION OF MOLECULAR
TRANSMITTANCE FUNCTIONS IN THE INFRARED REGION

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FINAL REPORT

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FINAL REPORT 12/31/79 FR1-79-UA-72

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with an assumed analytical transmittance function, using the same type of data. Computerized numerical techniques are presented in connection with the first method and a generalized transmittance function is adopted for the second method. Although the methodology is generally applicable to other gaseous species, it is specifically discussed in connection with the trace gases SO_2 , NO , NO_2 , and NH_3 . As a secondary effort a structural breakdown of the Lowtran code is presented for the purpose of incorporating the band models for the trace gases. The code is separated into basic functional modules or subroutines controlled by a main program. The modularization itself was primarily performed under a separate effort through the Atmospheric Sciences Laboratory.

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I. Introduction

Following the efforts of Elssasser¹ numerous workers have attempted to arrive at computationally-simple models for gaseous molecular transmittance, averaged over narrow spectral intervals in the infrared. These efforts may be naturally divided into those involving the analytical derivation of a mean transmittance function from Beer's Law, and those involving the extraction of the transmittance function itself from transmittance data. Traditionally, the former are called "analytical" and the latter are called "empirical". The method normally used in the empirical models consists of the extraction of the transmittance function through graphical techniques, with the adoption of a relationship between spectral and absorber parameters. In the development of analytical models a transmittance function is adopted at the offset, and the spectral and absorber parameters are afterward determined through computerized numerical procedures.

In the work reported here the authors present a totally computerized version of the classical graphical methods for the extraction of the empirical transmittance function. This is followed by a presentation of a numerical method which uses a double-exponential transmittance function for the development of analytical band models. Both methods are then applied to 20 cm^{-1} averaged line-by-line

transmittance data for the atmospheric trace gases SO_2 , NO , NO_2 , and NH_3 . The model parameters are listed at 5 cm^{-1} intervals throughout the major absorption bands of these gases for the convenience of the community of band model users. Although the methodology is applied specifically to the trace gases, no restrictions are immediately evident in the extension to other gaseous absorbers in the infrared. In fact, the analytical method was successfully applied earlier² to the principal band centers of the major absorbers H_2O vapor, O_3 and the uniformly-mixed gases.

As an application of the results found through this effort, the band models for the trace gases were incorporated in the widely-used code called Lowtran. To facilitate the inclusion of these models, as well as of others, the code was broken down into separate subroutines or modules controlled by a master program. The subroutines include the evaluation of the equivalent absorber amount, the selection of the spectrally-effective attenuation model and the individual attenuation models. The principal purpose of the modularization is to assist users with the modification of the code to suit their individual requirements on transmission models.

II. The Transmittance Equation

The monochromatic transmittance τ_ν at frequency ν for the passage of infrared radiation through a path length Z in an inhomogeneous medium with pressure and temperature distributions $P(Z)$ and $T(Z)$, respectively, is given by Beer's Law in the form

$$\tau_\nu = e^{-\int K_\nu(P,T) dU(Z)} \quad (1)$$

where K_ν is the resultant absorption coefficient for all contributing lines and gaseous absorbers, and U is the absorber amount. For broadband radiation detected by an instrument of spectral response ϕ_ν , the variable of interest is the weighted mean transmittance τ , defined as

$$\tau = \int \tau_\nu \phi_\nu d\nu / \int \phi_\nu d\nu \quad (2)$$

Equation (2) has been evaluated analytically over a spectral interval $\Delta\nu$ for the special case of Lorentzian broadened lines having assumed line distributions and intensities, leading to the classical band models^{1,3}. Numerous variations of the classical band models may be found in the literature, most of which specify the analytical form of τ in terms of mean line or meteorological variables. A notable exception is the model of King⁴ which expresses the homogeneous-path transmittance as

$$\tau = g(S\alpha^n U), \quad (3)$$

where g is a function to be determined empirically, S is the mean line intensity, α is the mean line half-width and n is an absorber parameter with the physical constraints of zero and one in the weak-line and strong-line limits, respectively. The path inhomogeneity may be accounted for in Eq. (3) through the Curtis-Godson equivalences

$$S\alpha^n U = \int S(Z)\alpha^n(Z)dU(Z). \quad (4)$$

From practical considerations, it is often desirable to transform the argument in Eq. (3) with the known relations

$$S = S_o \left(\frac{T_o}{T}\right)^a \quad (5)$$

$$\alpha = \alpha_o \left(\frac{P}{P_o}\right) \left(\frac{T_o}{T}\right)^{\frac{1}{2}} \quad (6)$$

in order to obtain

$$\tau = g \left\{ C \left(\frac{P}{P_o}\right)^n \left(\frac{T_o}{T}\right)^m U \right\}, \quad (7)$$

where C is a spectral parameter combining S_o and α_o^n , m is an absorber parameter combining the temperature exponents of S and α , a is an absorber constant, and the subscript "o" denotes standard conditions. For computational convenience Eq. (7) may be expressed as

$$\tau = f\{x\}, \quad (8)$$

where

$$x = C' + \log_{10} W \quad (9)$$

$$C' = \log_{10} C \quad (10)$$

$$W = \left(\frac{P}{P_0} \right)^n \left(\frac{T_0}{T} \right)^m U \quad (11)$$

Here, f is the transmittance function, C' is the spectral parameter, W is the equivalent absorber amount, and n and m are the absorber parameters; all of which are to be determined from transmittance data for each absorber.

III. Computerized Method of Empirical Model Development

3.1 Introduction

Assuming the availability of equal transmittance data, which is defined below, we have developed an algorithm, called ADSET, which evaluates absorber parameters n , m , spectral parameters $C'(\nu)$ and an empirical transmission function simultaneously. In the algorithm the transmission function is linearized and a linear regression technique is utilized for parameter evaluation. In order to evaluate the band model parameters and the empirical transmission function simultaneously, a set of auxiliary variables are introduced. Each data point is identified through the auxiliary variables to an absorption band and to a transmittance 'cut'. This enables us to obtain globally optimal set of parameters and the empirical transmission function simultaneously.

Based on the derived optimal pointwise transmission function, a piecewise analytical transmission function is developed. The commonly used computer code Lowtran for the evaluation of atmospheric transmittance can be greatly simplified by the use of this piecewise analytical transmission function to model the major absorbers.

Finally, the code ADSET also contains a subroutine which can compute the spectral parameter value $C'(\nu)$ for non-major absorption bands.

3.2 Data Structure

Several transmittance values τ_j , $j=1, 2, \dots, \text{NCUT}$ are chosen a priori, where NCUT is the number of chosen transmittance values. Curves of growth data (i.e. τ versus U) for each layer of atmosphere are assumed to be given at these transmittance values. Therefore, the curves of growth have 'cut' structure, namely, all data points are on one of the transmittance cuts $\tau = \tau_j$, $j=1, 2, \dots, \text{NCUT}$ (See Fig. 1). We call a data set with this cut structure an 'equal transmittance' data in the sequel.

3.3 Linearization of Transmission Function

Since f in Eq.(8) is known to be strictly monotone decreasing from one to zero as x changes from $-\infty$ to ∞ , there exists an inverse function f^{-1} defined on $(0,1)$ such that

$$\begin{aligned} x &= f^{-1}(\tau) \\ &= C' + \log W \\ &= C' + n \log\left(\frac{P}{P_0}\right) + m \log\left(\frac{T_0}{T}\right) + \log U. \end{aligned} \quad (12)$$

Let us define x_j , $j=1, 2, \dots, \text{NCUT}$ be the inverse image of the prechosen transmittance values τ_j , $j=1, 2, \dots, \text{NCUT}$ i.e.,

$$x_j = f^{-1}(\tau_j), \quad j=1, 2, \dots, \text{NCUT}, \quad (13)$$

i-th BAND

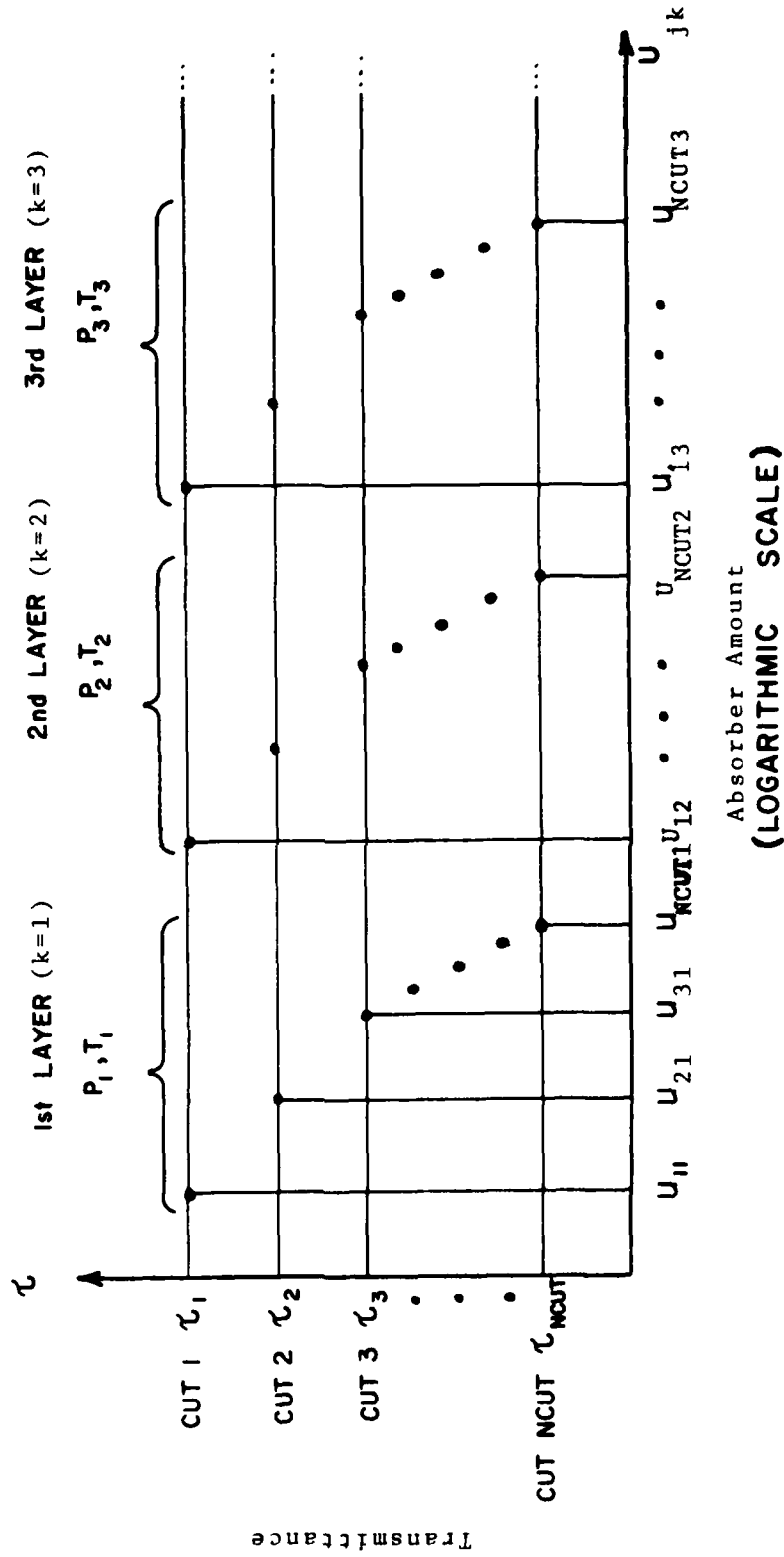


Fig. 1. Schematic representation of "equal transmittance" data structure.

Then, the set of points (x_j, τ_j) , $j = 1, 2, \dots, \text{NCUT}$ is nothing but the empirical transmission function, which is to be found. From Eq. (12), we reach the following regression equation.

$$n \log\left(\frac{P}{P_o}\right) + m \log\left(\frac{T_o}{T}\right) + C' - x = -\log U. \quad (14)$$

Note that this equation is linear in the unknown parameters n , m , C' and x . Therefore, the linear regression technique can be used to evaluate the optimum values for the parameters.

3.4 Formation of the Square Error

The square error corresponding to the k -th data point in i -th absorption band's j -th cut, denoted by E_{ijk} , is given by

$$E_{ijk} = \left\{ n \log\left(\frac{P_{ijk}}{P_o}\right) + m \log\left(\frac{T_o}{T_{ijk}}\right) + C'_i - x_j - (-\log U_{ijk}) \right\}^2 \quad (15)$$

Hence, the total square error E_{ij} for this cut is

$$E_{ij} = \sum_{k=1}^{L_{ij}} E_{ijk}, \quad (16)$$

where L_{ij} is the number of layers in this cut. Similarly, the total square error E_i for i -th band and the grand total square error E are given by

$$E_i = \sum_{j=1}^{J_i} E_{ij} = \sum_{j=1}^{J_i} \sum_{k=1}^{L_{ij}} E_{ijk}, \quad (17)$$

$$E = \sum_{i=1}^{NB} E_i = \sum_{i=1}^{NB} \sum_{j=1}^{J_i} \sum_{k=1}^{L_{ij}} E_{ijk}, \quad (18)$$

where J_i and NB are the numbers of the cuts in i -th absorption band and of the absorption bands, respectively. The final expression can be simplified if we assume that the number of layers (L_{ij}) in every cut is equal to a constant L_i . For this case

$$E = \sum_{i=1}^{NB} \sum_{j=1}^{J_i} \sum_{k=1}^{L_i} E_{ijk}. \quad (19)$$

Our objective is to find optimum set of parameters (n^* , m^* , C'_1 , C'_2 , ..., C'_{NB} , x_1^* , x_2^* , ..., x_{NCUT}^*) which minimizes this grand total error E .

3.5 Auxiliary Variables

In order to perform the minimization of E with respect to the above parameters simultaneously, we modify the square error E_{ijk} so that it contains all the parameters. This is done by introducing two sets of auxiliary variables u_i , $i=1, 2, \dots, NB$ and v_j , $j=1, 2, \dots, NCUT$. Using them, E_{ijk} is redefined as

$$E_{ijk} = \left\{ n \log \left(\frac{P_{ijk}}{P_o} \right) + m \log \left(\frac{T_o}{T_{ijk}} \right) + u_{1,ijk} C'_1 + \dots + u_{NB,ijk} C'_{NB} + v_{1,ijk} K_1 + \dots + v_{NCUT,ijk} K_{NCUT} - (-\log U_{ijk}) \right\}^2 \quad (20)$$

where $K_j = -x_j$, $j=1, 2, \dots, \text{NCUT}$. The auxiliary variables act as identifiers of the band and the cut. If a data point is for f -th band's j -th cut, then $u_f = 1$ and $u_i = 0$ for all $i \neq f$ and $v_j = 1$ and $v_j = 0$ for all $j \neq j$. Thus, only the spectral parameter C'_j and the cut parameter K_j corresponding to the current data are active and all other spectral and cut parameters disappear. Hence, Eq. (20) reduces to Eq. (15). The change from x_j to $K_j = -x_j$ is made in order to symmetrize the coefficient matrix of the resulting normal equation. This change makes it possible to utilize any specialized solution method for the symmetric normal equation when the space conservation is important.

3.6 Regression Analysis

Using the grand total error E with the redefined E_{ijk} in Eq. (20), the best parameter values n^* , m^* , $C'_1{}^*$, $\dots$, $C'_{\text{NB}}{}^*$, $K_1{}^*$, $\dots$, $K_{\text{NCUT}}{}^*$ are simultaneously determined by the linear regression. Setting the partial derivatives of E with respect to parameters equal to zero results in a linear normal equation of the form $AX = B$, where A , B and X are, respectively, a symmetric coefficient matrix, a constant vector and a parameter vector defined by

$$A = \begin{bmatrix} \Sigma v^2_{\text{NCUT}} & & \\ & \Sigma u^2_{\text{NB}} & \\ & & \Sigma \left(\log \frac{T}{T_0} \right)^2 \\ \text{---} & \text{---} & \text{---} \end{bmatrix} \quad (21)$$

Σv^2_1 Σu^2_2 $\Sigma \left(\log \frac{P}{P_0} \right)^2$

$$B = \left[\sum (-v_{\text{NCUT}} \log U), \dots, \sum (-v_1 \log U), \sum (-u_{\text{NB}} \log U), \dots, \right. \\ \left. \sum (-u_2 \log U), \sum \left(-\log\left(\frac{T_0}{T}\right) \log U\right), \sum \left(-\log\left(\frac{P}{P_0}\right) \log U\right) \right]^t, \quad (22)$$

$$X = \left[K_{\text{NCUT}}, \dots, K_1, C'_{\text{NB}}, \dots, C'_{2, m, n} \right]^t \quad (23)$$

The * in Eq. (21) represents some nonzero elements. Also the Σ in the above equations represents the triple sum $\sum_{\text{NB}} \sum_{j=1} \sum_{L_i}$ in Eq. (19). One may realize that C'_1 does not

appear in Eq. (23) and hence the corresponding auxiliary variable u_1 is also absent from Eqs. (21) and (22). This is because one of $C'_1, \dots, C'_{\text{NB}}$ is dependent on other C'_i so that $C'_1, \dots, C'_{\text{NB}}$ cannot be determined uniquely. It is necessary that one of C'_i s be given a number *a priori*. Here C'_1 is chosen and is given the value zero, and therefore is eliminated from the parameter vector X . This choice calls for some explanation. On τ vs. $\log W$ diagram the optimum empirical transmission function can be placed anywhere. What it amounts to is that a different placement results in a different set of C'_i values which is a linear shift (addition or subtraction of a constant) of another set of C'_i values. Only the relative relationship among C'_i is unique. This is clearly indicated in Fig. 2.

Since the placement of the empirical transmission function is arbitrary, we may position it on the data points corresponding to the first absorption band. In other words, the first absorption band is taken as the

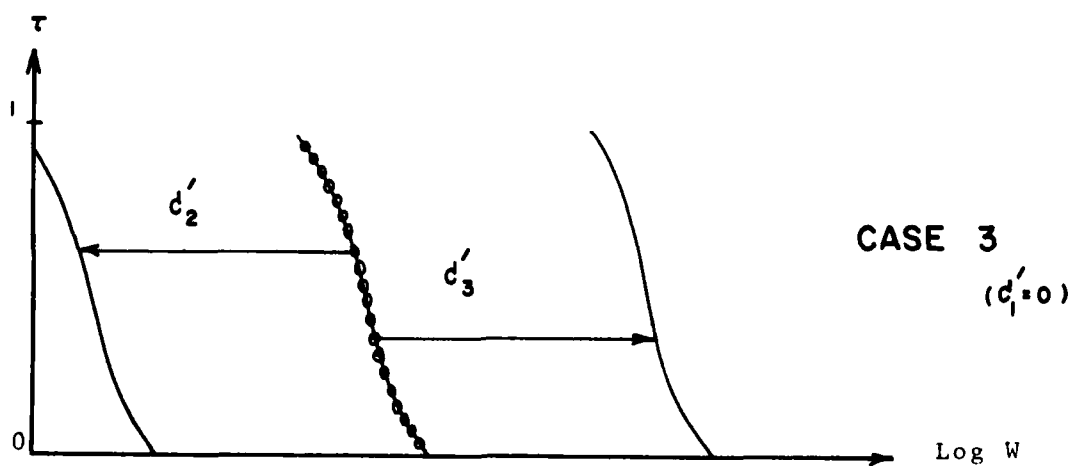
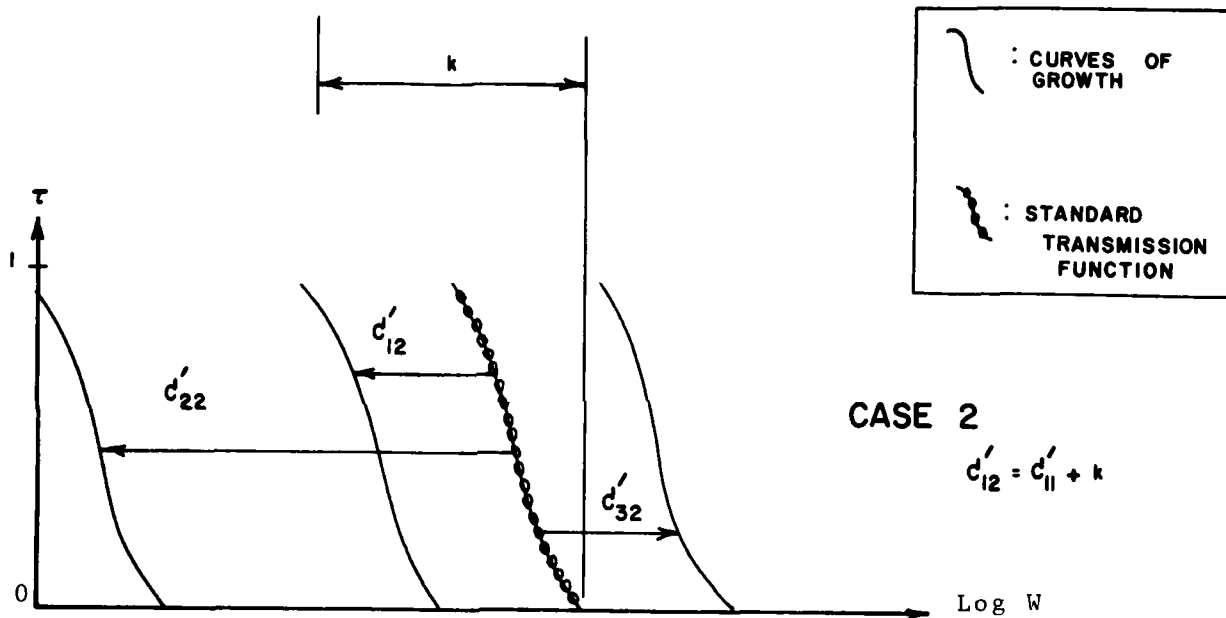
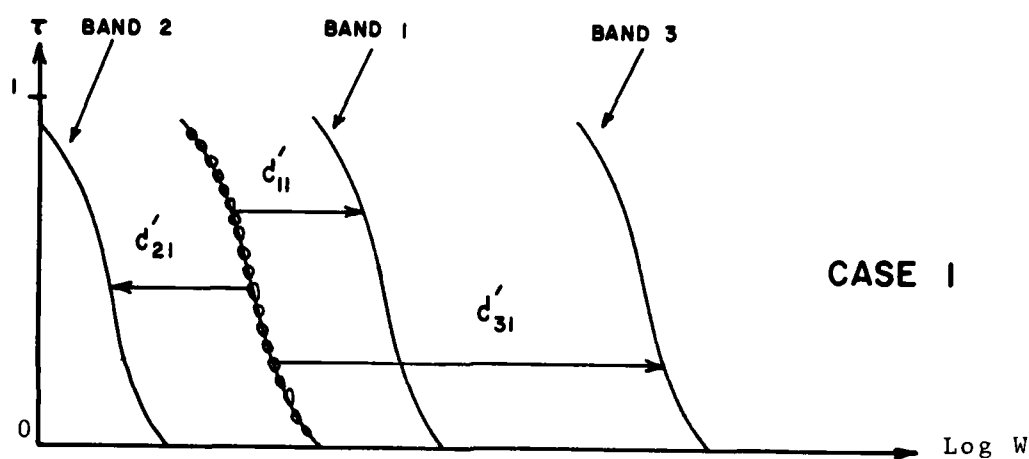


Fig. 2. Schematic representation of linear shift accounting for spectral dependence of transmittance.

reference band and the corresponding spectral parameter C_1' is set to be zero.

The queuing of parameters in X vector is determined in such a way that as many upper principal minor matrices as possible become diagonal (See Eq. (21)). This arrangement can reduce the amount of computation in the early stage of Gauss elimination steps when the normal equation is solved, and can result in less computational error.

3.7 Piecewise Analytical Transmission Function

After the best parameter values are computed, the piecewise analytical transmission function is generated by the piecewise interpolation. The transmittance region $(0,1)$ is divided into $NCUT - 1$ subregions by the transmittance cuts $\tau_2, \tau_3, \dots, \tau_{NCUT-1}$. Let $\tau_1 > \tau_2 > \dots > \tau_{NCUT}$, then the subregions are given by

Subregion 1	$[\tau_2, 1)$,
Subregion 2	$[\tau_3, \tau_1]$,
.	.
.	.
.	.
Subregion $NCUT-2$	$[\tau_{NCUT-1}, \tau_{NCUT-2}]$,
Subregion $NCUT-1$	$(0, \tau_{NCUT-1}]$.

The top and bottom subregions contain τ_1 and τ_{NCUT} as an inner point, respectively. The interpolation in each

subregion is done by the double exponential function defined by

$$\tau(x) = \exp \{-10^{a_1 + a_2 x + a_3 x^2}\}. \quad (24)$$

The generally-used linear interpolation is not used here since subregions cannot be assumed small enough for the linear approximation to be valid. Furthermore, the linear interpolation is totally inadequate for the top and bottom subregions. On the other hand, the double exponential function takes the values between and is asymptotic to one and zero as the argument varies from $-\infty$ to ∞ . It is also known that this function closely approximates the standard empirical transmission function used in the Lowtran code.^{2,16}

The parameters a_1 , a_2 , and a_3 for each subregion are determined by two different methods. The first method assumes that $a_3 = 0$ and uses no further data to compute a_1 and a_2 . They are simply determined by the condition that the interpolation function in each subregion passes through the end points. In the top and bottom subregions, the function is required to pass through two points; (τ_1, x_1) and (τ_2, x_2) for the top and $(\tau_{\text{NCUT}-1}, x_{\text{NCUT}-1})$ and $(\tau_{\text{NCUT}}, x_{\text{NCUT}})$ for the bottom subregions.

The second method does not assume that $a_3 = 0$ and requires additional data to compute parameter values. The same condition that each interpolation function passes

through two points reduces the number of unknown parameters to one. The last parameter is determined by minimizing the subregional square error E_i defined by

$$E_i = \sum_{i=1}^{L_i} (\tau_i - \exp \{-10^{a_1 + a_2 x_i + a_3 x_i^2}\})^2 \quad (25)$$

for those data points in respective subregions.

3.8 C' for Non-major Bands

Finally, the spectral parameters C' for non-major bands are computed by a straightforward method. The discrepancies between x_i^* and $\log W_i$ values computed for all cuts for one band are averaged to obtain the spectral parameter $C'(v)$ for that band, i.e.,

$$C' = \frac{1}{N} \sum_{i=1}^N (x_i^* - \log W_i), \quad (26)$$

where W_i are computed by Eq. (11) with optimal n^* and m^* .

IV. Computerized Method of Analytical Model Development

4.1 Introduction

In the last chapter, we assumed no analytical form for the transmission function $\tau = f(x)$ when the standard transmission function was computed. Here, by assuming the double exponential form given by Eq. (24) as the transmission function for the entire transmittance range, we derive an algorithm which can evaluate the best function parameter values a_1 , a_2 , and a_3 ; together with the band model parameters n , m , and C'_1 . Note that the double exponential function was used for the piecewise interpolation in the last chapter. But the computation of the function parameters was performed after the band model parameters and the empirical transmission function were obtained. In other words, the computation in the last chapter was sequential but not simultaneous. The algorithm we present in this chapter is, on the contrary, the simultaneous evaluation of all parameters. The preliminary development of this algorithm can be found in Ref. 5.

4.2 Basic Equations

The basic equations are Eq. (8) and Eq. (24) of the last chapter, which are cited here for the ease of reference.

$$\tau = f(x) \quad (27)$$

$$f(x) = \exp \{-10^{a_1 + a_2 x + a_3 x^2}\}. \quad (28)$$

Now, since we have assumed the function form, we can compute the transmittance if we have the value of x . Hence, we do not have to take the inverse function as we did before to perform the regression analysis. Instead, we take the square difference of the given and computed τ directly from this expression. Thus, we get

$$E_{ij} = [\tau_{ij} - \exp\{-10^{a_1 + a_2 x_{ij} + a_3 x_{ij}^2}\}]^2, \quad (29)$$

for i -th absorption band's j -th data point, where, as before, x_{ij} is given by

$$x_{ij} = C'_i + n \log\left(\frac{P_{ij}}{P_o}\right) + m \log\left(\frac{T_o}{T_{ij}}\right) + \log U_{ij}. \quad (30)$$

By summing this individual error for all data in i -th band, we have the total error for this band as

$$E_i = \sum_{j=1}^{J_i} E_{ij}, \quad (31)$$

where J_i is the number of data in i -th band.

Again, we introduce auxiliary variables u_i , $i=1,2,\dots,NB$ in order to introduce all C'_i , $i=1,2,\dots,NB$ into the x_{ij} expression Eq.(30). By this we get

$$x_{ij} = \sum_{k=1}^{NB} u_{k,ij} C'_k + n \log\left(\frac{P_{ij}}{P_o}\right) + m \log\left(\frac{T_o}{T_{ij}}\right) + \log U_{ij}, \quad (32)$$

We use this expression for x_{ij} in the following total error E

$$E = \sum_{i=1}^{NB} E_i = \sum_{i=1}^{NB} \sum_{j=1}^J E_{ij}. \quad (33)$$

Now, we are ready to take partial derivatives with respect to the parameters n , m , C_1' , ..., C_{NB}' , a_1 , a_2 , and a_3 to form the normal equation for this regression problem. Theoretically speaking, we can evaluate the 'best' parameter values by solving the normal equation. But obviously the grand total Eq. (33), which is to be minimized, is not a quadratic function of the unknown parameters and, therefore, the resulting normal equation is not a linear function of them. Hence, we need to adopt a different numerical method for the evaluation of the 'optimal' parameter values.

4.3 Nonlinear Optimization Method

The computational technique we use here is a recursive technique which is referred to as the conjugate gradient method¹⁷. In essence, this technique improves a set of guesses of the parameter values recursively by locating a new set of guesses which yields smaller error. For a given guess $(\alpha^n, \beta^n, \dots, \gamma^n)$ of the minimizing parameter vector, at which the error is minimized, the best direction of the search in the parameter space for a new guess is first determined using up to second order derivatives of the error. Then the one-dimensional search for the minimizing point is performed along this direction from $(\alpha^n, \beta^n, \dots, \gamma^n)$ to find a new guess $(\alpha^{n+1}, \beta^{n+1}, \dots, \gamma^{n+1})$.

which yields locally the smallest error. Now this procedure is repeated recursively to obtain a sequence of guesses until the gradients become less than a small positive number which is chosen *a priori*.

Actual computation was done by utilizing the packaged subroutine FMCG in SSP library available from IBM¹⁸. The necessary gradients are

$$\frac{\partial J}{\partial a_1} = -2 \sum D_j \delta f_j,$$

$$\frac{\partial J}{\partial a_2} = -2 \sum D_j \delta f_j x_j,$$

$$\frac{\partial J}{\partial a_3} = -2 \sum D_j \delta f_j x_j^2,$$

(34)

$$\frac{\partial J}{\partial n} = -2 \sum D_j \delta f_j (a_2 + 2a_3 x_j) \log\left(\frac{P_j}{P_0}\right),$$

$$\frac{\partial J}{\partial m} = -2 \sum D_j \delta f_j (a_2 + 2a_3 x_j) \log\left(\frac{T_0}{T_j}\right),$$

$$\frac{\partial J}{\partial C'_i} = -2 \sum D_j \delta f_j (a_2 + 2a_3 x_j) u_i,$$

where, Σ represents $\sum_{i=1}^{NB} \sum_{j=1}^{J_i}$ and D_j and δf_j are given by

$$D_j = \{E_{ij}\}^{\frac{1}{2}}, \quad (35)$$

$$\delta f_j = (\ln 10) 10^{a_1 + a_2 x_j + a_3 x_j^2} f(x_j), \quad (36)$$

and $f(x)$ is given by Eq. (28).

Note that there exists a linear dependence among the gradients which is

$$a_2 \frac{\partial J}{\partial a_1} + 2a_3 \frac{\partial J}{\partial a_2} = \sum_{i=1}^{NB} \frac{\partial J}{\partial C'_i} \quad (37)$$

Therefore, the parameter set $\{n, m, C'_1, \dots, C'_{NB}, a_1, a_2, a_3\}$ cannot be determined uniquely. As it was explained in the previous section, this is due to the arbitrariness in the positioning of the standard transmission function. Hence, the spectral parameter C'_1 is again set to be zero, so that we can evaluate unique set of optimal parameters.

V. Comparison of the Two Methods

5.1 Introduction

Both methods can evaluate the optimal n , m and $C'(v)$ values for major and non-major bands and also a standard transmission function. But there are some basic differences which are discussed in the sequel.

5.2 Final Products

The final product of the ADSET code is a piecewise analytical standard transmission function together with the band model parameters. Each analytical piece of the standard transmission function covers only one of the pre-chosen subintervals of $(0,1)$ transmittance range. On the other hand, SIMMIN produces only one analytical transmission curve for the entire range. Therefore, ADSET has more flexibility to adjust to the transmittance curve variations. This feature of ADSET can be very valuable for the gases with non-standard curves of growth.

This difference is amplified when the number of the transmittance sub-regions used in ADSET is increased. However, as the number of subregions increase, the requirement on the usable data becomes severer and more spaces are necessary to store the computed results. Hence, the determination of the number of subregions should be resorted to compromise.

5.3 Installation of the Results in Lowtran

The final products of two codes ADSET and SIMMIN were installed in the widely-used Lowtran code, as discussed in Section VII of this report. The SIMMIN results require less memory space, less time for transmittance computation and simpler coding than the ADSET result. In fact, for the SIMMIN result, all that have to be stored are the five band model parameters n , m , a_1 , a_2 , and a_3 , and a set of spectral parameters $C'(\nu_i)$ for each absorber. Furthermore, the computation of τ can be done by only one FORTRAN statement. On the other hand, the ADSET result requires the storage of NCUT-1 of a_1 , a_2 , and a_3 values, n and m and a set of $C'(\nu)$ values for each absorber. There can be a large difference in the number of the sets of a_1 , a_2 , and a_3 values to be stored. Moreover, some judging statements are necessary to select the right set of a_1 , a_2 , and a_3 for each transmittance computation.

5.4 Data Requirements

The ADSET code requires the cut structured data such that the transmittance of each data point must fall in one of prechosen values. But the SIMMIN code does not impose any conditions on the data set.

Some considerations on the requirement of equal transmittance data for ADSET are due here. Even if the available data do not have equal transmittance structure,

it can be transformed into the required form using interpolation/extrapolation. This constitutes the pre-processing of the raw data. Curves of growth data τ vs. $\log U$ with τ values not necessarily coinciding with the prechosen values can be locally interpolated/extrapolated using an analytical function. This procedure is indicated in Fig. 3. Again, the double exponential function is an excellent choice for the interpolation function. We note that an almost exact technique as the one used in obtaining a piecewise analytical transmission function can be used for this purpose. In fact, only a minor modification of the interpolation subroutine used in ADSET can accomplish this task.

5.5 Computation Time

The numerical methods used in ADSET and SIMMIN for solving normal equations are essentially different. The method in SIMMIN is a recursive algorithm and the other in ADSET is a non-iterative one. Therefore, the computation time for ADSET is determined by the size of the data set only, whereas, the one for SIMMIN depends on both the actual data values and the initial guesses. It is difficult to estimate the computation time for SIMMIN due to this dependence. One way of controlling the time is to limit the number of iterations performed. This feature is included in the packaged subroutine FMCG which is used for actual

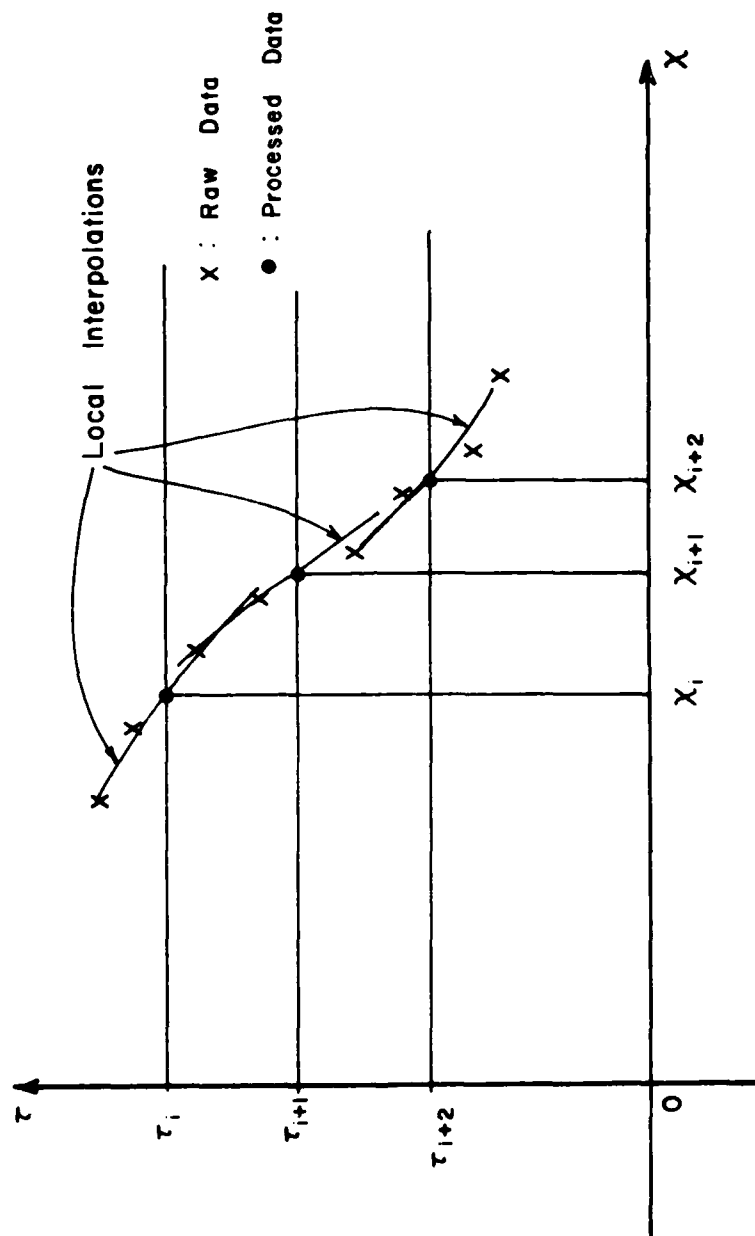


Fig. 3. Pre-processing of Data
 (τ_j, x_j) , and the derived equal transmission data.

computations. Actual time ranges required for ADSET and
SIMMIN computations will be given in a later section.

VI. Lowtran Capabilities and Functions

6.1 Introduction

The Lowtran code consists of a computer model for the calculation of transmittance through atmospheres containing absorbing and scattering molecules and aerosols. The models used in the code were for the most part developed in 1972⁶ but later editions incorporated computational changes and other capabilities⁷⁻¹⁰. It covers the spectral range from 0.25 to 28.5 μm at intervals of 5 cm^{-1} with a resolution for the major absorbers of 20 cm^{-1} . The transmittance calculation is made on six model atmospheres and two haze models on a 33-level basis for altitude, pressure, temperature and density from sea-level to 100 km. The path of the transmission is considered to be refracted by changes in atmospheric density, a fact taken into account in an optional subroutine. In its present form the Lowtran code consists of a single main program that inputs the path data and model parameters, computes the equivalent absorber amount, and performs the transmittance calculations. The only present subroutines are associated with the path, and are optional. The difficulties of understanding and, especially, updating such a program structure are considerable.

The principal objective of this effort is to modify the program structure of the Lowtran code in accordance

with the following criteria:

1. The basic functions, calculations and print-outs remain nearly identical to the original.
2. The basic operations involving the reading of data, the calculation of the equivalent path and the transmittance calculations are all separate, independent programs, but are connected as subroutines to a main control program.
3. The structure modification is performed on the latest version of the code, i.e., Lowtran 4.

As an exercise in the use of the modularized version, the present authors added empirical band models for transmittance through the trace gases. Also, continuous functions were made to replace their transmission tables for the principal molecular absorbing species.

6.2 General Features

In this section an effort is made to summarize the basic structure, fundamental calculations and models used in the Lowtran code for estimating atmospheric attenuation by gases and aerosols. Reference is specifically made to the latest fourth version, although at the present time the authors are aware of a recent effort by AFGL on a fifth version. From the authors' evaluation of their recent efforts, it appears that the modularization presented here may be incorporated in their latest version. For instance, the latter is known to have a single separate subroutine for the emission and transmission calculations. The major contribution of the work presented here lies in the separation of that emission and transmission loop into a subroutine for model selection, a subroutine for the equivalent path and individual subroutines for all of the attenuation models in the code.

The Lowtran code is designed for the specific purpose of calculating at low resolutions either atmospheric radiance or transmittance between any two locations in the Earth's atmosphere at frequencies ranging from the ultraviolet (UV) to the infrared (IR). This is accomplished through the use of band models accounting for

resonant gaseous absorption (e.g. H_2O vapor, O_3 , HNO_3 vapor and the uniformly-mixed gases), resonant aerosol absorption, non-resonant gaseous absorption (e.g. N_2 and H_2O vapor continua) and scattering by molecules and aerosols. The spectral intervals over which the band models are provided vary from 5 cm^{-1} to 500 cm^{-1} , as shown in Table 1. It should be pointed out that the spectral resolution is generally much lower than the interval over which they are defined. For instance, the models for the principal absorbers are given at 5 cm^{-1} intervals, while their spectral resolution is 20 cm^{-1} . The spectral resolutions for the remaining models is not specified anywhere in the available literature on the code. In this table the spectral definition of the models for aerosol absorption, and for aerosol and molecular scattering are not shown because they are spectrally continuous.

The spectral regions over which the attenuation models are effective are summarized in Table 2. It may be seen in this table that over some regions only a few species attenuate and, therefore, a transmittance of unity may be specified in the calculation of the total transmittance. This table forms the basis for the model selection subroutine introduced in the modularized version for the purpose of simplifying the code structure.

In the discussion that follows, the individual

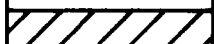
ATTENUATING SPECIE	MODEL FREQUENCY INTERVAL (cm ⁻¹)			
	5	50	200	500
H ₂ O				
UNIFORMLY- MIXED GASES				
O ₃				
N ₂ CONTINUUM				
H ₂ O CONTINUUM				
HNO ₃				
VISIBLE O ₃				
ULTRA VIOLET O ₃				

Table 1. Frequency interval of the attenuation band models in the Lowtran code. The models for aerosol absorption and aerosol and molecular scattering are spectrally continuous and, therefore, not shown.

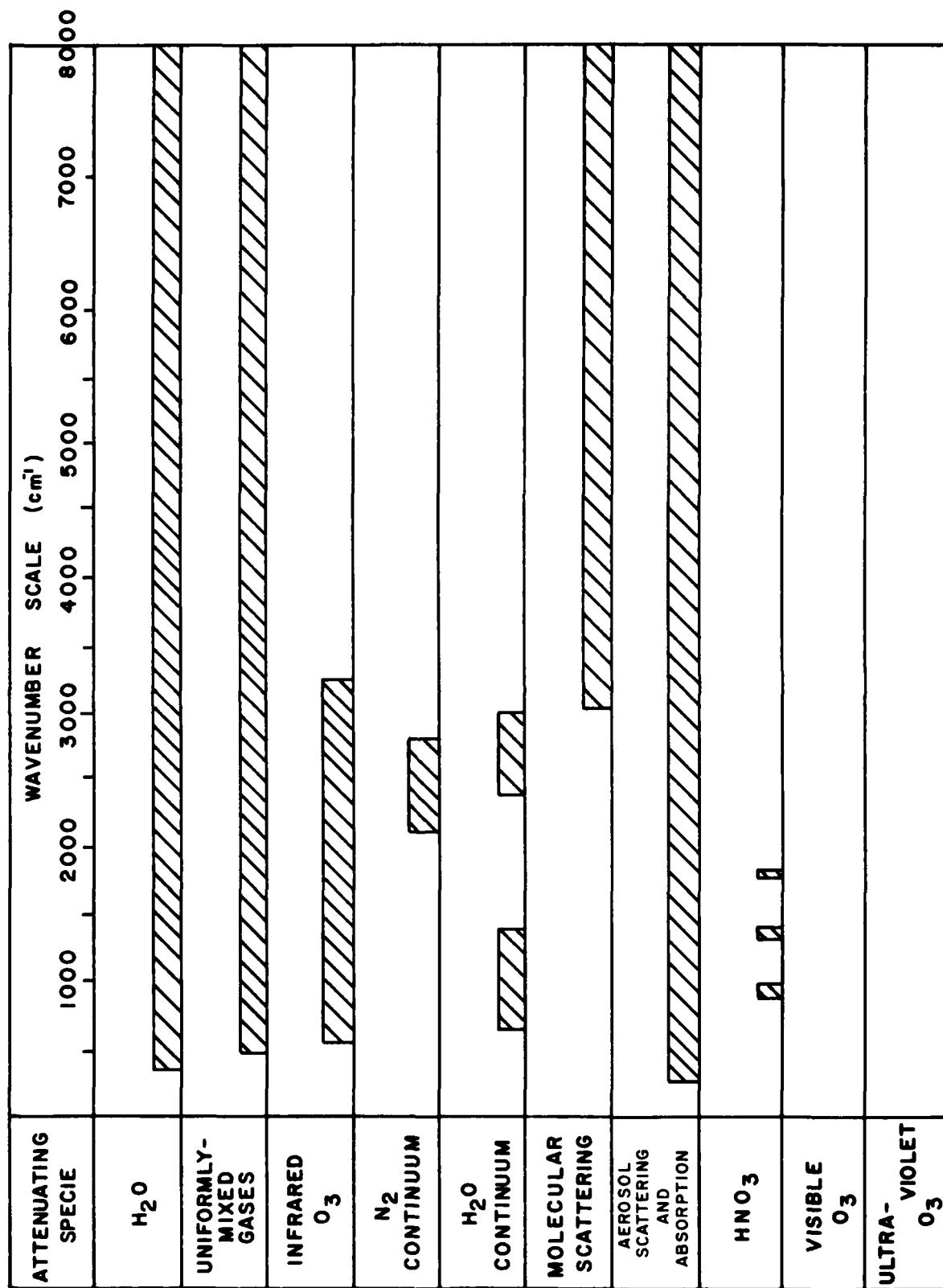


Table 2. Spectral region over which the attenuation models in LOWTRAN are effective.

ATTENUATING SPECIE	WAVENUMBER	SCALE (cm ⁻¹)
H ₂ O	9000	16000
UNIFORMLY-MIXED GASES	13000	14000
INFRARED O ₃	13000	14000
N ₂ CONTINUUM		
H ₂ O CONTINUUM		
MOLECULAR SCATTERING		
AEROSOL SCATTERING AND ABSORPTION		
HNO ₃		
VISIBLE O ₃		
ULTRA-VIOLET O ₃		

Table 2. (Continued)

ATTENUATING SPECIE	WAVENUMBER SCALE (cm ⁻¹)
H ₂ O	20000 25000 30000 35000 40000 45000 50000
UNIFORMLY-MIXED GASES	
INFRARED O ₃	
N ₂ CONTINUUM	
H ₂ O CONTINUUM	
MOLECULAR SCATTERING	
AEROSOL SCATTERING AND ABSORPTION	
HNO ₃	
VISIBLE O ₃	
ULTRA-VIOLET O ₃	

Table 2. (Continued)

attenuation models are grouped together in certain classes and are briefly discussed. Generally speaking, the discussion is restricted to the extent of illustrating the function and parameters which had to be identified in Lowtran for the modularization purpose that followed. An exception is made in the case of the major molecular absorption models (i.e. H_2O vapor, infrared O_3 and the uniformly-mixed gases) because they are replaced with continuous functions in the modularized version. For a comprehensive discussion on the theory of all of the original models the reader is encouraged to study the series of AFGL reports⁶⁻¹⁰ on the code, as well as the references therein.

6.3 Resonant Molecular Absorption Models

Molecular resonant absorption is modeled in the code for H_2O vapor, infrared O_3 , the uniformly-mixed gases, and HNO_3 vapor. Different approaches are used for the first three listed as compared with the approaches used in connection with O_3 in the visible and ultraviolet regions and with HNO_3 vapor in the infrared.

The models used to account for gaseous absorption by the molecules of H_2O vapor, infrared O_3 , and the uniformly-mixed gases are based on Eq.(8), namely

$$\tau = f\{x\}. \quad (8)$$

The developers of Lowtran obtained the parameters n , m , the function f and the spectral constant C' at 5 cm^{-1} intervals using experimental and calculated transmittance data of 20 cm^{-1} resolution. Table 3 shows the values of the parameters, as well as, the equations for the calculation of the absorber amount. The spectral constant C' over the entire spectrum of definition may be found as part of the data input presented in the Appendix. The transmission model for the uniformly-mixed gases was obtained by combining the data for all of these gases in the proportions listed in Table 4. It should be pointed out that the temperature and pressure exponents used in Lowtran for the major absorbers and listed in Table 3 are not the same as the ones developed from the original transmission data. This inconsistency was introduced during the digitizing of the curves for inclusion in the computer code, in order to account more accurately for the temperature dependence².

The method used for modeling HNO_3 vapor and the visible and ultraviolet O_3 is similar to the one described above for the major absorbers, except that the function f was specified *a priori* to be an exponential. Thus,

$$\tau = \exp(-CW), \quad (38)$$

where for HNO_3

$$W = \left(\frac{P}{P_0}\right) \left(\frac{T_0}{T}\right) U, \quad (39)$$

$$U = M Z \times 10^5, \quad (40)$$

and for O_3

$$W = U = 46.667 \rho Z. \quad (41)$$

In Eq. (40) M is the mixing ratio profile as tabulated in the Appendix together with the C 's, and ρ is the absorber density.

The last of the molecular absorption models is the one for the resonant absorption by atmospheric aerosols. The exponential function in Eq. (38) is assumed

$$\tau = \exp(-CW),$$

where

$$W = U = 3.5336 \times 10^{-6} NZ, \quad (42)$$

and N is the vertical distribution of the number of haze particles. Tabulations are provided of distributions for 5 Km and 23 km visibility, as listed in the Appendix. Other visibilities are treated in the code itself through linear interpolation.

6.4 Non-Resonant Molecular Absorption Models

Non-resonant gaseous molecular absorption is represented by the N_2 and H_2O vapor continuums. The same

modeling approach is used for N_2 as for resonant molecular absorption, that is

$$\tau = \exp(-CW),$$

where

$$W = \left(\frac{P}{P_o}\right)^2 \left(\frac{T_o}{T}\right)^{1.5} U \quad (43)$$

$$U = 0.8 Z. \quad (44)$$

For the H_2O vapor continuum an exponential function is also used, but with a more elaborate exponent. Thus,

$$\tau = \exp(-\gamma), \quad (45)$$

where

$$\gamma = C_s \left[P_w + \frac{C_n}{C_s} (P - P_w) \right] U. \quad (46)$$

Here, P_w is the partial pressure of water and C_s and C_n are the self-broadening and nitrogen-broadening spectral constants. The values of these spectral constants depend on the spectral region where the continuum is effective.

In the 8 to 14 μm region

$$C_s = C_o \exp\left[6.08 \left(\frac{296}{T} - 1\right)\right], \quad (47)$$

and

$$\frac{C_n}{C_s} = 0.002, \quad (48)$$

while in the 3.5 to 4.2 μm region

$$C_s = C_o \exp[4.56 (\frac{296}{T} - 1)], \quad (49)$$

and

$$\frac{C_n}{C_s} \approx 0.120. \quad (50)$$

In these equations the value of C_o is given by

$$C_o = 4.18 + 5578 \exp(-7.87 \times 10^{-3} v). \quad (51)$$

ATTENUATING SPECIE	SPECTRAL REGION (cm^{-1})	PRESSURE EXPONENT n	TEMPERATURE EXPONENT m	ABSORBER AMOUNT U
H ₂ O Vapor	350- 9,195 9,875-12,795 13,400-14,520	0.90	0.45	0.1 ρZ
Uniformly-Mixed Gases	500- 8,070 12,950-13,245	1.75	1.375	Z
Infrared O ₃	575- 3,270	0.40	0.20	46.667 ρZ
N ₂ Continuum	2,080- 2,740	2.00	1.50	0.8 Z
Aerosol Absorption	333-50,000	0.00	0.00	3.5336×10^{-6} NZ
Aerosol Scattering	333-50,000	0.00	0.00	3.5336×10^{-4} NZ
Molecular Scattering	3,000-50,000	1.00	1.00	9.87×10^{-20} Z
HNO ₃ Vapor	850- 920 1,275- 1,350 1,675- 1,735	1.00	1.00	1×10^5 MZ
Visible and Ultraviolet O ₃	13,000-24,000 27,500-50,000	0.00	0.00	46.667 ρZ

Table 3. Absorber parameters in Lowtran for the attenuation models, where ρ is the density, Z the range and M the mixing ratio. The H₂O continuum model is excluded because of its different functional form.

GAS	MOLECULAR WEIGHT	PARTS PER MILLION BY VOLUME (ppm)
CO ₂	44	330.0
N ₂ O	44	0.28
CO	28	0.075
CH ₄	16	1.60
O ₂	32	2.095 x 10 ⁵

Table 4. Concentrations of the uniformly-mixed gases
used in the combined model.

6.5 Scattering Models

In order to account for atmospheric scattering exponential functions were used again. For scattering by molecules the model is defined as in Eq. (38)

$$\tau = \exp(-CW)$$

where

$$W = \left(\frac{P}{P_0}\right) \left(\frac{T_0}{T}\right) U \quad (52)$$

$$U = 9.87 \times 10^{-20} Z \quad (53)$$

$$C = \nu^4 \quad (54)$$

For aerosol scattering the argument of the assumed exponential function is

$$W = U = 3.5336 \times 10^{-4} NZ \quad (55)$$

VII. Modularization of Lowtran Including the Trace Gases

7.1 Introduction

Considering the generality and broadness in scope of this code it is not surprising that the program structure shows in its present form great complexity. Although the program user is not normally interested in aspects of the code other than the input and output, there are many cases where a basic understanding helps in specific applications. Situations are likely to occur, for instance, where a replacement of one of the several attenuation models is highly desirable. To assist in the implementation of model additions or changes as well as in the extension to other spectral regions and media, the concept of the modularized version was conceived. This version¹⁵ was designed to represent exactly the same calculations as the original, except for the simplification of the program structure into modules or subroutines. However, upon the termination of that task the authors proceeded to add models for the trace gases, as developed during the present scientific effort.

7.2 Structure of Modularized Version

The basic design used was that of a main program which reads input data, computes total transmittance and radiance and generates outputs, and a series of subroutines

which select individual models and compute individual transmittances and absorber amounts. This is shown in Fig. 4. The main operational flow chart follows in Fig. 5. Excluding the four subroutines for the trace gases, the modularized version breaks down the original into one program with 11 subroutines. The flow chart for subroutine ABSORB is shown in Fig. 6. This subroutine computes the equivalent absorber amount for all of the attenuation models according to Eq.(4), which in terms of the meteorological variables becomes

$$W = \int \left(\frac{P(Z)}{P_0} \right)^n \left(\frac{T_0}{T(Z)} \right)^m dU \quad (56)$$

Figure 7 gives details of the Transmittance/Radiance Loop of program Main. It is worth noting that the modularized version of Lowtran being done by AFGL separates this loop into a subprogram. The modularization discussed in this text leaves the loop as part of the main program, but extracts individual subroutines for the calculation of the equivalent absorber amount, the frequency selection, and the attenuation models.

The flow chart for FREQSL subroutine is shown in Fig. 8. This subroutine is designed to simplify the process of arriving at the individual models effective at the frequency of interest. It should also assist the

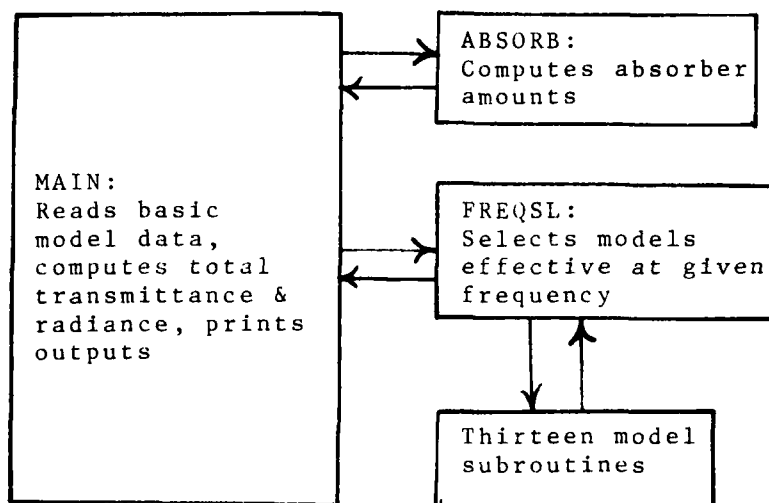


Fig. 4. Conceptual flow chart of modularized Lowtran.

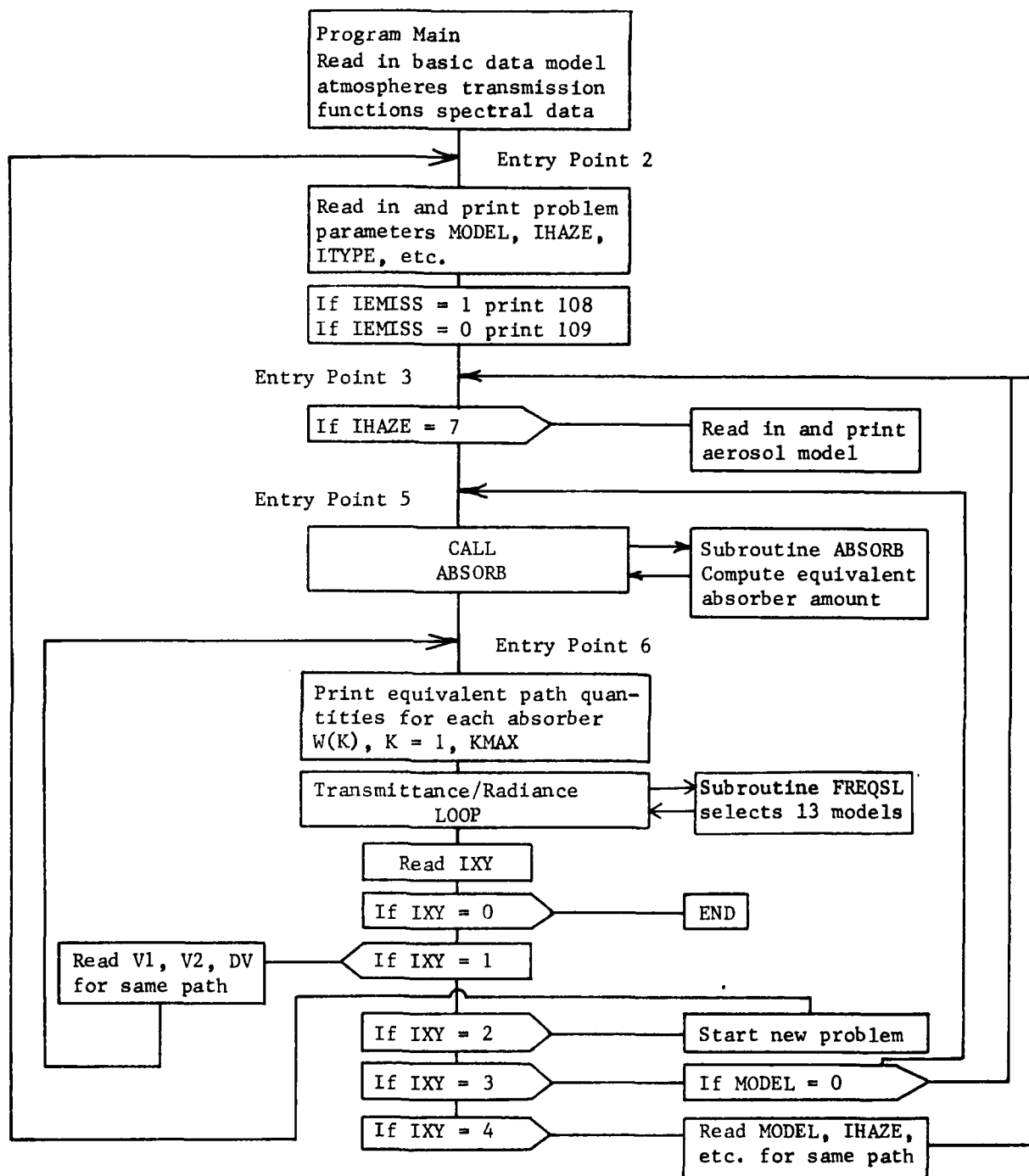


Fig. 5. General flow chart for Modularized Lowtran 4

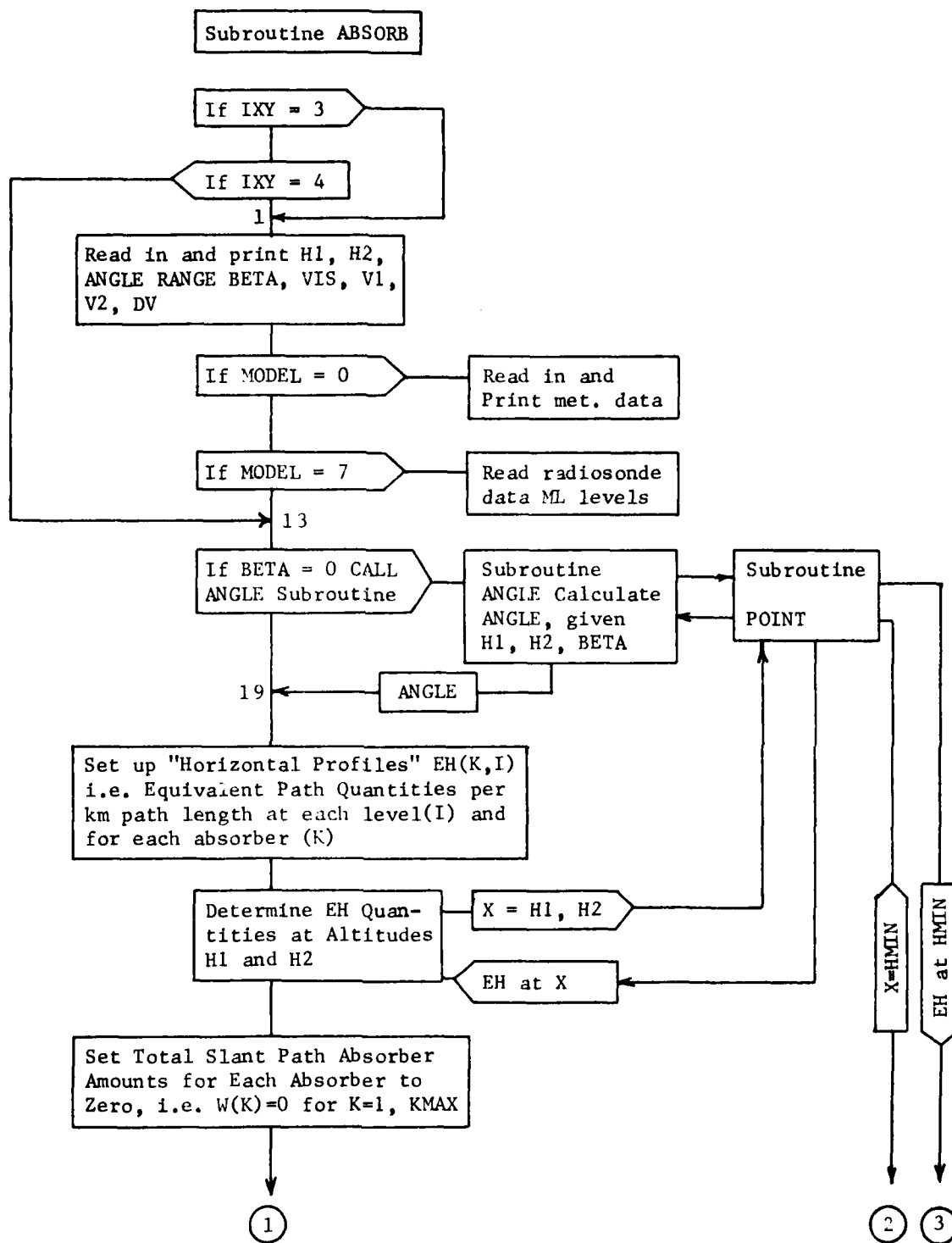


Fig. 6.

Flow chart for subroutine
 ABSORB, computing equivalent
 path quantities

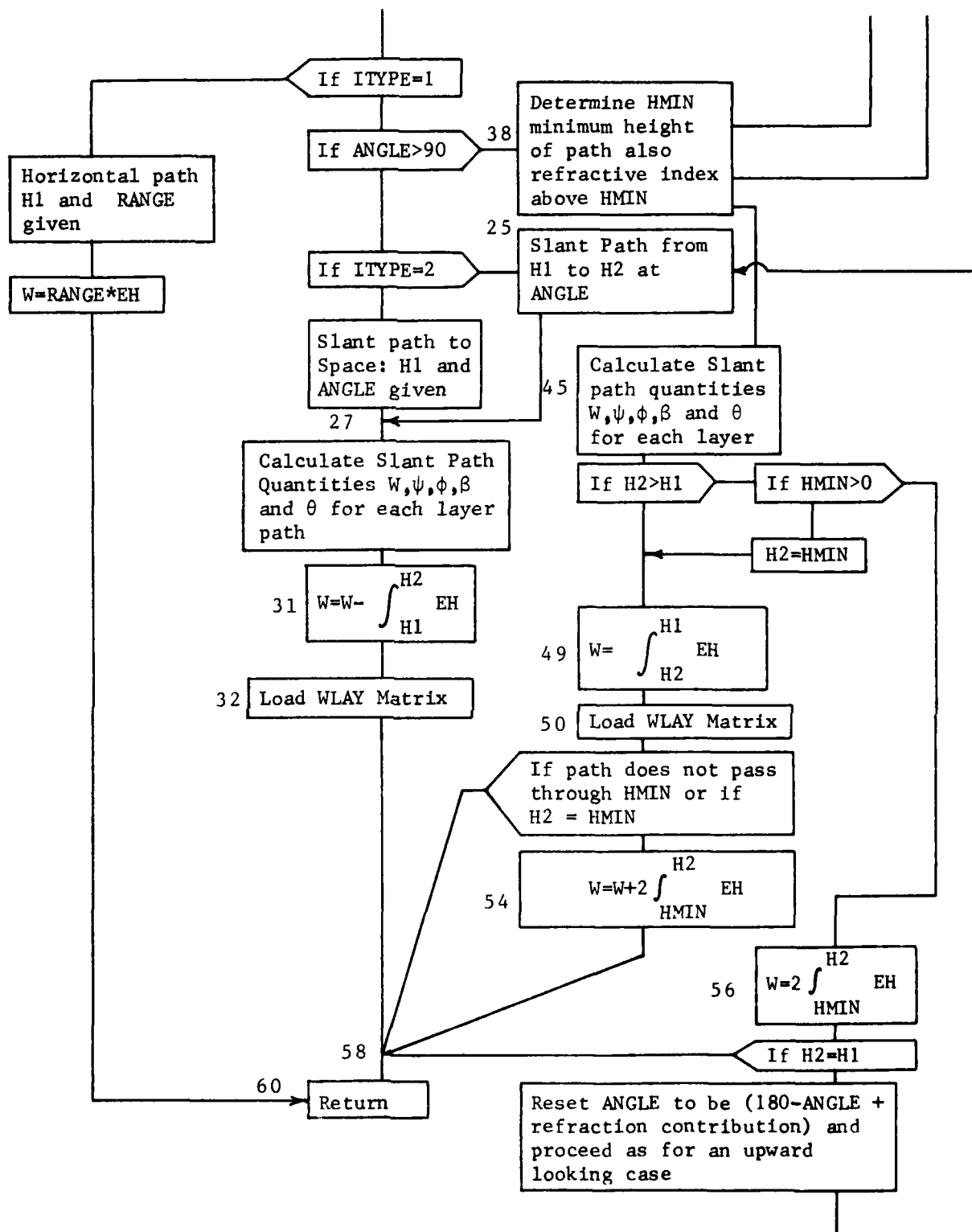
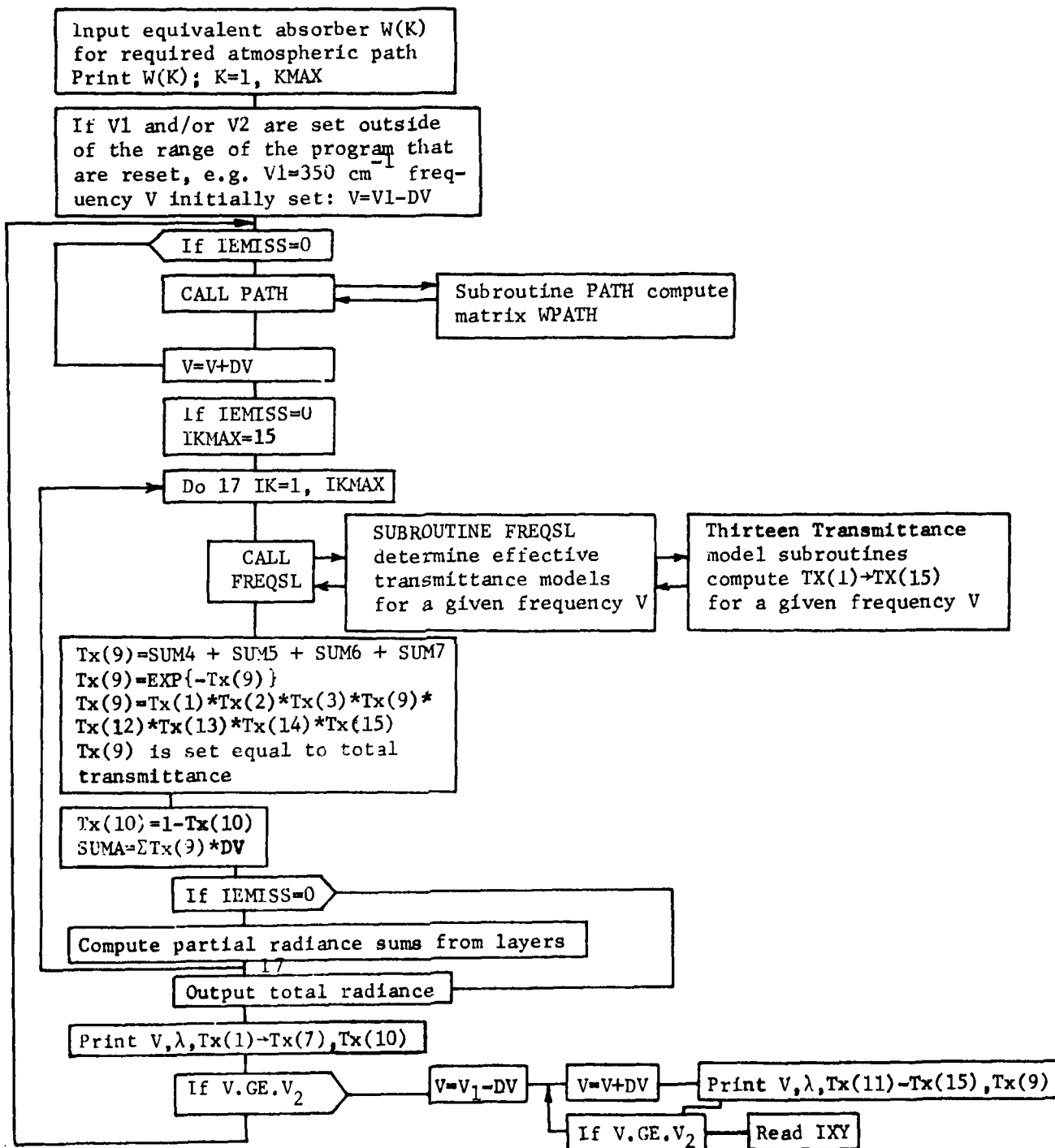


Fig. 6. (cont'd)



See Fig. 6.

Fig. 7. Flow chart for transmittance/radiance loop.

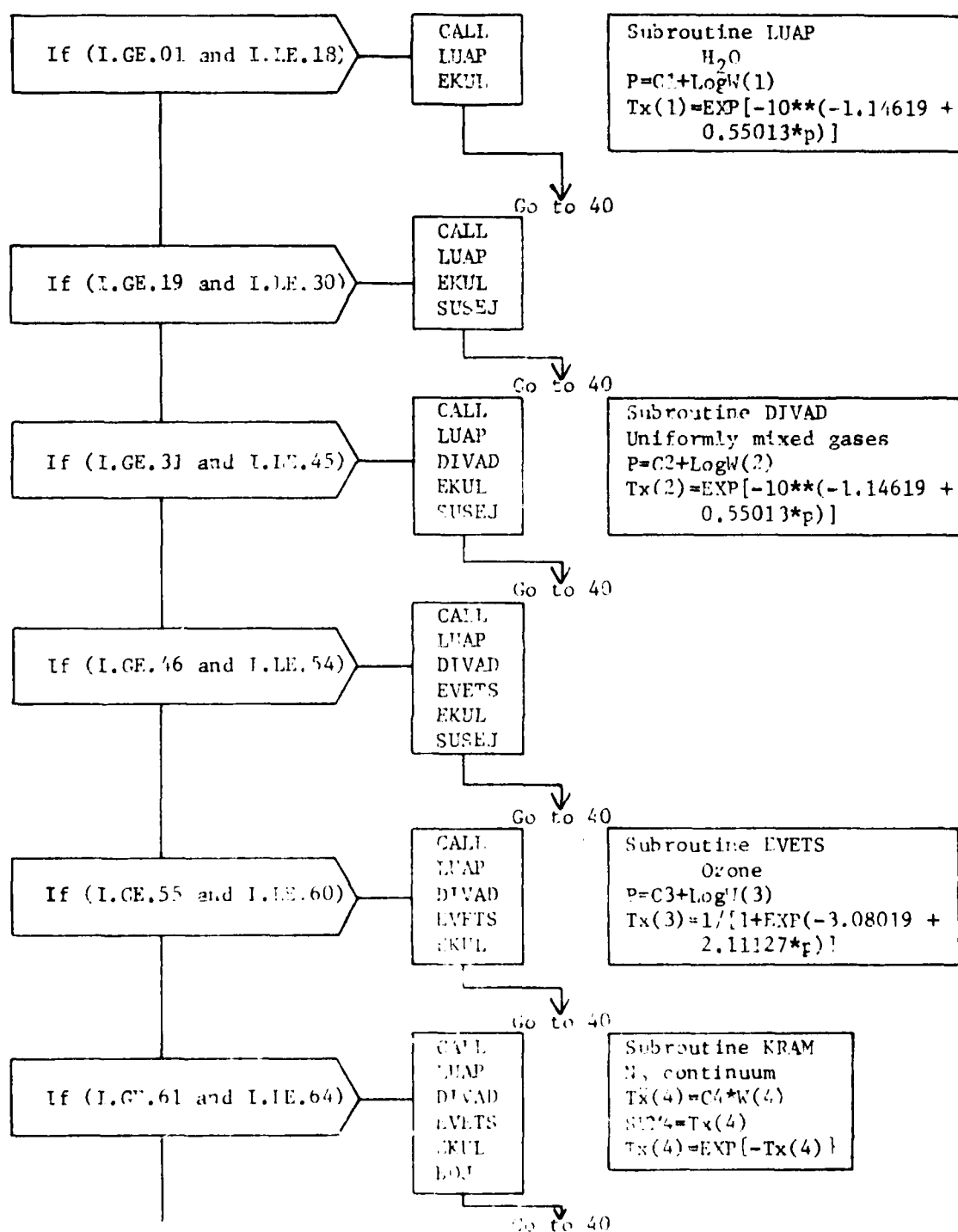


Fig. 8. Flow chart for subroutine TIEQSL and thirteen transmittance model subroutines.

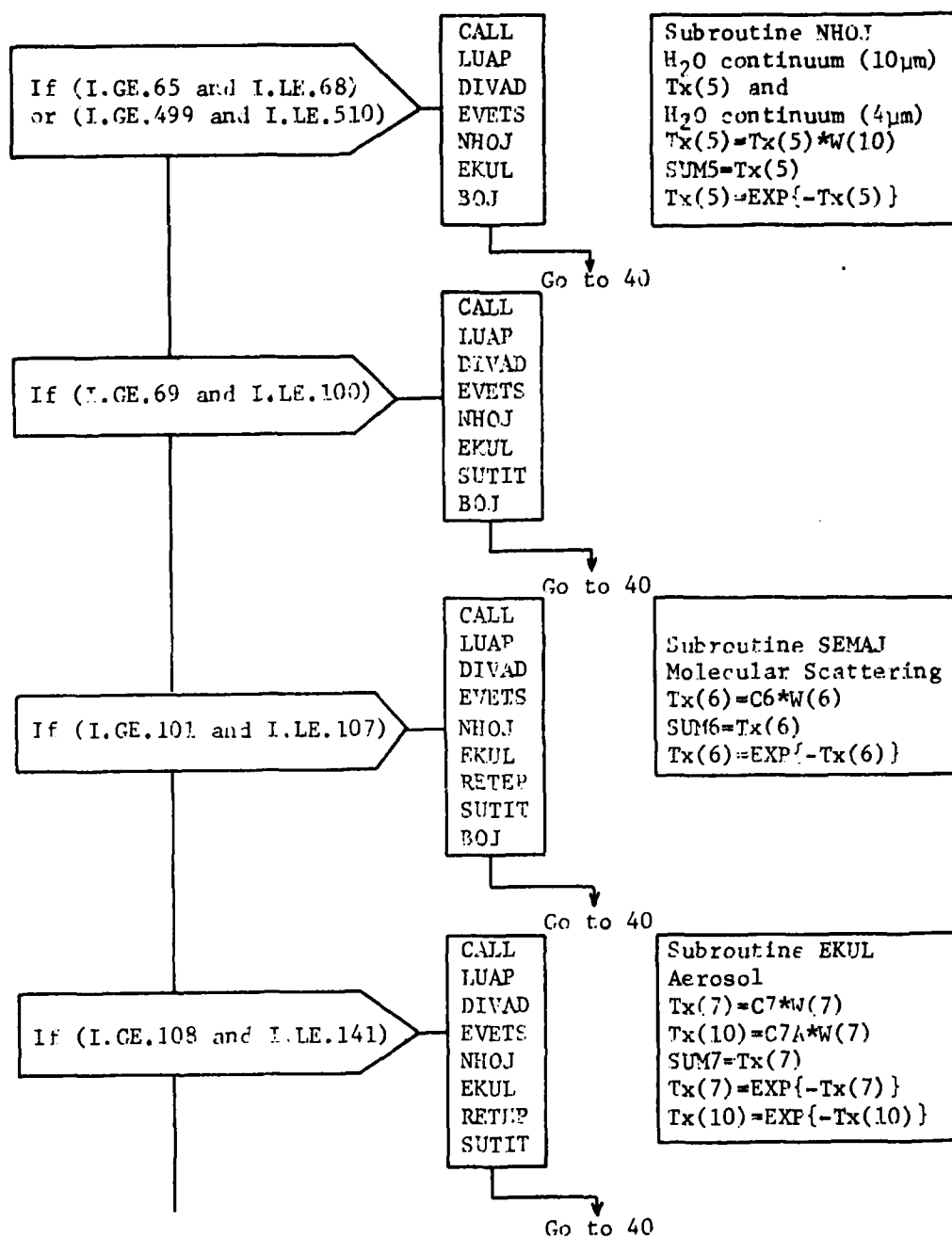


Fig. 8.

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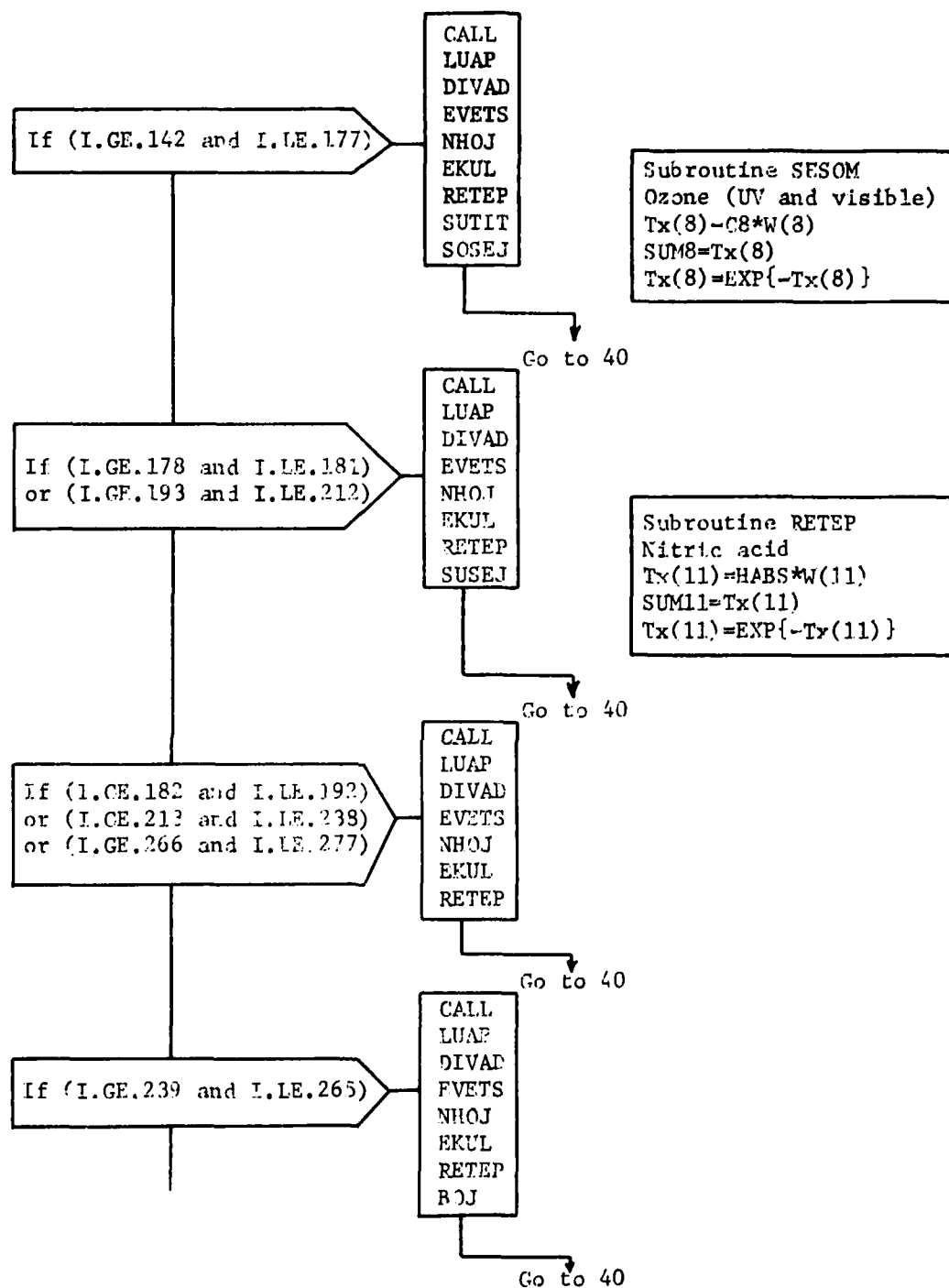


Fig. 8.

Continued

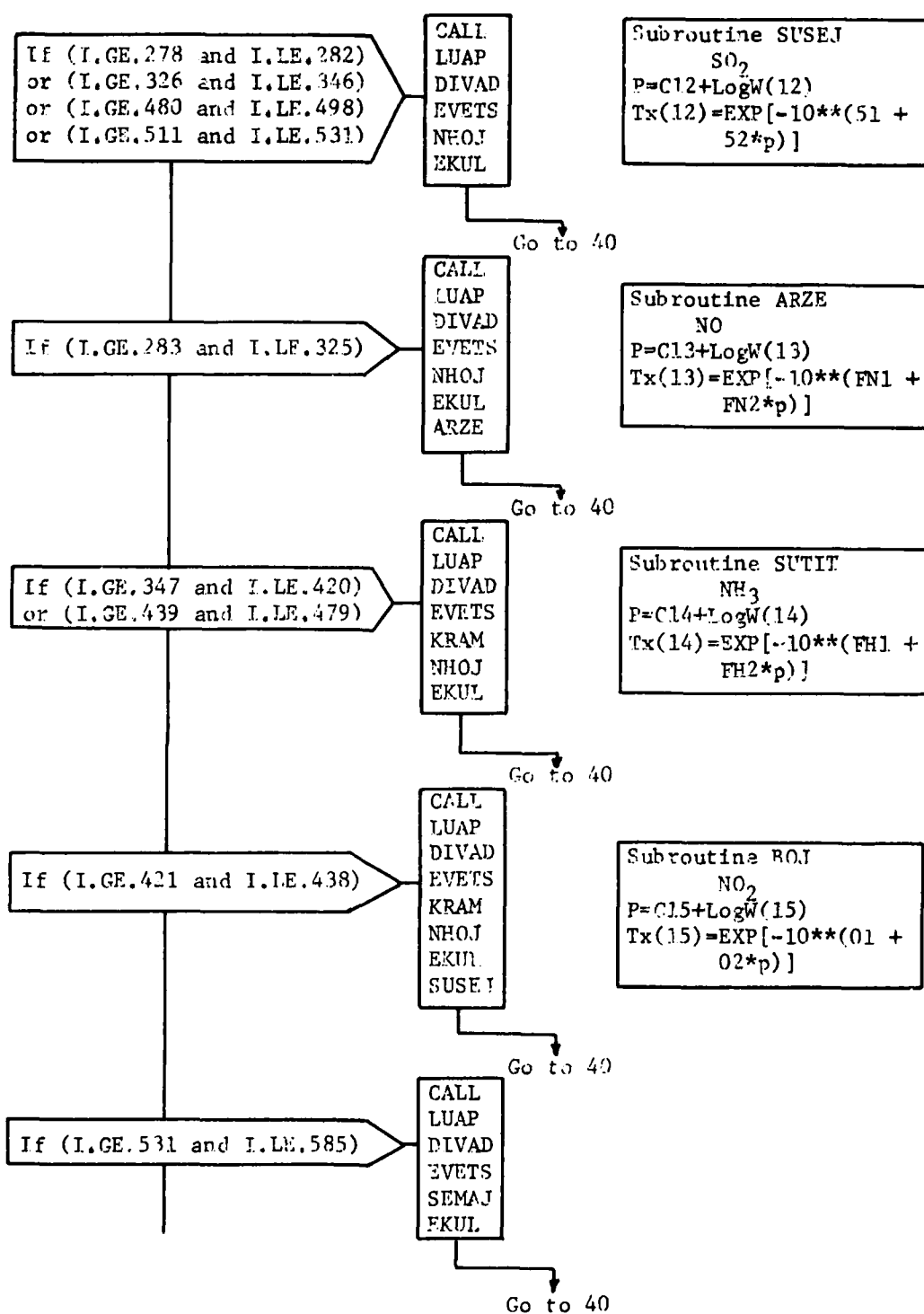


Fig. 8. Continued

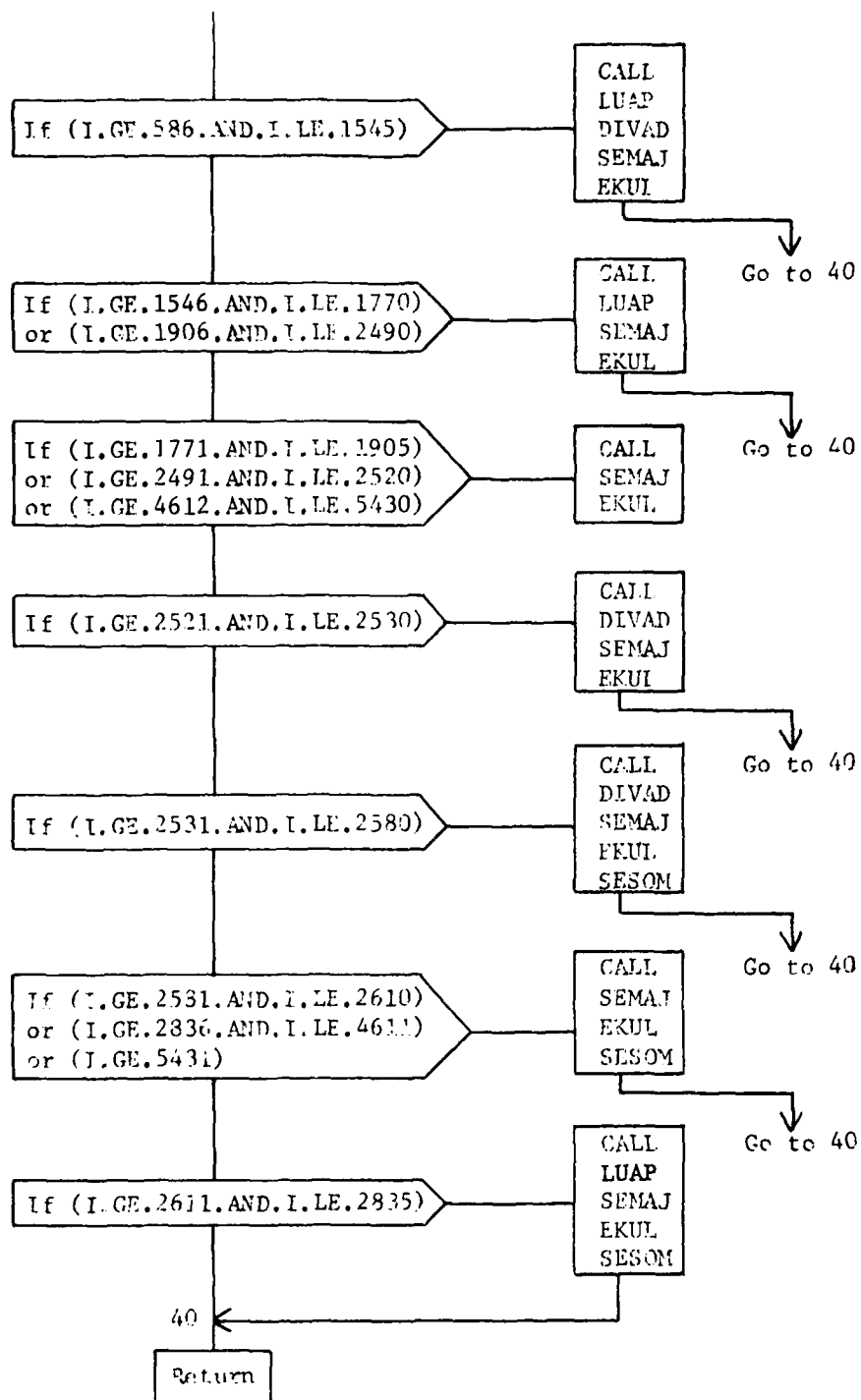


Fig. 8.

Continued

user who desires to replace or add models to the program and it should reduce the overall computational time. This subroutine is based on Tables 2 and 8.

7.3 Models for H₂O Vapor, Infrared O₃ and the Uniformly-Mixed Gases

As indicated above, all the attenuation models were extracted from the main program and placed into subroutines. The models were left basically in the same structural form except for the models for HNO₃ and H₂O vapor, infrared O₃ and the uniformly-mixed gases. The change in the first was to arrange it along the same form as in the other models originally available in Lowtran. That is, the spectral parameters were extracted from the subroutine and read at the beginning of program MAIN. The changes in the latter three gases (i.e. H₂O vapor, O₃ in the infrared and the uniformly-mixed gases) were based on a previous work by Pierluissi et al.² on the representation of the tabulated transmission functions by analytical functions. The other principal change consisted of adding models for the trace gases SO₂, NO, NO₂ and NH₃.

To arrive at the analytical function for modeling H₂O vapor and the uniformly-mixed gases the double exponential expression

$$\tau = \exp(-10^{a_0 + a_1 x}) \quad (57)$$

where x is as in Eq. 3 and a_0 and a_1 are absorber

constants, was curve-fitted to the 134 values of τ and x tabulated in Lowtran. The values found are $a_0 = -1.14619$ and $a_1 = 0.55013$, and it reproduced the tabulated transmittance with a standard deviation of 0.005. For O_3 the function adopted is given by

$$\tau = \frac{1}{1 + e^{a_0 + a_1 x}} \quad (58)$$

where $a_0 = -3.08019$, $a_1 = 2.11127$, and the tabulated data is reproduced with a standard deviation of 0.007. Note in each one of these functions that the 134 tabulated values are replaced with two and, hence, their adoption reduces the computer storage requirements. Also, they inherently offer exponential interpolation while with the present tabulation linear interpolation is being used. Finally, there is no need for the small optical thickness (i.e. $0.999 \leq \tau \leq 1$) correction inserted in Lowtran 4, as required by its radiance calculational scheme.

7.4 Models for Trace Gases SO_2 , NO , NO_2 , and NH_3

Absorption by the trace gases was incorporated in Lowtran using a somewhat similar procedure. Empirical transmission functions were first obtained from a computerized procedure which replaced the classical manual graphical techniques. The procedure is explained in Chapter III of this report and has been proposed to the scientific community¹¹.

Instead of either representing the transmission function by a table or by a single function, it was divided into nine segments for each absorber. The individual curve segments are summarized in Table 5, each one being represented by the function

$$\tau = \exp(-10^{a_0 + a_1 x}) \quad (59)$$

For each absorber x is computed with Eqs. (8) through (11) and the relation

$$U = 0.772 \times 10^{-4} \text{ ppm } \rho_a Z \quad (60)$$

where ppm is the parts per million by volume, ρ_a is the air density in gm/m^3 and Z is the range in kilometers. Table 6 lists the ppm and temperature and pressure exponents used in the modularized code for the individual trace gases. The ppm values are read as input through a separate card which may be easily changed according to the needs of the user. The constants C' are tabulated in Table 7. The spectral coverage for each gas is depicted in Table 8. The models are for a resolution of 20 cm^{-1} and are defined at 5 cm^{-1} through their spectral regions of effectiveness. Their mean standard deviation in fitting the original line-by-line data is about 0.008. Figure 9 depicts the transmission functions for the four trace gases considered.

CURVE SEGMENT	TRANSMITTANCE INTERVAL	x- INTERVAL	FUNCTION CONSTANTS	
			a ₀	a ₁
1	1.000 ~ 0.900	$x \leq -1.057$	0.0682	0.9894
2	0.900 ~ 0.800	-1.057 ~ -0.725	0.0594	0.9811
3	0.800 ~ 0.700	-0.725 ~ -0.514	0.0492	0.9670
4	0.700 ~ 0.600	-0.514 ~ -0.350	0.0408	0.9506
5	0.600 ~ 0.500	-0.350 ~ -0.208	0.0343	0.9319
6	0.500 ~ 0.400	-0.208 ~ -0.074	0.0295	0.9091
7	0.400 ~ 0.300	-0.074 ~ 0.061	0.0273	0.8792
8	0.300 ~ 0.200	0.061 ~ 0.212	0.0300	0.8353
9	0.200 ~ 0.0	$x \geq 0.212$	0.0466	0.7568

Table 5a. Constants for the curve segments in the empirical transmission function for SO₂.

CURVE SEGMENT	TRANSMITTANCE INTERVAL	x- INTERVAL	FUNCTION CONSTANTS	
			a_0	a_1
1	1.000 ~ 0.900	$x \leq -1.158$	-0.0228	0.8240
2	0.900 ~ 0.800	-1.158 ~ -0.684	-0.1822	0.6864
3	0.800 ~ 0.700	-0.684 ~ -0.333	-0.2537	0.5818
4	0.700 ~ 0.600	-0.333 ~ -0.047	-0.2660	0.5450
5	0.600 ~ 0.500	-0.047 ~ 0.199	-0.2663	0.5388
6	0.500 ~ 0.400	0.199 ~ 0.419	-0.2685	0.5497
7	0.400 ~ 0.300	0.419 ~ 0.626	-0.2785	0.5737
8	0.300 ~ 0.200	0.626 ~ 0.833	-0.3000	0.6080
9	0.200 ~ 0.0	$x \geq 0.833$	-0.3373	0.6528

Table 5b. Constants for the curve segments in the empirical transmission function for NO.

CURVE SEGMENT	TRANSMITTANCE INTERVAL	x- INTERVAL	FUNCTION CONSTANTS	
			a_0	a_1
1	1.000 ~ 0.900	$x \leq 0.215$	-1.1877	0.9771
2	0.900 ~ 0.800	0.215 ~ 0.556	-1.1835	0.9577
3	0.800 ~ 0.700	0.556 ~ 0.775	-1.1668	0.9277
4	0.700 ~ 0.600	0.775 ~ 0.949	-1.1416	0.8952
5	0.600 ~ 0.500	0.949 ~ 1.104	-1.1063	0.8580
6	0.500 ~ 0.400	1.104 ~ 1.252	-1.0615	0.8174
7	0.400 ~ 0.300	1.252 ~ 1.406	-1.0055	0.7727
8	0.300 ~ 0.200	1.406 ~ 1.579	-0.9400	0.7260
9	0.200 ~ 0.0	$x \geq 1.579$	-0.8683	0.6807

Table 5c. Constants for the curve segments in the empirical transmission function for NO_2 .

CURVE SEGMENT	TRANSMITTANCE INTERVAL	x - INTERVAL	FUNCTION CONSTANTS	
			a ₀	a ₁
1	1.000 ~ 0.900	x ≤ -1.444	0.2775	0.8692
2	0.900 ~ 0.800	-1.444 ~ -1.005	0.0962	0.7436
3	0.800 ~ 0.700	-1.005 ~ -0.661	-0.0570	0.5913
4	0.700 ~ 0.600	-0.661 ~ -0.340	-0.1261	0.4867
5	0.600 ~ 0.500	-0.340 ~ -0.033	-0.1450	0.4312
6	0.500 ~ 0.400	-0.033 ~ 0.267	-0.1459	0.4037
7	0.400 ~ 0.300	0.267 ~ 0.575	-0.1409	0.3852
8	0.300 ~ 0.200	0.575 ~ 0.921	-0.1290	0.3645
9	0.200 ~ 0.0	x ≥ 0.921	-0.1224	0.3573

Table 5d. Constants for the curve segments in the empirical transmission function for NH₃.

TRACE GAS	SPECTRAL REGION (cm^{-1})	PRESSURE EXPONENT n	TEMPERATURE EXPONENT m	PARTS PER MILLION BY VOLUME ppm
SO ₂	440- 615	0.07122	0.06159	0.221
	1,055-1,250			
	1,310-1,410			
NO	1,760-1,970	0.90098	1.01192	0.250
NO ₂	655- 880	0.18066	0.20911	0.090
	1,540-1,670			
	2,840-2,895			
NH ₃	670-1,230	0.52125	-0.60438	0.200

Table 6. Absorber parameters in Modularized Lowtran used with the models for the trace gases.

WAVENUMBER (cm ⁻¹)	C'	WAVENUMBER (cm ⁻¹)	C'	WAVENUMBER (cm ⁻¹)	C'
440	-2.987	1070	-1.653	1320	-1.237
445	-2.330	1075	-1.443	1325	-0.494
450	-1.791	1080	-1.252	1330	0.139
455	-1.370	1085	-1.080	1335	0.613
460	-1.041	1090	-0.926	1340	0.899
465	-0.795	1095	-0.787	1345	1.043
470	-0.613	1100	-0.661	1350	1.090
475	-0.469	1105	-0.544	1355	1.097
480	-0.346	1110	-0.434	1360	1.104
485	-0.233	1115	-0.329	1365	1.093
490	-0.126	1120	-0.230	1370	1.118
495	-0.037	1125	-0.139	1375	1.088
500	0.0	1130	-0.073	1380	0.926
505	-0.008	1135	-0.047	1385	0.534
510	-0.052	1140	-0.057	1390	-0.067
515	-0.102	1145	-0.083	1395	-0.804
520	-0.102	1150	-0.098	1400	-0.768
525	-0.044	1155	-0.071	1405	-1.687
530	0.013	1160	-0.020	1410	-2.469
535	0.039	1165	0.014	2450	-3.669
540	0.014	1170	0.011	2455	-2.855
545	-0.056	1175	-0.040	2460	-2.131
550	-0.141	1180	-0.123	2465	-1.528

Table 7a. The spectral coefficient $C'(\nu)$ for SO_2 .

WAVENUMBER (cm ⁻¹)	C'	WAVENUMBER (cm ⁻¹)	C'	WAVENUMBER (cm ⁻¹)	C'
555	-0.221	1185	-0.213	2470	-1.076
560	-0.294	1190	-0.301	2475	-0.805
565	-0.366	1195	-0.388	2480	-0.647
570	-0.442	1200	-0.481	2485	-0.571
575	-0.529	1205	-0.586	2490	-0.549
580	-0.635	1210	-0.707	2495	-0.539
585	-0.766	1215	-0.843	2500	-0.536
590	-0.934	1220	-0.996	2505	-0.517
595	-1.157	1225	-1.165	2510	-0.528
600	-1.457	1230	-1.351	2515	-0.691
605	-1.862	1235	-1.554	2520	-1.073
610	-2.420	1240	-1.777	2525	-1.673
615	-3.094	1245	-2.033	2530	-2.414
1055	-2.604	1250	-2.369	2535	-2.207
1060	-2.156	1310	-3.010		
1065	-1.884	1315	-2.080		

Table 7a.

(Continued)

WAVENUMBER	C'	WAVENUMBER	C'	WAVENUMBER	C'
1760	-2.691	1835	-0.231	1910	0.003
1765	-2.521	1840	-0.176	1915	-0.032
1770	-2.328	1845	-0.144	1920	-0.105
1775	-2.115	1850	-0.143	1925	-0.211
1780	-1.894	1855	-0.188	1930	-0.352
1785	-1.685	1860	-0.244	1935	-0.529
1790	-1.485	1865	-0.342	1940	-0.742
1795	-1.296	1870	-0.434	1945	-0.992
1800	-1.117	1875	-0.471	1950	-1.282
1805	-0.947	1880	-0.483	1955	-1.610
1810	-0.792	1885	-0.392	1960	-1.975
1815	-0.649	1890	-0.266	1965	-2.374
1820	-0.519	1895	-0.151	1970	-2.806
1825	-0.407	1900	-0.046		
1830	-0.311	1905	-0.001		

Table 7b. The spectral coefficient $C'(\nu)$ for NO.

WAVENUMBER	C'	WAVENUMBER	C'	WAVENUMBER	C'
655	-0.844	800	-0.255	1,600	2.616
660	-0.760	805	-0.286	1,605	2.616
665	-0.676	810	-0.315	1,610	2.606
670	-0.608	815	-0.334	1,615	2.608
675	-0.543	820	-0.352	1,620	2.643
680	-0.496	825	-0.366	1,625	2.682
685	-0.450	830	-0.396	1,630	2.672
690	-0.414	835	-0.423	1,635	2.576
695	-0.383	840	-0.459	1,640	2.350
700	-0.326	845	-0.498	1,645	1.955
705	-0.289	850	-0.541	1,650	1.346
710	-0.217	855	-0.586	1,655	0.596
715	-0.140	860	-0.630	1,660	-0.258
720	-0.097	865	-0.676	1,665	-1.214
725	-0.034	870	-0.720	1,670	-1.951
730	-0.031	875	-0.766	2,840	-1.220
735	-0.082	880	-0.809	2,845	-0.644
740	-0.139	1,540	-2.428	2,850	-0.253
745	-0.216	1,545	-1.494	2,855	0.052
750	-0.249	1,550	-0.647	2,860	0.326
755	-0.207	1,555	0.122	2,865	0.574
760	-0.117	1,560	0.756	2,870	0.792

Table 7c. The spectral coefficient $C'(v)$ for NO_2 .

WAVENUMBER	C'	WAVENUMBER	C'	WAVENUMBER	C'
765	-0.047	1,565	1.230	2,875	0.978
770	0.000	1,570	1.568	2,880	1.122
775	0.009	1,575	1.855	2,885	1.216
780	-0.046	1,580	2.104	2,890	1.252
785	-0.100	1,585	2.310	2,895	1.249
790	-0.148	1,590	2.469		
795	-0.214	1,595	2.573		

Table 7c.

(Continued)

WAVENUMBER	C'	WAVENUMBER	C'	WAVENUMBER	C'
690	-2.603	875	-1.124	1,060	-0.589
695	-2.456	880	-1.155	1,065	-0.565
700	-2.290	885	-1.161	1,070	-0.537
705	-2.128	890	-1.143	1,075	-0.510
710	-1.980	895	-1.139	1,080	-0.512
715	-2.225	900	-1.117	1,085	-0.528
720	-1.823	905	-1.107	1,090	-0.575
725	-1.744	910	-0.844	1,095	-0.625
730	-1.674	915	-0.558	1,100	-0.668
735	-1.577	920	-0.238	1,105	-0.694
740	-1.481	925	-0.042	1,110	-0.717
745	-1.372	930	-0.002	1,115	-0.740
750	-1.284	935	-0.157	1,120	-0.774
755	-1.207	940	-0.436	1,125	-0.834
760	-1.128	945	-0.610	1,130	-0.905
765	-1.061	950	-0.548	1,135	-0.977
770	-1.004	955	-0.352	1,140	-1.042
775	-0.947	960	-0.139	1,145	-1.133
780	-0.886	965	-0.095	1,150	-1.219
785	-0.876	970	-0.365	1,155	-1.301
790	-0.872	975	-0.729	1,160	-1.383
795	-0.869	980	-1.048	1,165	-1.488
800	-0.872	985	-1.275	1,170	-1.594

Table 7d. The spectral coefficient $C'(v)$ for NH_3 .

WAVENUMBER	C'	WAVENUMBER	C'	WAVENUMBER	C'
805	-0.848	990	-1.257	1,175	-1.696
810	-0.811	995	-1.142	1,180	-1.796
815	-0.772	1,000	-1.053	1,185	-1.873
820	-0.773	1,005	-0.963	1,190	-1.936
825	-0.793	1,010	-0.920	1,195	-1.991
830	-0.825	1,015	-0.944	1,200	-2.080
835	-0.869	1,020	-0.889	1,205	-2.183
840	-0.894	1,025	-0.829	1,210	-2.292
845	-0.890	1,030	-0.736	1,215	-2.404
850	-0.873	1,035	-0.644	1,220	-2.529
855	-0.868	1,040	-0.596	1,225	-2.639
860	-0.907	1,045	-0.569	1,230	-2.732
865	-0.965	1,050	-0.572		
870	-1.045	1,055	-0.590		

Table 7d.

(Continued)

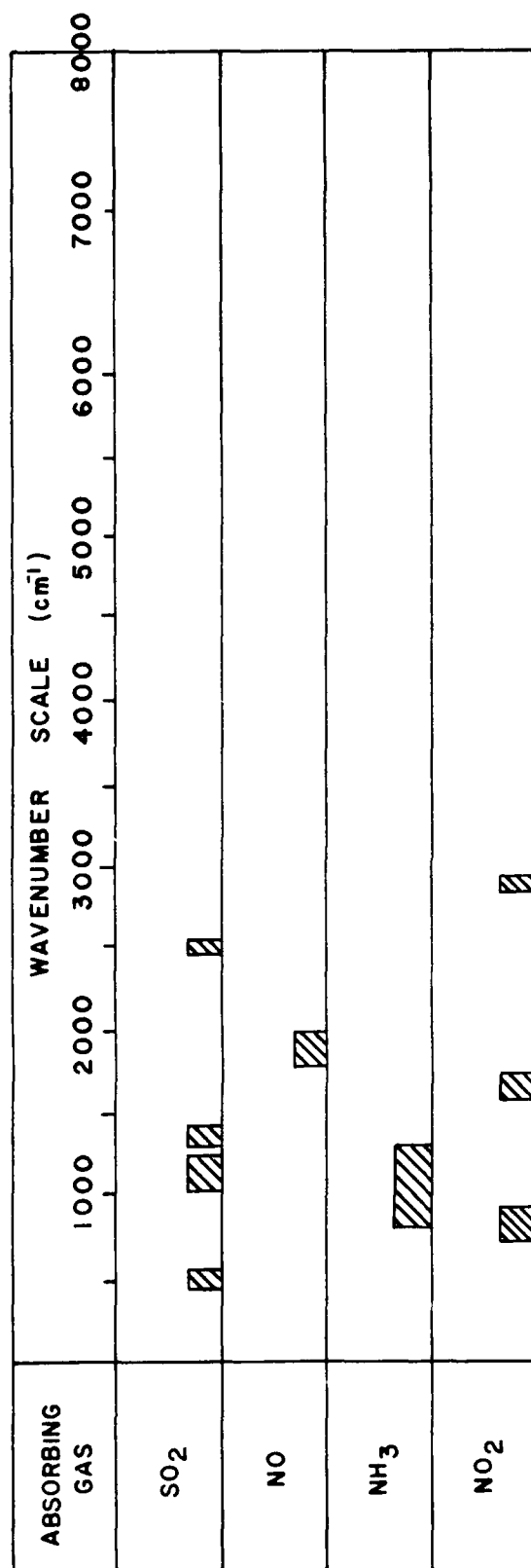


Table 8. Absorption frequency region of the trace gases in the atmosphere.

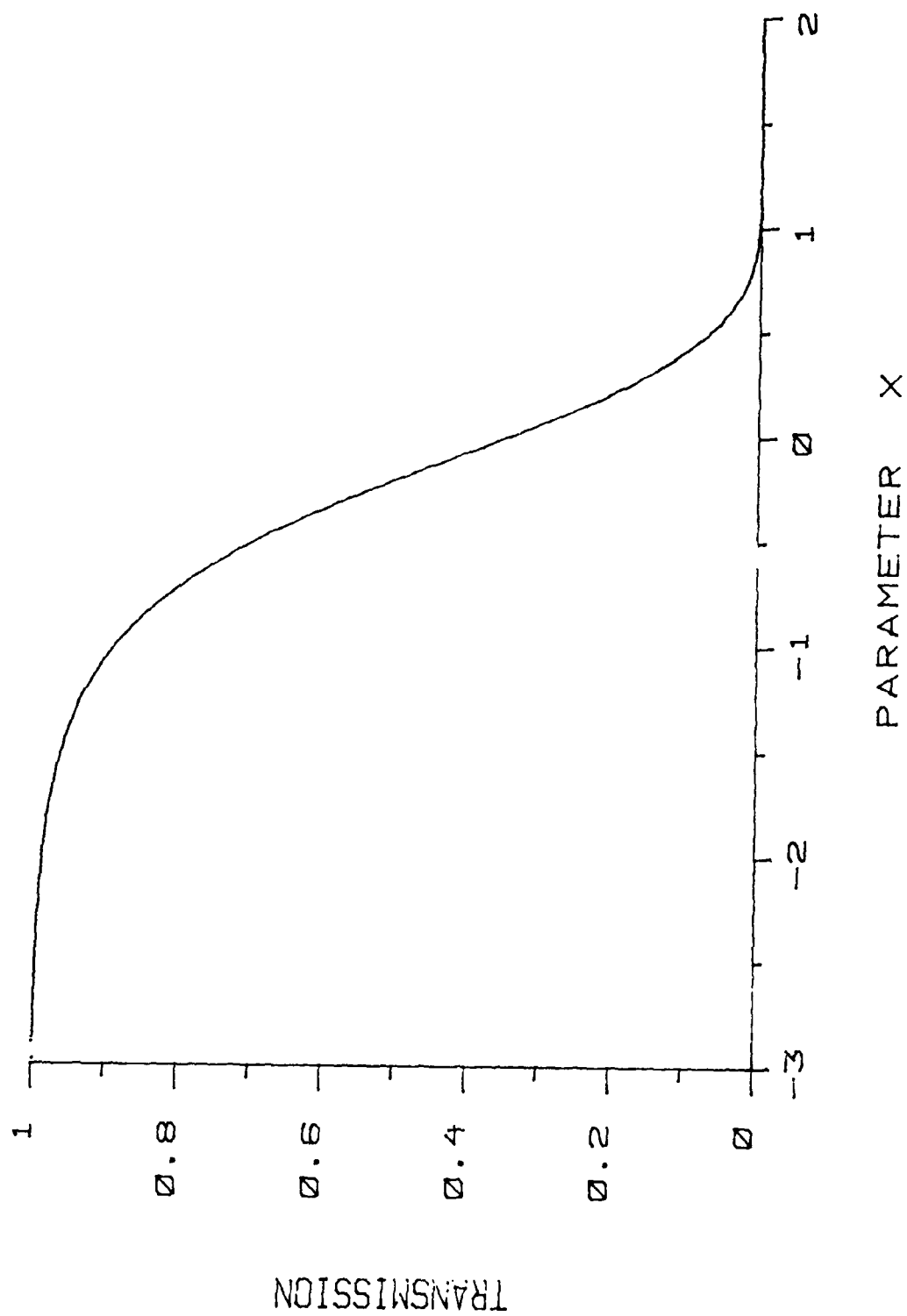


Fig. 9a. Empirical transmission function for SO_2 .

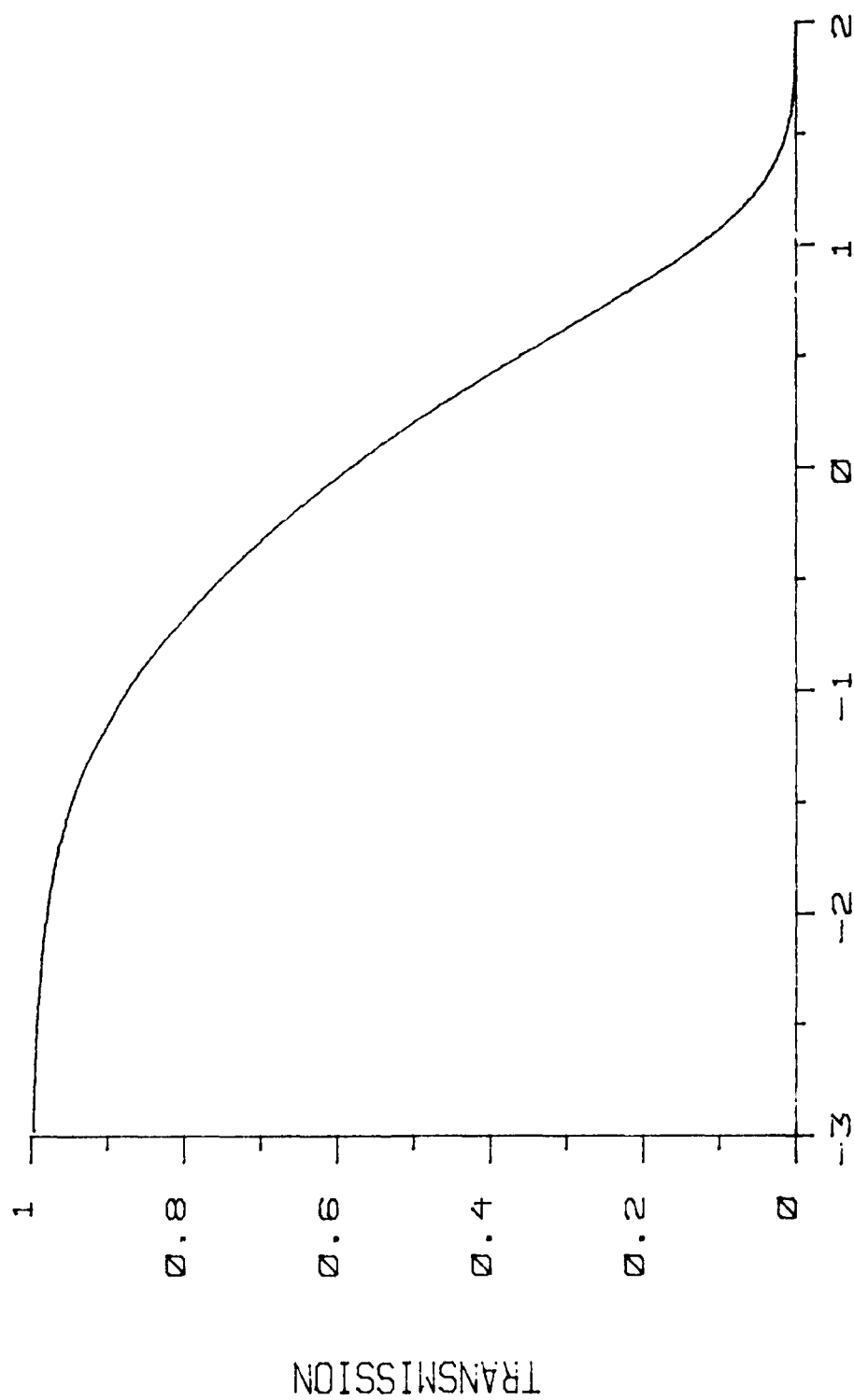


Fig. 9b. Empirical transmission function for NO.

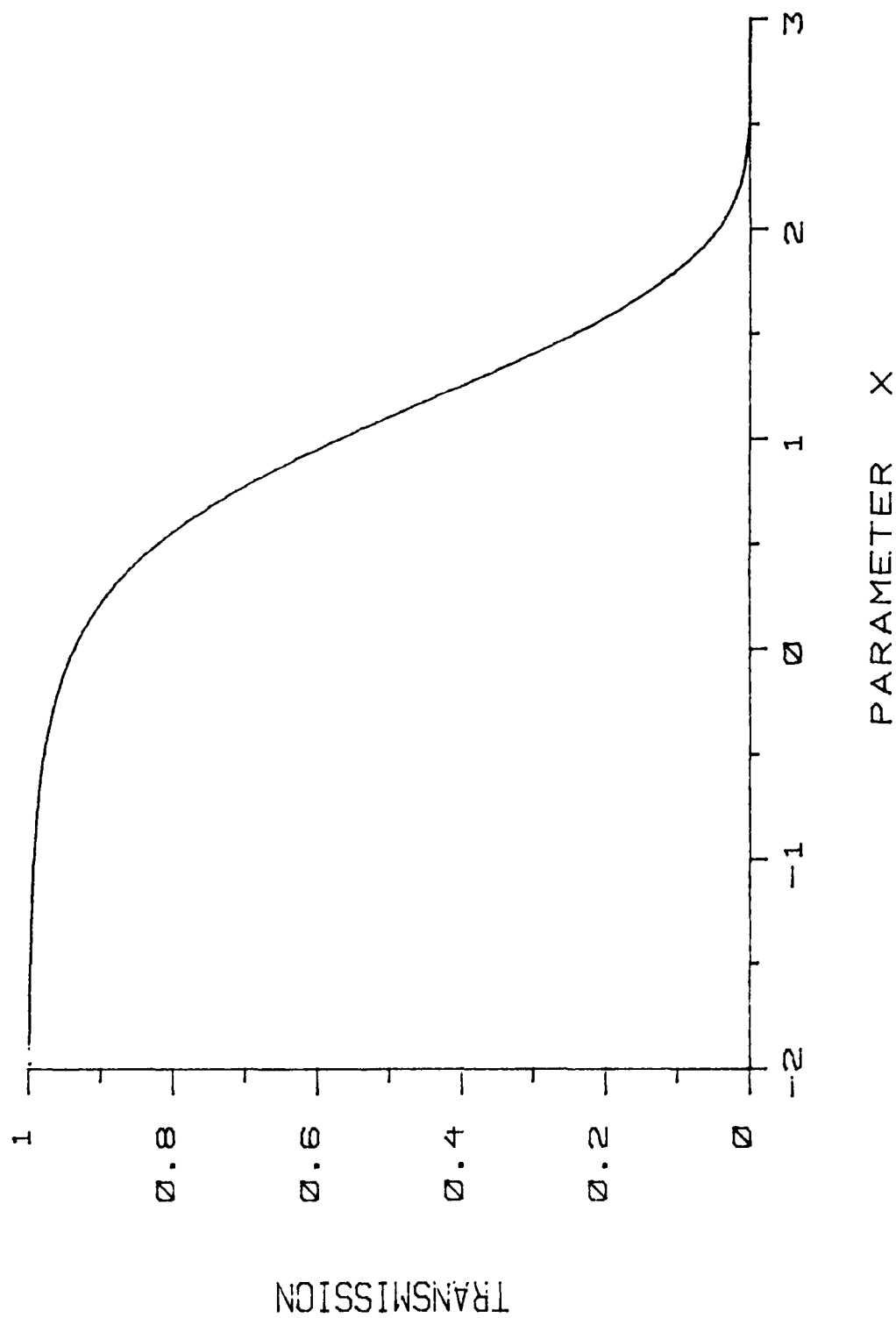


Fig. 9c. Empirical transmission function for NO_2 .

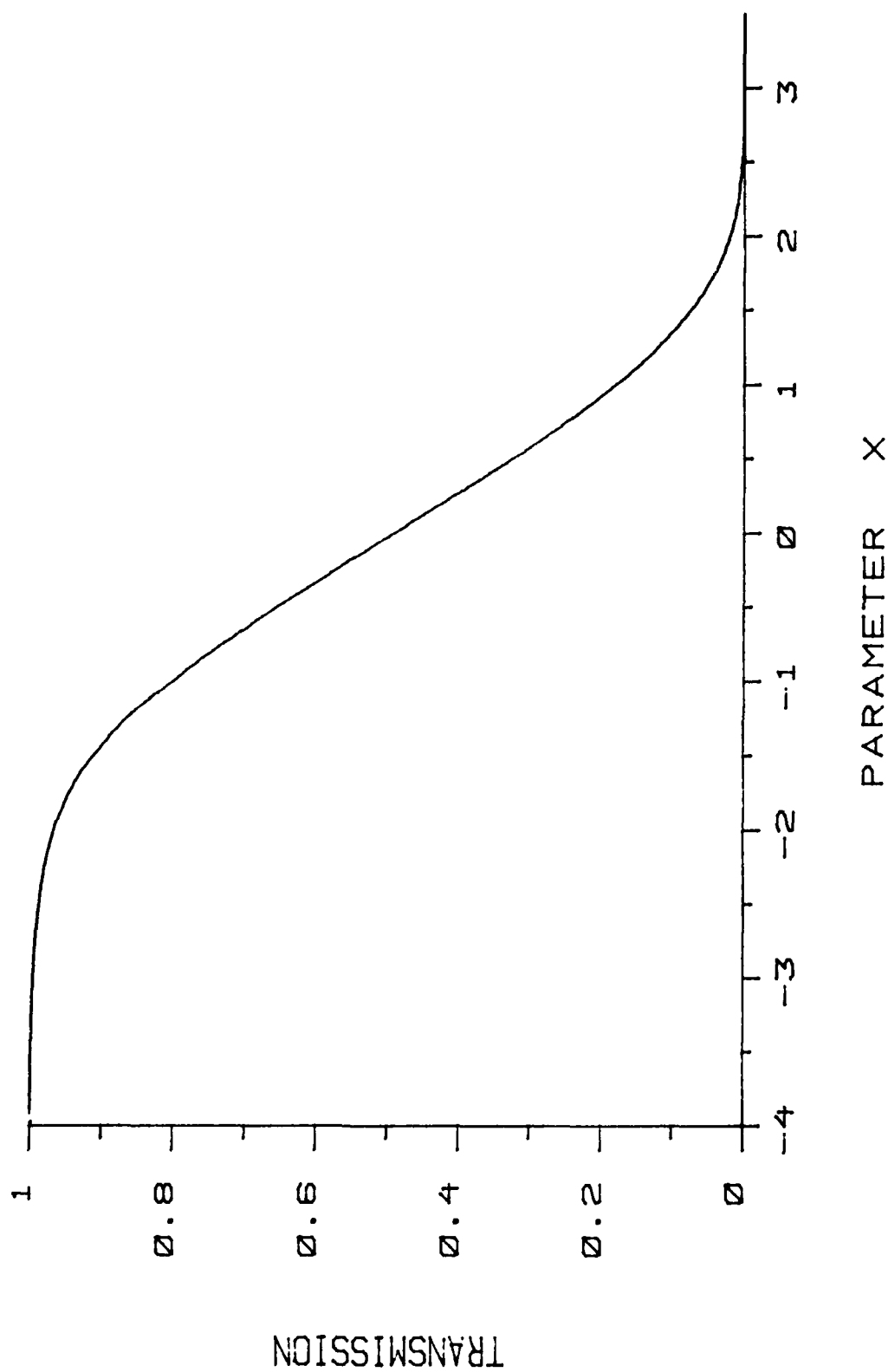


Fig. 9d. Empirical transmission function for NH_3 .

VIII. Calculations and Results

8.1 Introduction

The procedure for the use of the Modularized Lowtran in calculations is identical to that of the original and, hence, deserves no further explanation. There are some input and output alterations that deserve some explanatory remarks. Changes in the input format include:

1. Reading of the spectral constants for all band models at the beginning of the main program rather than in the subroutines.
2. Elimination of the transmittance tables for H_2O vapor, infrared O_3 and the uniformly-mixed gases.
3. Reading of the spectral constants for the newly added band models for the trace gases.
4. Reading of the air density profile for the U.S. Standard atmosphere, and of the ppm for the calculation of the equivalent amounts of the trace gases.
5. Changes in the dimension statements to include the additional subscripted variables.

Changes in the output format include:

1. Modification of the print out of the input data.
2. Modification of the output table of computations to include the transmittance for the trace gases.

It should be stressed, however, that the code is operated using exactly the same four control cards as in the original code.

8.2 Testing of Modularized Version

The first step in the testing of the modularization consisted of running identical calculations using the original code and the modularized code before the replacement of the transmittance tables and before the addition of the trace gases. Numerous cases were considered during this effort. A particular case in which the spectral range varied from 2350 to 2450 cm^{-1} for a path at 65° from a height of 2.5 km to a height of 8.5 km and a 23 km visual range, is shown in the Appendix. This output is identical to the output obtained from the original Lowtran.

The second step in the testing procedure consisted of running calculations using the original code and the modularized version with the transmittance tables replaced with the continuous functions, but before the addition of the trace gases. For this purpose, 10 frequencies were selected such that different combinations of models would be effective in the calculation of the total transmittance. The calculations were for a 5 km path at sea level in a sub-arctic winter atmosphere with a 23 km visibility. The results are summarized in Table 9. The columns listed under Transmittance Deviations represent the differences between the calculations using the tabulated and the continuous functions. Note that the average total transmittance deviation is 0.0034, which is below the standard deviation obtained in the curve fitting of

TRANSMITTANCE DEVIATIONS

WAVENUMBER (cm^{-1})	H ₂ O VAPOR	INFRARED O ₃	UNIFORMLY- MIXED GASES	TOTAL TRANSMITTANCE
455	0.0022	0.0000	0.0000	0.0021
555	0.0035	0.0000	0.0026	0.0018
655	0.0041	0.0003	0.0000	0.0000
755	0.0007	0.0003	0.0047	0.0038
955	0.0057	0.0002	0.0050	0.0096
1155	0.0026	0.0003	0.0050	0.0058
1355	0.0044	0.0000	0.0013	0.0006
1855	0.0007	0.0001	0.0034	0.0007
2455	0.0015	0.0000	0.0054	0.0045
3155	0.0037	0.0001	0.0027	0.0053

Table 9. Transmittance difference between calculations using the tabulation of the transmittance functions and calculations using the continuous function representation for a 5 km path at sea level in a sub-arctic winter atmosphere.

the functions to the individual transmittance tables. This deviation amounts to an error of about 0.7% in the middle of the curve-of-growth, which far exceeds the accuracy of Lowtran (between 10 to 20%). The following are attractive features of the continuous functions:

1. They inherently provide for continuous exponential interpolation in transmittance, which is superior to the linear interpolation used in connection with the transmittance tables.
2. They provide for analytical operations such as differentiation and interpolation often needed in radioactive transfer problems.
3. They can be used easily for curve fitting to new transmittance data using computerized procedures.
4. Their use reduces significantly the computer storage requirements for the individual models.
5. They continuously provide for transmittance calculations for small argument values where $0.9999 \leq \tau \leq 1$, for which range Lowtran 4 includes an additional exponential function.

It should be pointed out that the deviations listed in Table 9, although insignificant, do not represent errors solely attributed to the analytical functions. Since they are smaller than the uncertainties in the original data used to develop the tabulated transmittances, they primarily represent differences in the calculational procedures. In fact, in the region between the tabulations the use of the analytical functions are likely to provide more accurate results than the use of the original method in Lowtran.

The last effort in the testing of the modularized code consisted of calculations involving the newly added trace gases. For this purpose ten frequencies were run at which the trace gas models are effective. The same frequencies were run with the modularized Lowtran without these models. The results are summarized in Table 10. The table is primarily intended to show the absorptive effects of the trace gases.

MOLECULAR TRANSMITTANCE

WAVENUMBER (cm ⁻¹)	SO ₂	NO	NO ₂	NH ₃	TOTAL (with T.G.)	TOTAL (without T.G.)
455	0.9948	1.0000	1.0000	1.0000	0.0000	0.0000
555	0.9308	1.0000	1.0000	1.0000	0.0185	0.0199
655	1.0000	1.0000	0.9997	1.0000	0.0000	0.0000
755	1.0000	1.0000	0.9995	0.9783	0.0029	0.0030
955	1.0000	1.0000	1.0000	0.8878	0.1155	0.1300
1155	0.8929	1.0000	1.0000	0.9820	0.1657	0.1890
1355	0.2728	1.0000	1.0000	1.0000	0.0000	0.0000
1855	1.0000	0.9034	1.0000	1.0000	0.0000	0.0000
2455	0.9998	1.0000	1.0000	1.0000	0.5734	0.5735

Table 10. Calculations of trace gas (T.G.) transmittances for a 5 km path at sea level in a tropical atmosphere with a 23 km visual range. The columns on total transmittance include all the attenuators and the trace gases, except for the rightmost column which excludes the trace gases.

Table 11: (a) Atmospheric regions included in the data calculations

Model	P (mbar)	T (°K)
Standard	1013	288.1
	898.6	281.6
	795.0	275.1
	701.2	268.7
	616.6	262.2
Tropical	805.0	288.0
Subarctic Winter	1013	257.1

(b) Transmittance cuts chosen from the curve of growth

τ_1	0.99
τ_2	0.95
τ_3	0.9
τ_4	0.8
τ_5	0.7
τ_6	0.6
τ_7	0.5
τ_8	0.4
τ_9	0.3
τ_{10}	0.2
τ_{11}	0.1
τ_{12}	0.065

		Absorber Parameters		Spectral Parameter C' (cm ⁻¹)				Coefficients of Analytical Function				Standard Deviation
		n	m	v ₁	v ₂	v ₃	v ₄					
	SUM	0.07844	0.06037	0.0	0.019	1.108	-0.566	a ₁ = 0.02292 a ₂ = 0.86759 a ₃ = -0.08578				0.006259
	Band Model Parameters	0.07130	0.06186	0.0	0.014	1.104	-0.571					
A	Empirical											
	$\tau_i =$ $x_i =$	0.95 -1.3727	0.9 -1.0569	0.8 -0.7246	0.7 -0.5140	0.6 -0.3498	0.5 -0.2076	0.4 -0.0742	0.3 0.0606	0.2 0.2115	0.1 0.4170	
D	Piece-Wise Analytical											
	$a_1 =$ $\left(\begin{matrix} 1st \\ order \end{matrix} \right) a_2 =$ $a_3 =$	0.0682 0.9894 0	0.0594 0.9811 0	0.0492 0.9670 0	0.0408 0.9506 0	0.0343 0.9319 0	0.0295 0.9091 0	0.0273 0.8792 0	0.0300 0.8353 0	0.0466 0.7568 0		0.005749
E												
T	$a_1 =$ $\left(\begin{matrix} 2nd \\ order \end{matrix} \right) a_2 =$ $a_3 =$	0.0755 1.0016 0.0050	0.2247 1.3653 0.2157	0.2099 1.5013 0.4314	0.1356 1.4061 0.5273	0.0590 1.1214 0.3400	0.0285 0.8897 -0.0689	0.0299 0.8715 -0.8641	0.0151 1.1520 -1.1634	0.0296 0.8781 -0.1931		0.005604

Table 12a. Band model parameters for SO₂.

	Absorber Parameters		Spectral Parameter C' (cm ⁻¹)				Coefficients of Analytical Function				Standard Deviation	
			ν_1	ν_2	ν_3	ν_4						
	n	m	ν_1 1905	ν_2	ν_3	ν_4	$a_1 = -0.26287$ $a_2 = 0.58035$ $a_3 = -0.00926$	0.008667				
STIMUL	1.05084	1.08785	0.0									
Band Model Parameters			0.90099	1.01192	0.0							
A	Empirical	$\tau_1 =$ $x_1 =$	0.95 -1.5380	0.9 -1.1585	0.8 -0.6838	0.7 -0.3334	0.6 -0.0473	0.5 0.1988	0.4 0.4193	0.3 0.6260	0.2 0.3333	0.1 1.0715
D	Piece-Wise Analytical	$a_1 =$	-0.0278	-0.1822	-0.2537	-0.2660	-0.2663	-0.2685	-0.2785	-0.3000	-0.3373	
S	$\left(\begin{smallmatrix} \text{1st} \\ \text{order} \end{smallmatrix}\right)$	$a_2 =$	0.8240	0.6764	0.5818	0.5450	0.5388	0.5497	0.5737	0.6080	0.6528	0.005563
E		$a_3 =$	0	0	0	0	0	0	0	0	0	
T	$\left(\begin{smallmatrix} \text{2nd} \\ \text{order} \end{smallmatrix}\right)$	$a_1 =$	-0.1770	-0.1867	-0.2710	-0.2709	-0.2615	-0.3293	-0.4937	-0.6837	-0.2321	
		$a_2 =$	0.5906	1.0667	0.5046	0.4258	0.6162	1.0007	1.4307	1.6815	0.4283	0.005635
		$a_3 =$	-0.0866	0.2064	-0.0759	-0.3133	-0.5107	-0.7296	-0.8199	-0.7357	0.1179	

Table 12b. Band model parameters for NO.

	Absorber Parameters	Spectral Parameter C' (cm ⁻¹)							Coefficients of Analytical Function				Standard Deviation
		n	m	ν ₁	ν ₂	ν ₃	ν ₄						
SIEMIS		0.19941	0.22631	0.0	2.697	1.271			a ₁ = -1.2203 a ₂ = 1.0908 a ₃ = -0.1188	0.015395			
Band Model Parameters		0.17830	0.22484	0.0	2.689	1.259							
A	Empirical	0.95	0.9	0.8	0.7	0.6	0.5	0.4	0.3	0.2	0.1		
D	Empirical	-0.0009	0.2140	0.5542	0.7739	0.9483	0.1028	1.2511	1.4046	1.5784	1.8074		
S	Piece-wise Analytical	a ₁ = -1.1860 a ₂ = 0.9170 a ₃ = 0	-1.1324 0.9578 0	-1.1656 0.9276 0	-1.1404 0.8950 0	-1.1052 0.8579 0	-1.0604 0.8172 0	-1.0042 0.7723 0	-0.9381 0.7252 0	-0.8656 0.6793 0		0.015555	
I		a ₁ = -1.1864 a ₂ = 0.9777 a ₃ = -0.0065	-1.0811 0.3013 0.3544	-0.4268 -1.3600 1.7222	0.0792 -1.9671 1.6619	0.1053 -1.5164 1.1576	-0.9289 0.5929 0.0953	-3.6587 4.7838 -1.5105	-5.3854 6.7090 -2.0059	-0.9659 0.7984 -0.0352		0.015620	

Table 12c. Band model parameters for NO_2 .

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COMPUTERIZED METHOD FOR THE GENERATION OF MOLECULAR TRANSMITTAN--ETC(U)

DEC 79 J H PIERLUISSI, K TOMIYAMA

DAA629-79-C-0067

UNCLASSIFIED

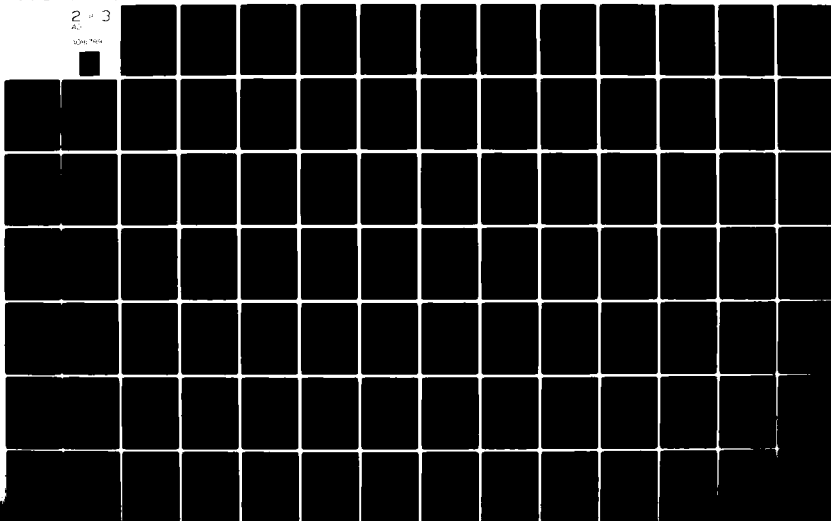
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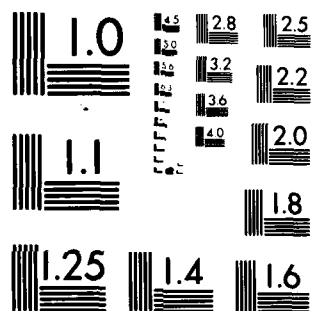
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MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS 1963 A

	Absorber Parameters		Spectral Parameter C' (cm ⁻¹)				Coefficients of Analytical Function				Standard Deviation
			n	m	v ₁	v ₂					
	SIMIN	0.53876	-0.71406	930						a ₁ = -0.14141 a ₂ = 0.44740 a ₃ = -0.06716	
	Band Model Parameters	0.52125	-0.60437	0.0							
A	Empirical										
	$\tau_i =$	0.95	0.9	0.8	0.7	0.6	0.5	0.4	0.3	0.2	0.1
	$x_i =$	-1.8032	-1.4438	-1.0054	-0.6608	-0.3403	-0.0330	0.2673	0.5751	0.9210	1.3562
D	Piece-Wise Analytical										
S	$a_1 =$	0.2775	0.0962	-0.0570	-0.1261	-0.1450	-0.1459	-0.1409	-0.1290	-0.1224	
	$a_2 =$	0.8692	0.7436	0.5913	0.4867	0.4312	0.4037	0.3852	0.3645	0.3573	0.005237
Z	$a_3 =$	0	0	0	0	0	0	0	0	0	
T	$a_1 =$	0.0894	0.9846	0.2095	-0.1135	-0.1475	-0.1419	-0.2291	-0.3829	-0.0196	
	$a_2 =$	0.6347	2.2425	1.2594	0.5427	0.3457	0.5098	0.8682	1.0318	0.1698	0.005484
	$a_3 =$	-0.0722	0.6120	0.4010	0.0559	-0.2290	-0.4530	-0.5734	-0.4794	0.0785	

Table 12d. Band model parameters for NH₃.

8.3 Band Model Development

Two sets of curves of growth data for each major absorption band for four trace gases SO_2 , NO , NO_2 , and NH_3 were generated by the line-by-line calculation from the AFGL trace gas parameter tape. One of them consists of 12-cut data for several layers of atmosphere and the other consists of 65-cut data for the standard atmosphere only. Considering the wide range of applications, we included not only the standard atmospheric conditions but also one condition each from the tropical and subarctic winter climates. They are listed in Table 11 together with the 12 chosen transmittance values. The major absorption bands for the four trace gases are given in Table 12 together with the corresponding computed C' values.

Ten middle cuts were chosen from the 12-cut data and used in both ADSET and SIMMIN for the computation of the band model parameters and the standard transmission function. Depending on the number of major absorption bands, the total numbers of data used differ but are in the range of 60-210. The 65-cut data was used in ADSET for the piecewise interpolation to compute piecewise analytical transmission functions.

The ADSET computations were done first. The obtained band model parameter values n , m , and C'_1 and nine sets of coefficients a_1 , a_2 , and a_3 are tabulated in

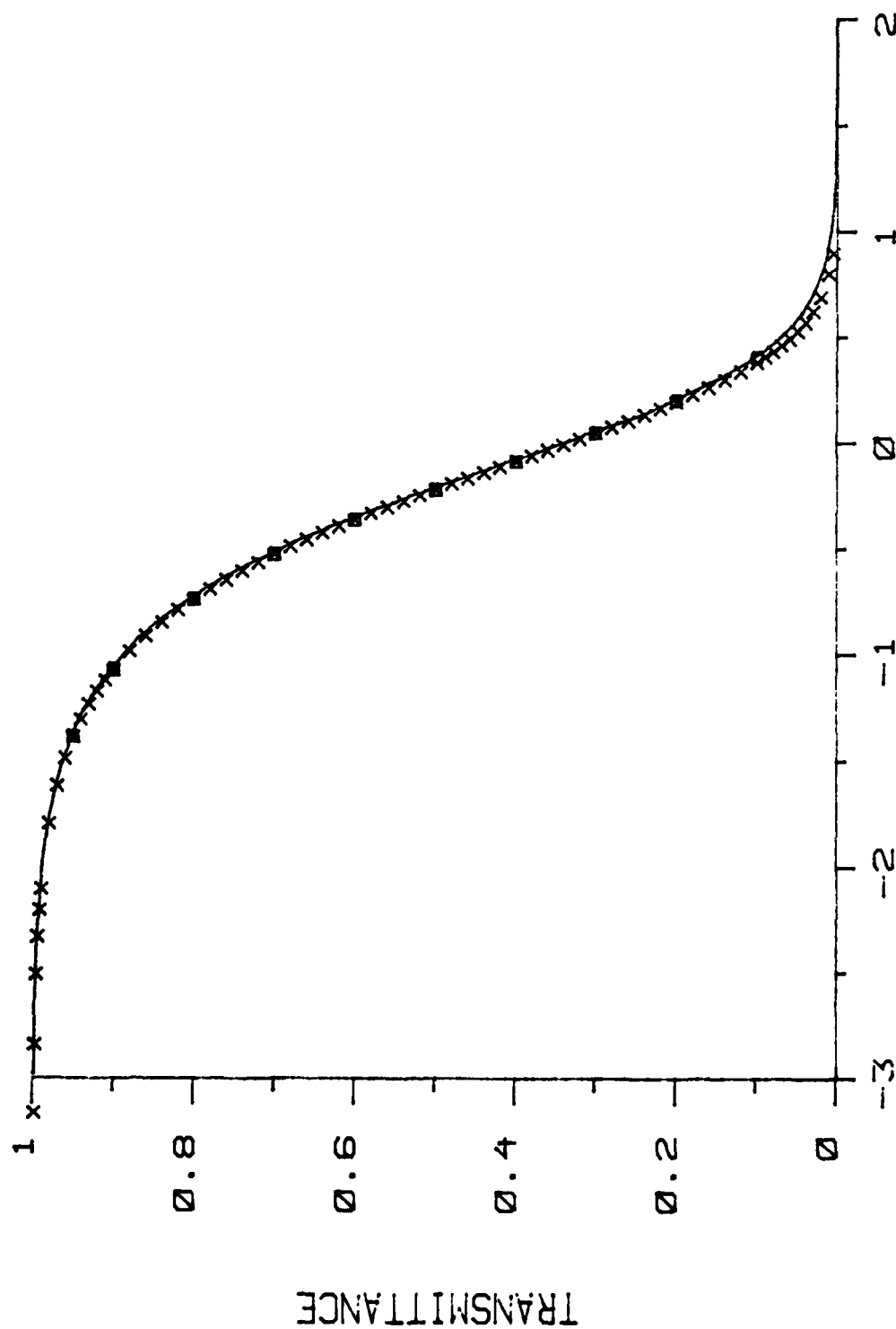
Table 12 for SO_2 , NO, NO_2 , and NH_3 in this order. The corresponding standard deviations are also listed in these tables.

We also have generated standard atmospheric condition data for non-major bands of each trace gases. These data were used to evaluate non-major $C'(v)$ values. The computed $C'(v)$ values were listed in Table 5. As we have discussed, these $C'(v)$ values and the band model parameters together with the first order piecewise-analytical standard transmission function were implemented in the modularized Lowtran.

We recall that the SIMMIN computation is a recursive one and we need a set of initial guesses of the parameter values to start the computation. For the band model parameters n , m , and C'_1 , we used the values computed by ADSET. For a_1 and a_2 , the respective averages of the first order piecewise interpolation results of ADSET were used. Finally, a_3 was set to be zero. We note that our initial guesses are fairly accurate, since these values were optimal or optimal in average for ADSET computation. A small number ϵ which was used for the check of convergence was chosen to be 10^{-6} . Since the parameter values are expected to be in the range $-10 \sim 10$, $\epsilon = 10^{-6}$ gives the limit of numerical accuracy of numbers in the computer. The SIMMIN results are also listed in Table 12.

Typical curve-fits by piecewise analytical standard transmission functions to actual data are shown in Fig. 10 for SO_2 at 500 wavenumber. The corresponding analytical standard transmission function are also compared to the data in Fig. 10. In all of the three graphs in this Figure, the 65-cut data were also plotted to show the fitness of the standard curves.

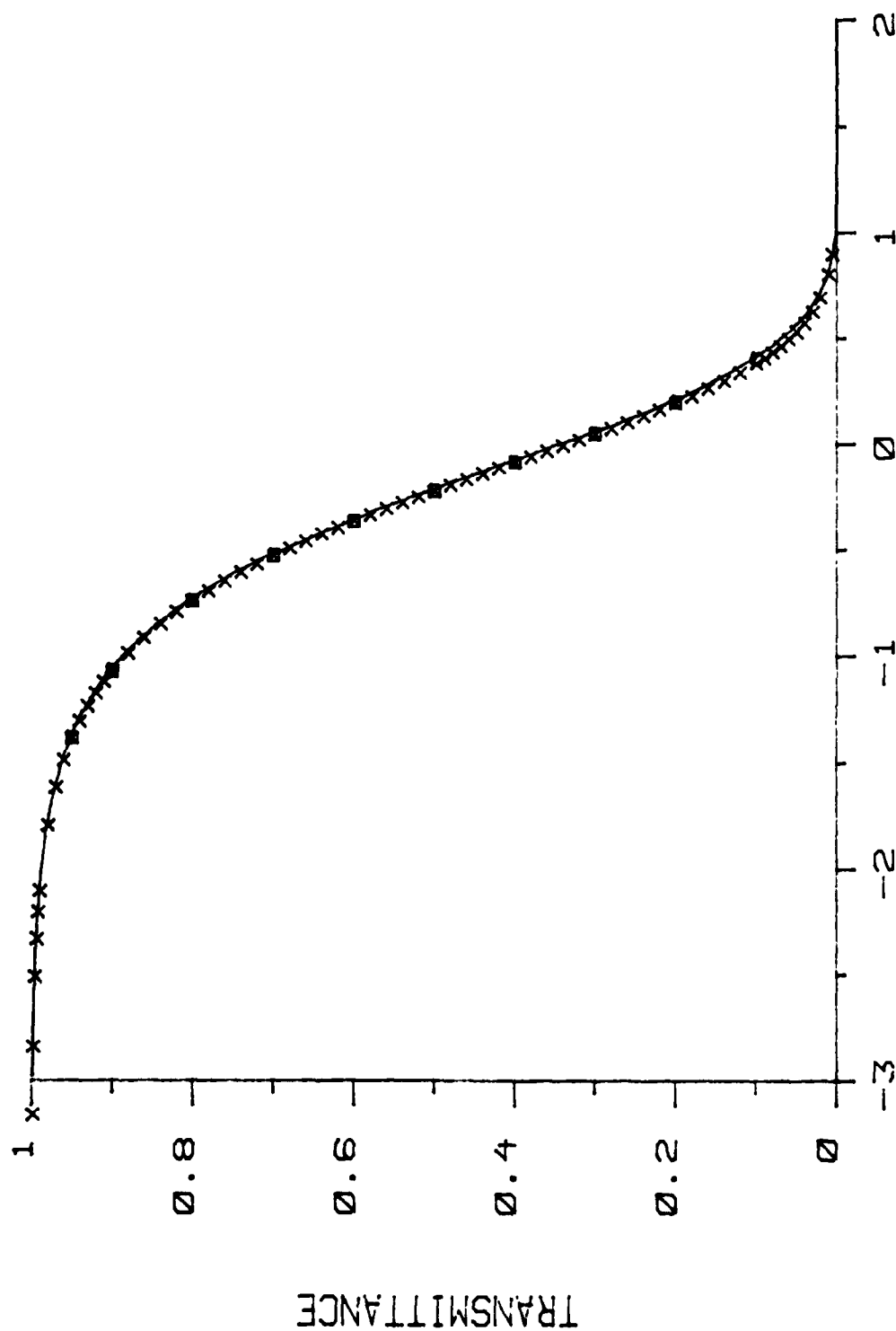
The computation was repeated using two smaller data sets with 6 and 4 cuts only. The chosen cuts were (0.95, 0.9, 0.8, 0.6, 0.4, and 0.1) for 6 cut data and (0.95, 0.9, 0.6, and 0.2) for 4 cut data. The derived band model parameter values were similar to those in Table 12 and, hence, were not repeated here. Instead, the corresponding standard deviations were listed and compared with the 10 cut cases in Table 13.



PARAMETER X

Fig. 10. (a) Standard transmission function from
ADSET with $a_3 = 0$ for SO₂ at 500 cm⁻¹

ADSET $a_3=0$
— Piecewise analytic
□ empirical
x 65 data



PARAMETER X

Fig. 10. (b) Standard transmission function from
ADSET with $a_3 \neq 0$ for SO_2 at 500 cm^{-1}

ADSET $a_3 \neq 0$
—piecewise analytic
□ empirical
x 65 data

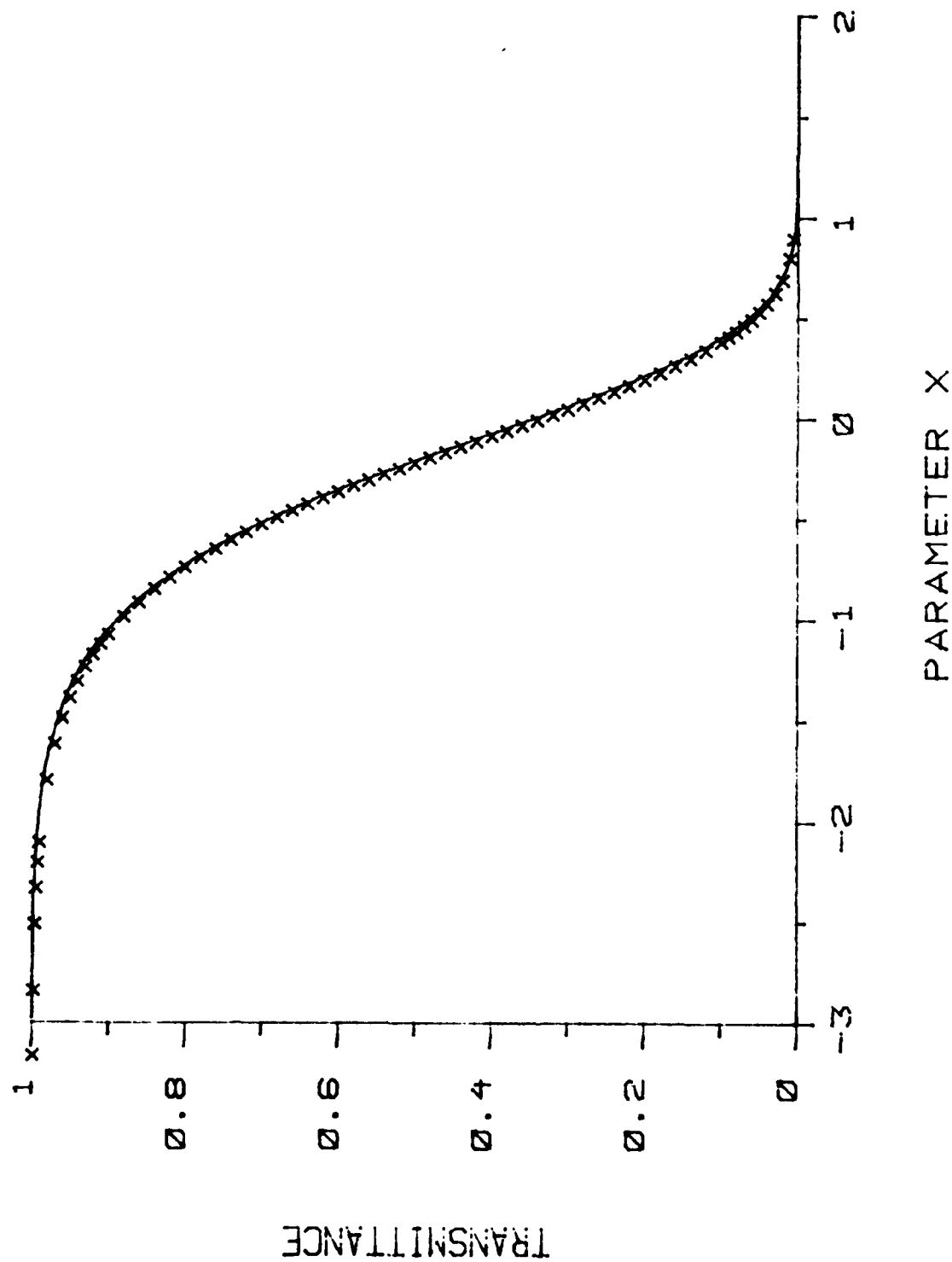


Fig. 10. (c) Standard transmission function from SIMMIN
for SO_2 at 500 cm^{-1}

SIMMIN
—: Computed
x: 65 data

ABSORBER	CODES	STANDARD DEVIATIONS IN τ		
		4 Cut Data	6 Cut Data	10 Cut Data
SO ₂	SIMMIN	0.004450	0.006636	0.006259
	ADSET	0.005344	0.006551	0.005749
	SIMMIN	0.004830	0.006036	0.005604
NO	SIMMIN	0.005349	0.009345	0.008667
	ADSET	0.009310	0.006934	0.005563
	SIMMIN	0.009210	0.006764	0.005635
NO ₂	SIMMIN	0.015009	0.014051	0.015395
	ADSET	0.01863	0.015355	0.015555
	SIMMIN	0.017377	0.014780	0.015620
NH ₃	SIMMIN	0.004661	0.010423	0.010558
	ADSET	0.006455	0.005454	0.005237
	ADSET	0.006594	0.005400	0.005484

Table 13. Comparison of standard deviations in τ . The two rows, ADSET 1 and 2 are, respectively, for the piecewise analytical transmission functions and linear and quadratic exponents.

IX Discussion and Conclusions

9.1 Introduction

The modularized version presented here is fundamentally the same Lowtran code except for the separation of its computation structure into separate modules or subroutines. Although it is based on the 4th version, it can be adapted with little modification to any future versions, such as the 5th version now in progress. In fact, this latter version already has been structured by AFGL such that the emission/radiance loop is in a subroutine. The modularized code presented here breaks down that loop into a frequency selection subroutine, an equivalent absorber amount subroutine and separate subroutines for each one of the attenuation codes. The use of modules in a complex code such as Lowtran has numerous advantages, among which the amenability for updating by individual users to suit their specific needs is at the top of the list. In the ever changing field of modeling it is highly desirable to be able to easily modify the code for changes in the spectral coverage, the spectral resolution, the absorber concentrations in abnormal environments, the original transmission data used in the development and in the models used for the individual attenuators. The modularized version presented here, although is not the final answer to all conceivable needs, it is a first basic step

in that direction. Practicing this predicament, the authors added transmission models for the trace gases to the code.

9.2 Changes and Recommendations

The following are the basic changes introduced in The Modularized Lowtran:

1. The original main program was separated into a central program and subroutines for the absorber amount and the individual attenuation models.
2. In the interest of efficiency and clarity, a new subroutine FGQSL was added for the selection of the attenuation model effective at the given frequency.
3. The subroutine HNO_3 was re-structured to the form of the other previously incorporated subroutines in Lowtran.
4. Continuous analytical models were provided to replace the transmittance curves for H_2O vapor, O_3 and the uniformly-mixed gases.
5. New subroutines for the trace gases SO_2 , NO , NO_2 and NH_3 were added.

A copy of the modularized version is found in the Appendix.

Some recommendations may be made at this time concerning future modifications of Lowtran. They are as follows:

1. AFGL should be informed of the modularization presented here as well as of the addition of the trace gases (SO_2 , NO , NO_2 and NH_3) so that they may modify their master copy accordingly.
2. As soon as they are available, vertical profiles for the concentrations of the trace gases should be added.
3. The uniformly-mixed gases (CO_2 , N_2O , CO , CH_4 , etc.) should be modeled and be included as separate subroutines.

4. The resolution of all resonant absorption models in the IR should be increased to about 10 cm^{-1} , which will also allow for model redevelopments with more recent and more accurate transmission data.
5. All model developments should adopt computerized numerical methods rather than the inaccurate manual graphical techniques used in the past.
6. The transmittance calculations should include the calculation of the standard deviation expected from known uncertainties in the input meteorological variables¹²⁻¹⁴.
7. The slant-path calculations should include corrections for the Lorentzian-Doppler broadening above the 10 mb-level.
8. Continuous functions should replace the tabulated transmittance functions, together with their awkward interpolation procedure.

9.3 Model Development

The values of band model parameters n and m and spectral parameters C_1' obtained by ADSET and SIMMIN agreed very well. Furthermore, as it was shown in Table 13, the standard deviations corresponding to different cases followed a same pattern for the ADSET and SIMMIN results. This consistency proves the validity of both methods.

In general, the SIMMIN and ADSET computations resulted in similar standard deviations. It was expected that the ADSET computation should result in lower standard deviations since it contained more parameters to adjust. However, for a half of the cases, the SIMMIN code produced lower standard deviations. This is due to the large computational error for the ADSET computations in solving the normal equation $AX = B$. When the condition number of the coefficient matrix A becomes large (i.e., A becomes close to be singular), the computational error becomes so large that it can exceed the directly minimized error of the SIMMIN computation.

We note that this reversal occurred for all four cut data cases. This suggests that the advantage for ADSET of having more parameters to be adjusted is not significant for these cases. Hence, we recommend the use of SIMMIN if the available data contains less than five or six cuts.

A comparison of the standard deviations for two

piecewise interpolation results in the ADSET computation showed no significant difference. Furthermore, the results with the second method using quadratic form of x on the exponent of the double exponential function were 'bumpy' for some cases. Since the nature of the transmittance does not predict this behavior, we conclude that the first method using linear function of x is accurate enough to be used in the actual application.

The standard deviations were much higher for NO_2 cases than the cases for the rest of absorbers. By inspecting each curve of growth in detail, it was found that this was mainly due to the difference in the steepness of the curves of growth for three absorption bands. This difference cannot be compensated by C'_1 values since they only shift the curves of growth linearly. In fact, within the current band model structure, it is impossible to compensate this difference. Hence, it may be necessary to modify some of the basic assumptions regarding the band model structure, if lower standard deviations are required.

As a side-effect of this discrepancy in the tangent of curves of growth, the SIMMIN computation took far more time for NO_2 cases than the rest. Most of the computations of ADSET were completed by 26-36 CPU seconds. The fluctuations in the computation time were very small. On the other hand, the SIMMIN computation time varied from 14 seconds to 270 seconds. NO_2 cases consumed about 200-270

seconds, which were about four times as much as that for the other cases. This is because the minimizing point in the parameter space is not well defined for NO_2 cases. In other words, the error surface in the parameter space has a very shallow bottom so that the updating step cannot produce large enough changes in the parameter guesses in order to have a rapid convergence.

Thus, it was found that the accuracy of the computed results and the time of execution depend heavily on the actual data. Hence, it is very important to give enough consideration for the data structure. This will be discussed in the next section.

9.4 Data Structure

As it was expressed earlier, we assumed that the number of layers (= the number of data points) in each cut is the same for an absorption band. This was done for the sake of easier coding in data handling. However, this assumption need not be valid. Especially in weaker absorption bands, it is required to use very large range values to have high enough equivalent absorber amounts in order to realize lower transmittances. In some cases the range becomes enormous (in the order of the radius of the earth) so that the corresponding data no longer possess physical significance. The ADSET code has a criterion that if the logarithm of the equivalent absorber, $\log W$, exceeds a certain critical value, then the corresponding data will be set aside and will not be used in the later computation. The critical value was set to be 2 for the actual computation, which corresponds approximately to a vertical path through the atmosphere.

In connection with this, if data are not available at some layers, then the data values are set at 0 to flag the nonavailability of data. ADSET can also detect this and will ignore the data.

A caution must be executed in choosing combinations of pressures and temperatures, i.e., atmospheric conditions. If a data set contains either the standard pressure or the

standard temperature or both only, then both ADSET and SIMMIN fail because of the fact that the coefficient of n or m or both in Eq.(12) becomes zero, since

$$\log \left(\frac{P_o}{P_o} \right) = \log 1 = 0, \quad (61)$$

$$\log \left(\frac{T_o}{T_o} \right) = \log 1 = 0. \quad (62)$$

For this case, the coefficient matrix A of the normal equation in ADSET becomes singular and the gradient corresponding to n or m or both in SIMMIN becomes zero all the time. Hence, the normal equation cannot be solved in ADSET and the initial guess of n or m or both cannot be changed in SIMMIN.

Another consideration which should be pointed out is to include different climate conditions. The standard climate condition for several layers of atmosphere contains sequence of pressures and temperatures both of which are monotone decreasing. Therefore, if only these conditions are used, then it is very difficult to distinguish the cause of changes in the transmittance due to the changes in pressure and in temperature. This leads to the shallow bottom of the error surface and hence, large computational error results in ADSET caused by the large condition number of the coefficient matrix and slow convergence in SIMMIN due to the small gradient. In the actual computation,

we included not only the standard climate conditions but also one condition each from the tropical and subarctic winter climates in consideration of wide applicability of the results. Numerically speaking, this also resulted in making the regression problem well-posed by breaking the monotonousness of the pressure and temperature combinations of the standard conditions. In fact, several computations were done for ADSET and SIMMIN with standard condition data only. SIMMIN took 10-45 minutes of CPU time to converge if it were convergent and ADSET resulted in a set of absurd values for n and m . Thus, the importance of the numerical consideration, which is ignored in many cases, is clearly indicated. The proper care should be taken when selecting controllable data values.

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0086      IF (5.105) (C49(1),C49(2),C49(3))
0087      IF (5.105) (C50(1),C50(2),C50(3))
0088      IF (5.105) (C51(1),C51(2),C51(3))
0089      IF (5.105) (C52(1),C52(2),C52(3))
0090      IF (5.105) (C53(1),C53(2),C53(3))
0091      IF (5.105) (C54(1),C54(2),C54(3))
0092      IF (5.105) (C55(1),C55(2),C55(3))
0093      IF (5.105) (C56(1),C56(2),C56(3))
0094      IF (5.105) (C57(1),C57(2),C57(3))
0095      IF (5.105) (C58(1),C58(2),C58(3))

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0096      ICOUNT=0
0097      IF (EMISS.EQ.0) GO TO 7
0098      RADSUM=0.0
0099      FACT=0.5
0100      CALL PATH(WLAY,WDPTH,TEHY)
0101      PRINT 113
0102      PRINT 114
0103      IF (EMISS.EQ.0) IKMAX=IKLC
C----- BEGINNING OF TRANSMITTANCE CALCULATIONS
7      IV=VAL*V
      AX=AX+1
0104      SUMV=0.
0105      TL=1.
0106      TS=1.
0107      TR=1.
0108      TR=1.
0109      IKLC=1
0110      IF (EMISS.EQ.0) IKLF=IKMAX
0111      DO 17 IV=IKLC,IKMAX
0112      IF (EMISS.EQ.0) GO TO 9
0113      DO 9 K=1,KMAX
      M=EMPATH(IK,K)
0114      CONTINUE
      L=IK
0115      IF (L=0) GO TO 11
0116      L=L-K
0117      IF (L=0) GO TO 11
0118      IF (ICOUNT.EQ.0) GO TO 10
0119      IF (ICOUNT.EQ.50) GO TO 10
0120      GO TO 11
0121      ICOUNT=0
0122      IF (EMISS.EQ.0) PRINT 115
0123      DO 12 K=1,KMAX
      TX(K)=1.0
0124      CONTINUE
0125      ICOUNT=ICOUNT+1
0126      V=IV
      I=(I+50)/5+1
0127      SUM4=0.
0128      SUM5=0.
0129      SUM6=0.
0130      SUM7=0.
0131      SUM8=0.
0132      SUM9=0.
0133      SUM11=0.
0134      CALL FFOEL(I,IV,M,IAZ=TX,ALAM)
0135      TX(9)=SUM4+SUM5+SUM6+SUM7+SUM8+SUM11
0136      IF (TX(9).EQ.0.0) GO TO 14
0137      IF (TX(9).LE.0.1) GO TO 13
0138      IF (TX(9).GT.2.0) GO TO 15
0139      TX(9)=EXP(-TX(9))
0140      GO TO 16
0141      TX(9)=1.0-TX(9)+0.5-TX(9)*TX(9)
0142      GO TO 16
0143      TX(9)=1.0
0144      GO TO 16
0145      TX(9)=0.
0146      TX(9)=TX(1)*TX(2)*TX(3)*TX(9)*TX(12)*TX(13)*TX(14)*TX(15)
0147      IF (IV.GE.1300) TX(3)=TX(9)
0148      IF (EMISS.EQ.0) GO TO 19
0149      ALAM=1.0E+04/V
0150      BIK=OFF(TRAY(IK),V)
0151      TL=TL*(TX(9)*TX(10))/(TX(7)*TX(6))
0152

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MAIN

FORTRAN IV SYSTEM 21

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0001 SURROUTINE ABSORB(XV,LENTOS,P2,MMIX,M,X,V1,V2,V3,VLAM,SUM,M,LAY)
0002 CMMON /M01/ 71341,P17,341,PH15,341,MH(7,341),M,UL,FE,CW,C
0003 CMMON /M02/ IFIND,C,19,JSTOP
0004 CMMON /M03/ HZ1(341),HZ2(16),MC(7,341)
0005 CMMON /M04/ THAZE,JP,14,M1,M2,M3,M4,P,TRODAD
0006 CMMON /M05/ RADMAX,320,M1N,VMAX,VPMIN
0007 CMMON /M06/ PDMSO2,PDMSO,PDMSO3,PDMSO2
0008 CMMON /M07/ IFMISS,MAX,ANGLE,LEN,MH,M1,J1,J2,JM1,J,EXTFA,ITYPE
0009 CMMON /M08/ H1,M2,M3,M4,MDEL
0010 CMMON /M09/ AM7(134),ASTJ(341),PHZ2(7),WLAV(341),VH(15),M(15),EL
0011 CMMON /M10/ MMIX(341),HZ(2)
0012 C*****
0013 C THIS SUBROUTINE CALCULATES THE EQUIVALENT ABSORBED AMOUNT FOR EACH
0014 C GAS AND FOR ANY PATH GEOMETRY
0015 C
0016 C FUEL=15) USE ABSORBER AMOUNTS PER CM AT LEVEL 15, M(1-15) ARE
0017 C EQUIVALENT ABS ORBE AMOUNTS AT A GIVEN DISTANCE.
0018 C*****
0019 F11=EXP(15.0764-14.3595EA-2.4392-0.51EA)
0020 IF(LAY,EO,31) GO TO 1
0021 IF(LAY,EO,31) GO TO 1
0022 IF(LAY,EO,31) GO TO 1
0023 IF(LAY,EO,31) GO TO 1
0024 IF(LAY,EO,31) GO TO 1
0025 IF(LAY,EO,31) GO TO 1
0026 IF(LAY,EO,31) GO TO 1
0027 IF(LAY,EO,31) GO TO 1
0028 IF(LAY,EO,31) GO TO 1
0029 IF(LAY,EO,31) GO TO 1
0030 IF(LAY,EO,31) GO TO 1
0031 IF(LAY,EO,31) GO TO 1
0032 IF(LAY,EO,31) GO TO 1
0033 IF(LAY,EO,31) GO TO 1
0034 IF(LAY,EO,31) GO TO 1
0035 IF(LAY,EO,31) GO TO 1
0036 IF(LAY,EO,31) GO TO 1
0037 IF(LAY,EO,31) GO TO 1
0038 IF(LAY,EO,31) GO TO 1
0039 IF(LAY,EO,31) GO TO 1
0040 IF(LAY,EO,31) GO TO 1
0041 IF(LAY,EO,31) GO TO 1
0042 IF(LAY,EO,31) GO TO 1
0043 IF(LAY,EO,31) GO TO 1
0044 IF(LAY,EO,31) GO TO 1
0045 IF(LAY,EO,31) GO TO 1
0046 IF(LAY,EO,31) GO TO 1

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FORTRAN IV G LEVEL 21          ABSORR          DATE = 79218          16/22/49          PAGE 0002

0047 IF (JLGE.32) FAC=(I7(K)-73.0)/30.
0048 IF (FAC.GT.1.0) FAC=1.0
0049 L=J+1
0050 IF (M1.GT.0) T(7,K)=T(M1,J)*(T(M1,L)/T(M1,J))**FAC
0051 Y=273.15/T(7,K)
0052 IF (M1.LE.0) Y=273.15/(273.15+DD)
0053 IF (M1(7,K).LE.0.0) WH(7,K)=F(Y)
0054 IF (M2.GT.0) WH(7,K)=WH(M2,J)*(WH(M2,L)/WH(M2,J))**FAC
0055 IF (M2.LE.0) WH(7,K)=0.01824+WH(7,K)
0056 IF (M3.GT.0) WH(7,K)=WH(M3,J)*(WH(M3,L)/WH(M3,J))**FAC
0057 WH(7,K)=0.
0058 IF (M1X(J).LE.0) GO TO 5
0059 HSTO(8)=WH(7,K)*WH(1X(L)/WH(1X(J))**FAC
0060 GO TO 4
0061 IF (Z(K).GT.5.0) GO TO 6
0062 IF (AMAZZ(K).EQ.0.0) HAZZ(K)=H2(J)*(H2(Z(L)/H2(Z(J))**FAC
0063 IF (AMAZZ(K).EQ.0.0) HAZZ(K)=H1(J)*(H1(Z(L)/H1(Z(J))**FAC
0064 IF (M1X(J).EQ.0) GO TO 13
0065 IF (M1X(J).GT.105
0066 PRINT 103,Z(K),H1(K),H2(K),HSTO(8),WH(7,K),H1(K),HAZZ(K)
0067 CONTINUE
0068 I=M
0069 AL=ML
0070 V1=0
0071 V2=0
0072 W3=0
0073
0074
0075
0076
0077
0078
0079
0080
0081
0082
0083
0084
0085
0086
0087
0088
0089
0090
0091
0092
0093
0094
0095
0096
0097
0098
0099
0100
0101
0102

C NOTE THAT Z(K) MAY NOT CORRESPOND TO THE VALUES GIVEN FOR STANDARD
C MODEL ATMOSPHERES
IF (IXY.GE.3) GO TO 13
GO TO 1
IF (RANGE.GT.0.0) GO TO 9
IF (H2.GT.0.0) AND (H2.LT.H1) IFIND=1
GO TO 13
I=VDEF7
ACT=ACOS(10.9*(RANGE+RANGE/(X1*X2)+X2/X1-X1/X2))/CA
IF (H2.EQ.0.0) GO TO 11
IFIND=1
PFT=CA*PETA
X2=DE+H2
ANGLE=ATAN(X2/SIN(PET))/(X2*COS(PET)-X1)/CA
RANGE=X2*SIN(PET)/SIN(ANGLE*CA)
PFT=PFTA
GO TO 13
FAC=X2/X1**2-(SIN(ANGLE*CA))**2
IF (RANGE.GT.0.0) X2=X1*(SQRT(1-((PFT-ARCSIN(X2/X1))**2)))
IF (ANGLE.NE.0.0) ANGLE=NE+180.0,PFT=ANGLE*ANGF*SIN(ANGLE-CA)/X2
IF (ANGLE.LT.0.0) ANGLE=ANGLE+PI
IF (RANGE.LT.0.0) RANGE=-RANGE
PFT=PFT/CA
PRINT 102, H1,H2,ANGLE,RANGE,PFT,VIS
CONTINUE
GO 14 I=1,34
DO 14 J=1,NMAX
MLAY(I,J)=0.
SUMA=0.
IF (IXY.LE.2) READ 100,V1,V2,DV
IF (IXY.LE.2) PRINT 100,V1,V2,DV

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FOURTEEN IV G LEVEL 21

ABSORP

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0133 IF (ITYPE.EQ.1) PRINT 106, H1, RANGE
0134 IF (ITYPE.EQ.2) PRINT 107, H1, H2, ANGLE
0135 IF (ITYPE.EQ.3) PRINT 108, H1, H2, ANGLE
0136 IF (MCEFL.EQ.0) M=7
0137 IF (VIS.GT.0.0) PRINT 109, VIS
0138 IF (VIS.LT.2.C.AND.VIS.GT.0.0) PRINT 110
0139 IF (V.EQ.1) PRINT 111, V
0140 IF (M.EQ.2) PRINT 112, M
0141 IF (M.EQ.3) PRINT 113, M
0142 IF (M.EQ.4) PRINT 114, M
0143 IF (V.EQ.5) PRINT 115, V
0144 IF (M.EQ.6) PRINT 116, M
0145 IF (H2.EQ.0.0) PRINT 117
0146 IF (H2.EQ.0.0) PRINT 118, H2, ANGLE, PETA, LEA, H1
0147 AV=10.000/V1
0148 ALAN=1.000/AV2
0149 CADMI=1.0E+74
0150 ZCMAX=0.
0151 VCMIN=0.
0152 VCMAX=0.
0153 PRINT 119, V1, V2, DV, ALAN, AV1
0154 AV=0.5E-6*(V1+V2)
0155 AV=AV*AVM
0156 CC=77.46+4.59*AVM
0157 CW=43.487+0.3473*AVM
0158 IF (IFIND.EQ.1) GO TO 19
0159 IF (IFIND.EQ.1) CALL ANGL (H1, H2, ANGLE, PETA, LEA, H1)
0160 IF (IFIND.EQ.1) GO TO 19
0161 IF (ITYPE.EQ.1) GO TO 19
0162 GO TO 10 K=1, KMAX
0163 WH(1)=0.0
0164 CONTINUE
0165 PETA=0.0
0166 C=0.0
0167 ID=0
0168
0169 ***** WITH DECREASING CONSTANT PRESSURE PAIR QUANTITIES *****
0170 Y=0.0
0171 SPH=SPH/1E1
0172 IF (H1.GT.7.0E1) GO TO 17
0173 GO TO 10
0174 IF (H1.GT.7.0E1) GO TO 14
0175 IF (SPH.GT.7.0E1) GO TO 14
0176 H1=7.0E1
0177 J1=0.0
0178 SPH=SPH/1E1
0179 ANGLE=180.0-ARC SIN(SPH)/CA
0180 PL=PL*(H1)*SPH
0181 GO TO 19
0182 HMIN=PL-RE
0183 PRINT 122, HMIN
0184 GO TO 59
0185 GO TO 22.1E1, NL
0186 PS=PI*H1/1013.0
0187 TS=273.15/T(M,1)
0188 IF (H1.GT.0.0) GO TO 14
0189 X=0.0
0190

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0160      PT=PSORSORT(TS)
0161      P=0.1*H(M,1)
0162      IF(M2.GT.0.4*W.W.L*7) GO=0.1*H(M2,1)
0163      FM(1,1)=Q*PT*W*0.9
0164      FM(2,1)=K*PT*W*0.75
0165      FM(4,1)=0.3*PT*W
0166      PP=0.5*P*W*273.15/TS
0167      TS=(296.7/273.15)*TS
0168      FM(5,1)=Q*PP*W*P(6.08*(TS-1.0)+3.032*P*(0.5*PP*W)
0169      FM(10,1)=P*(PP*W*0.12*(PS=PP*W))+FXD(1.5*P*(TS-1.0))
0170      CM(5,1)=X
0171      HAZ=FM(1,1)
0172      IF(M2.GT.7) HAZ=HAZE(1)
0173      IF(7.01.GE.5.0) GO TO 20
0174      IF(M2.GT.7) HAZ=HAZE(2) HAZ=HAZE(1)
0175      IF(M2.GT.7) HAZ=HAZE(2) HAZ=HAZE(1)
0176      IF(M2.GT.7) HAZ=HAZE(2) HAZ=HAZE(1)
0177      IF(M2.GT.7) HAZ=HAZE(2) HAZ=HAZE(1)
0178      IF(M2.GT.7) HAZ=HAZE(2) HAZ=HAZE(1)
0179      HAZ=6.339*(HAZE(1)+HAZE(2))/5.0=HAZE(1)/5.0=HAZE(1)/23.0
0180      IF(M2.GT.7) HAZ=HAZE(1)
0181      FM(7,1)=HAZE(1)
0182      FM(8,1)=6.667*HAZE(1)
0183      FM(9,1)=0.4*W.W.L*7) FM(9,1)=40.667*W(9,1)
0184      FM(3,1)=H(R,1)*PT*W*0.4
0185      FM(11,1)=H(R,1)*PT*W*0.4
0186      FM(11,1)=H(R,1)*PT*W*0.4
0187      FM(11,1)=H(R,1)*PT*W*0.4
0188      FM(11,1)=H(R,1)*PT*W*0.4
0189      FM(11,1)=H(R,1)*PT*W*0.4
0190      FM(11,1)=H(R,1)*PT*W*0.4
0191      FM(11,1)=H(R,1)*PT*W*0.4
0192      FM(11,1)=H(R,1)*PT*W*0.4
0193      FM(11,1)=H(R,1)*PT*W*0.4
0194      FM(11,1)=H(R,1)*PT*W*0.4
0195      FM(11,1)=H(R,1)*PT*W*0.4
0196      FM(11,1)=H(R,1)*PT*W*0.4
0197      FM(11,1)=H(R,1)*PT*W*0.4
0198      FM(11,1)=H(R,1)*PT*W*0.4
0199      FM(11,1)=H(R,1)*PT*W*0.4
0200      FM(11,1)=H(R,1)*PT*W*0.4
0201      FM(11,1)=H(R,1)*PT*W*0.4
0202      FM(11,1)=H(R,1)*PT*W*0.4
0203      FM(11,1)=H(R,1)*PT*W*0.4
0204      FM(11,1)=H(R,1)*PT*W*0.4
0205      FM(11,1)=H(R,1)*PT*W*0.4
0206      FM(11,1)=H(R,1)*PT*W*0.4
0207      FM(11,1)=H(R,1)*PT*W*0.4
0208      FM(11,1)=H(R,1)*PT*W*0.4
0209      FM(11,1)=H(R,1)*PT*W*0.4
0210      FM(11,1)=H(R,1)*PT*W*0.4
0211      FM(11,1)=H(R,1)*PT*W*0.4
0212      FM(11,1)=H(R,1)*PT*W*0.4
0213      FM(11,1)=H(R,1)*PT*W*0.4
0214      FM(11,1)=H(R,1)*PT*W*0.4
0215      FM(11,1)=H(R,1)*PT*W*0.4

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FORTRAN IV C LEVEL 21      ARSOPB      DATE = 79218      16/22/49      PAGE 0007

0325 IF (TX3.LT.0.0) TX3=TX(9)
0326 IF (J1.EQ.N.AND.H2.GE.M1) GO TO 43
0327 HMIN=AD/TX3=PE
0328 IF (ARS(X-HMIN).GT.0.0001) GO TO 42
0329 IF (J1.EQ.N.AND.H2.GE.M1) YN1=TX3
0330 IF (J2.EQ.N.AND.J1.NE.J2) YN2=TX3
0331 IF (H2.GE.M1) TX2=TX3
0332 IF (H2.GE.M1) J2=N
0333 IF (H2.GE.M1.OR.H2.LT.HMIN) H=HMIN
0334 PRINT 126, HMIN
0335 TFI=H2.LT.HMIN)J2=N
0336 IF (H2.LT.HMIN) PRINT 127, HMIN
0337 GO TO 45
0338 PRINT 126,HMIN
0339 IF (H2.LT.H1) GO TO 45
0340 IF (ITYPE.EQ.3.OR.H2.GE.M1) PRINT 128
0341 ITYPE=7
0342 TX2=HI(9,1)
0343 JMIN=0
0344 J2=1
0345 H2=0.0
0346 H=0.0

C**** NOW DEFINE VERTICAL PATH QUANTITIES VM(1-8)
0347 IF (J2.EQ.0) PRINT 129
0348 JSTOR=J=1
0349 DO 51 I=1,NL
0350 J=J-1
0351 FFE=EM(9,J)
0352 IF (I.EQ.1) REF=YMI
0353 IF (I.EQ.1.AND.K2.EQ.1) REF=YX2
0354 IF (J.EQ.J2.AND.K2.EQ.0) REF=TX2
0355 IF (I.NE.1) X1=Z(J+1)
0356 X2=Z(IJ)
0357 IF (J.EQ.J2.AND.K2.EQ.0) X2=H
0358 IF (J.EQ.JMIN.AND.K2.EQ.1) X2=HMIN
0359 HM=(REF+X1)*SPHI=RE
0360 IF (HM.GT.Z(J).AND.HM.GT.X2) X2=HM
0361 PX=IRE+X1/IPE+X2
0362 PS=X1-X2
0363 ALP=90.0
0364 THETA=ASIN(SPHI)/CA
0365 SALD=RX*SPHI
0366 IF (ABS(X2-HM).GT.1.0E-5) ALP=ASIN(SALD)/CA
0367 HCT=ALP-THET
0368 IF (SPHI.GT.1.0E-10) PS=(REF+X2)*SIN(REF+CA)/SPHI
0369 THETA=180.0-THET
0370 RETA=RETA+REI
0371 PSI=RETA-ALP=ANGLE+180.0
0372 SP=SP+PS
0373 DO 50 K=1,KMAX
0374 AJ=EM(K,J)
0375 IF (J.EQ.J1) BJ=E(K)
0376 IF (J.EQ.J2.AND.H2.LT.H1.AND.K2.GT.0.0) AJ=W(K)
0377 IF (J.EQ.JMIN.AND.H2.GE.M1) AJ=TX(K)
0378 IF (J.EQ.JMIN.AND.ABS(H2-HM1.LT.1.0E-5) AJ=TX(K)
0379 IF (K2.EQ.0) GO TO 46
0380 IF (J.EQ.J2) BJ=W(K)
0381

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0382 IF (J.FQ.JMIN) AJ=TX(K)
0383 IF (AJ.EQ.0.0) CF=AJ.EQ.0.0) GO TO 48
0384 IF (AJ.FQ.RJ) GO TO 47
0385 FV=DS(AJ=BJ)/ALOG(AJ/BJ)
0386 GO TO 49
0387 FV=DS*AJ
0388 GO TO 49
0389 FV=0.0
0390 VHI(K)=VHI(K)+FV
0391 VHI(K)=VHI(K)+FV
0392 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 50
0393 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 50
0394 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0395 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0396 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0397 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0398 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0399 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0400 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0401 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0402 CONTINUE
0403 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0404 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0405 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0406 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0407 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0408 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0409 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0410 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0411 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0412 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0413 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0414 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0415 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0416 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0417 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0418 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0419 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0420 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0421 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0422 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0423 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0424 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0425 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0426 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0427 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0428 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0429 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0430 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0431 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0432 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0433 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0434 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0435 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0436 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0437 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54
0438 IF (J.FQ.J2.AND.K2.EQ.1) GO TO 54

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[illegible]

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FORTRAN IV G LEVEL 21

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0044 TX1=TX(9)
0045 CALL POINT (M2,VN,N,NO,TX,10)
0046 IF (NP.EQ.1) N=N+1
0047 J2=N
0048 IF (J1.EQ.J2) TX1=TX1+VN*EH(9,J1)
0049 DO 7 J=J1,J2
0050 X1=OC+7(J)
0051 X2=OC+7(J+1)
0052 IF (1.6*Q.11) X1=CF+M1
0053 IF (1.6*Q.12) X2=CF+M2
0054 CALL POINT (M2,VN,N,NO,TX,10)
0055 ALPHASIN(SALP)
0056 EN=EH(9,J1)/EH(9,J1)
0057 IF (1.6*Q.11) EN=VN/EN(9,J1)
0058 IF (1.6*Q.12) EN=EH(9,J1)/TX1
0059 IF (1.6*Q.13) EN=EH(9,J1)/TX1
0060 IF (1.6*Q.14) EN=EH(9,J1)/TX1
0061 EN=EN*ALP
0062 IF (1.6*Q.15) EN=EN*TX1(THEY)
0063 FOR EN=EN
0064 RET=RET+EN*YF
0065 TH1=TH1/CA
0066 RE=REY/CA
0067 C=LO/CA
0068 PRINT *02, J,Z(J),TH1,ALP,RE,REY,CA,TX,NO,TX1,RE,C
0069 IF (X2.EQ.CF+M2) (=PI=ALP)
0070 IF (SALP.GE.PN) EN=1.
0071 SPH=5ALP/PN
0072 TH2=SPH*SIN(SPH)
0073 CONTINUE
0074 IF (1.6*Q.15) GO TO 99
0075 GO TO 26
0076 CONTINUE
0077 TX=EN*TX
0078 ANGLE=PI-ANGLE
0079 TANGLE
0080 ANGLE=PI/2
0081 PRINT *04, B1,ANG,TANG
0082 IF (1.6*Q.15) GO TO 3
0083 CONTINUE
0084 IF (J1)
0085 CALL POINT (M1,VN,N,NO,TX,10)
0086 TX1=TX(9)
0087 VN1=VN
0088 IF (MPL.EQ.1) N=N+1
0089 J2=N
0090 IF (1.6*Q.17) J2=M1
0091 J1=N
0092 IF (M2.GE.M1) GO TO 13
0093 CALL POINT (M2,VN,N,NO,TX,10)
0094 TX2=TX(9)
0095 VN2=VN
0096 J2=N
0097 IF (J1.EQ.J2) TX2=VN1+TX(9)=CF(9,11)
0098 J1=N
0099 X1=OC+7(J+1)
0100 X2=OC+7(J)

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0100 IF (J.EQ.J1) X1=RE+M1
0101 IF (J.EQ.J2) X2=RE+M2
0102 SALD=X1*SPH1/X2
0103 HMIN=X1*SPH1-ME
PRINT 402, J,X1,Z(J),SPH1,SALP,HMIN,RE
0104 IF (SALP.LE.1.0) GO TO 11
SALD=CHT
0105 IF (HMIN.GT.M2) GO TO 14
ZLP=ADST*(SALP)
THE=ADST*(SCM1)
RETALD=THET
ME=RET1+RET
RE=ZLP/LOI
0110 IF (J.EQ.J1) RE=RE+TAN(THET)
FRT1=RET1+RE
TH1=THEY/CA
RE=RET/CA
0115 AL=ALD/CA
PRINT 402, J,X2,THET,AL,RET1,RET,HMIN,HMIN,RET1,TH1,RE,AL
IF (X2.EQ.-E+M2) (EPI=ALP
REF=HMO,J)
0119 IF (J.EQ.J1) RE=RE+1
0120 IF (J.EQ.J2) REF=TX2
0121 IF (J.EQ.1) GO TO 12
PE=EM(9,J)/EM(9,J-1)
0122 IF (J.EQ.J1) RN=VAL/EM(9,J-1)
0123 IF (J.EQ.J2+1) RN=REF/TX2
0124 IF (J.EQ.J2) RN=REF/YX2
0125 IF (SALD.GE.54) RN=1.
SMD=SCALP*RN
0127 IF (Z(J).LE.-P2) GO TO 12
GO TO 10
0129 X1=X2
0130 IF (SMD/(J1+M2).LT.1.0E-10) (X2=X1,JE=J1) GO TO 13
GO TO 14
0132 IF (J1=1
X1=SE+Z(J+1)
0134 IF (J.EQ.1) X1=RE+M1
0135 IF (J.EQ.12+M2) (JANE,J1) X1=RE+M2
X2=SE+Z(J)
0137 HMIN=X1*SPH1-RE
0138 IF (HMIN.LE.0.0) GO TO 25
0139 IF (Z(J).LT.HMIN) GO TO 16
REF=EM(9,J)
0140 IF (J.EQ.J2) REF=Y1
0141 IF (HMIN.GE.1/X2
AL=RE*(SALP)
0142 THE=ADST*(SCM1)
0143 RETALD=THET
0144 FRT1=RET1+RET
0145 FRT2=RET2+RE
0146 RET2=RET2+RET
0147 RN=REF/EM(9,J-1)
0148 IF (SALD.GE.PN) RN=1.0
0149
0150
0151
0152
0153
0154

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FOSTRAN IV 5 LEVEL 21

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0211 IF (SP41,GE,RN) RN=1.
0212 SP41=SPH1/RN
0213 THE=ARSIN(SPH1)
0214 GO TO 5
0215 CALL POINT (H2,VN,AP,IX,IX)
0216 TX1=TX1+VN-FH(Q,J1)
0217 Q=TX1/VN
0218 J2=J1
0219 IF (SP41,GE,RN) RN=1.
0220 SP41=SPH1/QN
0221 THE=ARSIN(SPH1)
0222 GO TO 5
0223 H2=H2+V1
0224 LE=LE+1
0225 RET=RT1
0226 THE=ANGLE*(RI-RT1)/(1.4*RT1/TANG)
0227 QN=2*RT1/CA
0228 H2=H2+CA
0229 TH1=THEY/CA
0230 PRINT 404, RT1, DRTA, CAT, TH1, TANG
0231 IF (THE,GT,TR,THE,LT,TV) THE=(TV+TH)/2.
0232 TH1=THEY/CA
0233 PRINT 404, DRT1, B, CAT, TH1
0234 TH1=TN/CA
0235 TH1=TM/CA
0236 PRINT 405, TN, TM, T, L, TM
0237 SPH1=FIN(THEY)
0238 TANG=TAN(THEY)
0239 IT=IT+1
0240 QN=ARSIN(RT1)
0241 QN=ARSIN(ANGLE+THEY)
0242 IF (IT,EQ,10) THET=3.5*(ANGLE+THEY)
0243 IF (IT,EQ,10) GO TO 28
0244 IF (DHE,GT,1.0E-7,AND,OTH,GT,1.0E-7) GO TO 1
0245 ANGLE=THEY/CA
0246 DRT1=406, ANGLE, IT
0247 PERIEN
0248 29 HI=42
0249 ANGLE=CA/CA
0250 PRINT 406, ANGLE, IT
0251 EFF=IP1
0252 FORMAT (//, ITERATION NUMBER, 13, //)
0253 FORMAT (16, F16.7, F13.4)
0254 FORMAT (14, F10.4, F13.4, F10.4)
0255 FORMAT (1, MIN=, F14.6, , D1=, F14.6, , D2=, F10.4)
0256 FORMAT (1, TOTAL BETA =, F14.6, F15.6, F14.6, , F14.6, , THEY =, F10.4)
0257 1.6, TANG=, F10.6)
0258 FORMAT (5F12.6)
0259 FORMAT (8X, //, , ZENITH ANGLE =, F7.3, , DEGREES : RECOMPUTED
0260 1 FROM SUBROUTINE ANGL (ITERATION, 13, , , )
0261 EN)

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FORTRAN IV G LEVEL 21 FREOSL DATE = 79218 16/22/49

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0001 SUBROUTINE FREOSL(IV,M,HAZE,TX,ALAM)
0002 COMMON /M05/ C1(2580),C2(1575),C3(540),C4(133),C5(15),C8(102),C11(
0003 144),C12(115),C13(43),C14(13),C15(185)
0004 COMMON /M06/ VX(45),CT(45),CTAL(45)
0005 COMMON /M07/ TR(67),FM(67),FC(67)
0006 COMMON /M08/ SUM4,SUM5,SUM6,SUM7,SUM8,SUM9,SUM11
0007 COMMON /M09/ FS(9),S1(9),S2(5)
0008 COMMON /M10/ FN(19),FN1(9),FN2(9)
0009 COMMON /M11/ FMH3(9),FMH(9),FM2(9)
0010 COMMON /M12/ FMH3(9),FMH(9),FM2(9)
0011 COMMON /M13/ FMH2(9),C1(9),C2(9)
0012 DIMENSION M(15),X(15)
0013
0014 *****
0015 C THIS SUBROUTINE SELECTS THE ATTENUATION EFFECTIVE AT THE FREQUENCY
0016 C INPUT FROM 13 MODEL SUBROUTINES.
0017 C *****
0018 IF (I.GE.-01.AND.I.LE.18) GO TO 4
0019 IF (I.GE.-19.AND.I.LE.30) GO TO 3
0020 IF (I.GE.-31.AND.I.LE.45) GO TO 2
0021 IF (I.GE.-46.AND.I.LE.54) GO TO 1
0022 IF (I.GE.-55.AND.I.LE.60) GO TO 6
0023 IF (I.GE.-61.AND.I.LE.63) GO TO 4
0024 IF (I.GE.-65.AND.I.LE.68) GO TO 9
0025 IF (I.GE.-69.AND.I.LE.100) GO TO 10
0026 IF (I.GE.-101.AND.I.LE.107) GO TO 11
0027 IF (I.GE.-108.AND.I.LE.141) GO TO 12
0028 IF (I.GE.-142.AND.I.LE.177) GO TO 15
0029 IF (I.GE.-178.AND.I.LE.181) GO TO 16
0030 IF (I.GE.-182.AND.I.LE.192) GO TO 17
0031 IF (I.GE.-213.AND.I.LE.238) GO TO 16
0032 IF (I.GE.-277) GO TO 13
0033 IF (I.GE.-239.AND.I.LE.265) GO TO 17
0034 IF (I.GE.-278.AND.I.LE.282) GO TO 17
0035 IF (I.GE.-283.AND.I.LE.346) GO TO 14
0036 IF (I.GE.-347.AND.I.LE.420) GO TO 14
0037 IF (I.GE.-421.AND.I.LE.438) GO TO 19
0038 IF (I.GE.-439.AND.I.LE.470) GO TO 19
0039 IF (I.GE.-531.AND.I.LE.585) GO TO 21
0040 IF (I.GE.-586.AND.I.LE.1549) GO TO 22
0041 IF (I.GE.-1546.AND.I.LE.1770) GO TO 16
0042 IF (I.GE.-1771.AND.I.LE.1905) GO TO 16
0043 IF (I.GE.-1906.AND.I.LE.2490) GO TO 16
0044 IF (I.GE.-2491.AND.I.LE.2520) GO TO 16
0045 IF (I.GE.-2521.AND.I.LE.2530) GO TO 25
0046 IF (I.GE.-2531.AND.I.LE.2580) GO TO 26
0047 IF (I.GE.-2581.AND.I.LE.2610) GO TO 26
0048 IF (I.GE.-2611.AND.I.LE.2835) GO TO 24
0049 IF (I.GE.-2836.AND.I.LE.2835) GO TO 24
0050 CALL EVTS(IV,M,C3,TX)
0051 CALL EVTS(IV,M,C3,TX)
0052 CALL EVTS(IV,M,C3,TX)
0053 CALL EVTS(IV,M,C3,TX)
0054 CALL EVTS(IV,M,C3,TX)
0055 CALL EVTS(IV,M,C3,TX)
0056 CALL EVTS(IV,M,C3,TX)
0057 CALL EVTS(IV,M,C3,TX)
0058 CALL EVTS(IV,M,C3,TX)
0059 CALL EVTS(IV,M,C3,TX)
0060 CALL EVTS(IV,M,C3,TX)
0061 CALL EVTS(IV,M,C3,TX)
0062 CALL EVTS(IV,M,C3,TX)
0063 CALL EVTS(IV,M,C3,TX)
0064 CALL EVTS(IV,M,C3,TX)
0065 CALL EVTS(IV,M,C3,TX)
0066 CALL EVTS(IV,M,C3,TX)

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FORTRAN IV G LEVEL 21 FREQSL
 0047 GO TO 6
 0048 CALL NHQJII,IV,d,C5,TX,SUM5)
 0049 GO TO 8
 0050 CALL SUTYII,IV,C14,TX)
 0051 GO TO 9
 0052 CALL PETEPI,IV,C11,SJW11,TX)
 0053 GO TO 10
 0054 CALL SUTYII,IV,C14,TX)
 0055 CALL PETEPI,IV,C11,SJW11,TX)
 0056 CALL NHQJII,IV,d,C5,TX,SUM5)
 0057 GO TO 6
 0058 CALL SUSEJII,IV,C12,TX)
 0059 GO TO 12
 0060 CALL SUSEJII,IV,C12,TX)
 0061 GO TO 13
 0062 CALL FJII,IV,C15,TX)
 0063 GO TO 13
 0064 CALL AFZFI,IV,C13,TX)
 0065 GO TO 14
 0066 CALL KRAMII,IV,C4,TX,SUM4)
 0067 GO TO 14
 0068 CALL SUSEJII,IV,C12,TX)
 0069 GO TO 19
 0070 CALL SEMAJII,IV,d,TX,SUM6)
 0071 GO TO 5
 0072 CALL SEMAJII,IV,d,TX,SUM6)
 0073 GO TO 7
 0074 CALL SEMAJII,IV,d,TX,SUM6)
 0075 GO TO 4
 0076 CALL SEMAJII,IV,d,TX,SUM6)
 0077 GO TO 5
 0078 CALL CIVACII,IV,C2,TX)
 0079 GO TO 24
 0080 CALL SESOMII,IV,C8,TX,SUM8)
 0081 GO TO 25
 0082 CALL SESOMII,IV,C8,TX,SUM8)
 0083 GO TO 24
 0084 CALL CIVACII,IV,C2,TX)
 0085 GO TO 27
 0086 RETURN
 0087 END

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FORTRAN IV G LEVEL 21      LUMP      DATE = 79218      16/22/49      PAGE 0001

0001      SUBROUTINE LUAP(L,W,C1,TX)
0002      DIMENSION C1(2580),TX(11),WS(11),W(11)
0003      C*****
0004      C TRANSMITTANCE FOR WATER VAPOR *****
0005      C
0006      C THIS SUBROUTINE USES A CONTINUOUS FUNCTION FOR THE ORIGINAL
0007      C TRANSMITTANCE TABLE.
0008      C*****
0009      IF (W(1),LT,1.0E-20) GO TO 5
0010      IF (1.0E-1170) 11=1
0011      IF (1.0E-1905,AND,1.0E-2490) 11=1+135
0012      IF (1.0E-2610) 11=1+255
0013      WS(11)=4.0610(W(1))**C1(11)
0014      TX(11)=EXP(-10**(-1.1+619*0.55013**WS(11)))
0015      RETURN
0016      END

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FORTRAN IV G LEVEL 21          DIVAD          DATE = 79218          10/22/49          PAGE 0001

0001      SUBROUTINE DIVAD(I1,W,C2,TX)
0002      DIMENSION C2(1575),TX(2),WS(2),W(2)
*****
C      TRANSMITTANCE FOR UNIFORMLY MIXED GASES
C
C      THIS SUBROUTINE USES A CONTINUOUS FUNCTION FOR THE ORIGINAL
C      TRANSMITTANCE TABLE.
C*****
0003      IF (4(2).LT.1.0E-20) G1 TO 5
0004      I1=1)
0005      IF (1.0E-2520) I1=1-1005
0006      WS(2)=1.05104(2)+C2(11)
0007      TX(2)=EXP(-10*(1-1+619+0.55C1)*WS(2)))
0008      RETURN
0009      END

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0001      SUBROUTINE EVETS(I,M,C3,TX)
0002      DIMENSION C3(50),TX(3),MS(3),M(3)
0003      C*****
0004      C TRANSMITTANCE FOR OPEN
0005      C
0006      C THIS SUBROUTINE USES A CONTINUOUS FUNCTION FOR THE ORIGINAL
0007      C TRANSMITTANCE TABLE.
0008      C*****
0009      IF (M(3).LT.1.0E-20) GO TO 5
0010      M=1E-45
0011      MS(1)=E(2)E(3)E(3)+C3(1)
0012      TX(1)=1/(1+C3P(-3.0,0)M+2.1112E+5(3)))
0013      C*****
0014      END

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FORTRAN IV G LEVEL 21          VMCJ          DATE = 79218          16/22/49          PAGE 0001

0001      SUBROUTINE WMOJ(I,IV,M,C5,TX,SIMS)
0002      *****TRANSMITTANCE FOR WATER VAPOR (CONTINUUM & WIGOR) AND 10 MICRON REGION
0003      DIMENSION C5(15),TX(5),W(10)
0004      IF(I.LT.65.C6-1.GT.531) GO TO 2
0005      IF(I.GT.201) GO TO 1
0006      TX(5)=(4.18+5578.0*EXP(-7.87E-3*IV))*W(5)
0007      GO TO 3
0008      1  IF(I.LT.401) GO TO 2
0009      XT=(1-401.01/13.0+1.3
0010      XM=XT*FLCAT(NH)
0011      TX(5)=C5(NH)
0012      TX(5)=TX(5)*XM*(C5(NH)-C5(NH-1))
0013      TX(5)=TX(5)*W(10)
0014      GO TO 3
0015      2  TX(5)=0.0
0016      3  SUMS=TX(5)
0017      IF (TX(5).EQ.0.0) GO TO 5
0018      IF (TX(5).LE.0.1) GO TO 4
0019      IF (TX(5).GT.23.0) GO TO 6
0020      TX(5)=EXP(-TX(5))
0021      GO TO 7
0022      4  TX(5)=1.0-TX(5)+0.5*TX(5)*TX(5)
0023      GO TO 7
0024      5  TX(5)=1.0
0025      6  TX(5)=0.0
0026      7  RETURN
0027      END
0028

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FORTRAN IV C LEVEL 21      KPM      DATE = 79218      16/22/49      PAGE 0001

0001      SUBROUTINE GRAM(M,N,TX,SJM4)
0002      *****TRANSMITTANCE FOR NITE-OPEN CONTINUOUS*****
0003      DIMENSION C(113),TX(4),M(4)
0004      IF (I.LT.307) GO TO 4
0005      I1=1346
0006      TX(4)=C(411)*M(4)
0007      SUM4=TX(4)
0008      IF (TX(4).EQ.0.0) GO TO 4
0009      IF (TX(4).LE.0.1) GO TO 3
0010      IF (TX(4).GT.2.0) GO TO 5
0011      TX(4)=301-TX(4)
0012      GO TO 5
0013      TX(4)=1.0-TX(4)*.5+TX(4)*TX(4)
0014      GO TO 5
0015      TX(4)=1.0
0016      GO TO 5
0017      TX(4)=0.0
0018      GO TO 5

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FORTRAN IV C LEVEL 21          SEMAJ          DATE = 79218          16/22/49          PAGE 0001

0001      SUBROUTINE SEMAJ(L,IV,M,TR,SUM6)
0002      C*****TRANSMISSION COEFF FOR MULTIPLE SCATTERING *****
0003      DIMENSION TR (3,M(6))
0004      V=IV
0005      C6=9.837E-20*(V**6,C(17)
0006      TR(6)=C6*M(6)
0007      SUM6=TR(6)
0008      IF (TR(6).GT.0.0) GO TO 4
0009      IF (TR(6).LT.0.1) GO TO 3
0010      IF (TR(6).GT.2.0) GO TO 5
0011      TR(6)=END(-TR(6))
0012      GO TO 5
0013      TR(6)=1.0-TR(6)*C6*(M(6)+TR(6))
0014      GO TO 4
0015      TR(6)=1.0
0016      C6=C(17)
0017      TR(6)=C6
0018      RETURN
0019      END

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FORTRAN IV G LEVEL 21      EKUL      DATE = 79218      16/22/49      PAGE 0001

0001      SUBROUTINE EKUL(IV,W,IMAZE,TX,SUM7,ALAM)
0002      ***** TRANSMITTANCE FOR AEROSOL *****
0003      COMMON /A06/ VX(45),CT(45),CTA(65)
0004      DIMENSION TX(1),W(7)
0005      V=IV
0006      ALAM=1.0E+4/W
0007      XX=0.0
0008      YV=0.0
0009      I=1
0010      N=144
0011      XD=ALAM*VX(I)
0012      IF(XD) 2,1,1
0013      CONTINUE
0014      XX=(CT(N)-CT(N-1))*XD/(VX(N)-VX(N-1))*7(5)
0015      TX(7)=XX*W(7)
0016      SUM7=TX(7)
0017      IF (TX(7).LE.0.0) GO TO 5
0018      IF (TX(7).LE.0.1) GO TO 4
0019      IF (TX(7).GT.20.1) GO TO 6
0020      TX(7)=EXP(-TX(7))
0021      GO TO 7
0022      TX(7)=1.0*TX(7)+0.5*TX(7)*TX(7)
0023      GO TO 7
0024      TX(7)=1.0
0025      TX(7)=0.0
0026      CONTINUE
0027      YV=(CTA(N)-CTA(N-1))*XD/(VX(N)-VX(N-1))+CTA(N)
0028      TX(10)=YV*W(7)
0029      IF (TX(10).EQ.0.0) GO TO 9
0030      IF (TX(10).LE.0.1) GO TO 8
0031      IF (TX(10).GT.20.1) GO TO 10
0032      TX(10)=EXP(-TX(10))
0033      GO TO 11
0034      TX(10)=1.0-TX(10)+0.5*TX(10)*TX(10)
0035      GO TO 11
0036      TX(10)=1.0
0037      TX(10)=0.0
0038      GO TO 11
0039      TX(10)=0.0
0040      LETJ=J
0041      END

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FORTRAN IV G LEVEL 21 SESUM DATE = 79218 16/22/49 PAGE 0001

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0001  SUBROUTINE SESUM(I,M,CR,TX,SUP8)
0002  C***** TRANSMITTANCE FOR UV RZONE *****
0003  DIMENSION CR(102),TX(8),W(8)
0004  AT=1
0005  IF(I,LE,4611) GO TO 1
0006  IF(I,GT,5431) GO TO 2
0007  XX=40.0
0008  XI=141-2531.0/XX+1.0
0009  LI=1
0010  L2=53
0011  GO TO 3
0012  XX=100.0
0013  XI=(XI-5+31.0/XX+57.0
0014  L1=57
0015  L2=102
0016  DO 4 N=1,L2
0017  XO=XI-ELCAY(N)
0018  IF (XO) 6,5,4
0019  CONTINUE
0020  TX(8)=W(8)*C8(N)
0021  GO TO 9
0022  TX(8)=CR(N)*XD*(C8(N)-C4(N-1))
0023  TX(8)=4(8)*TX(8)
0024  SUM8=TX(8)
0025  IF (TX(8)-EQ,0.0) GO TO 10
0026  IF (TX(8)-LE,0.1) GO TO 9
0027  IF (TX(8)-GT,20.0) GO TO 11
0028  TX(8)=EXP(-TX(8))
0029  GO TO 12
0030  TX(8)=1.0-TX(8)+0.5*TX(8)*TX(8)
0031  GO TO 12
0032  TX(8)=1.0
0033  GO TO 12
0034  TX(8)=0.0
0035  RETURN
0036  END
  
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FORTRAN IV G LEVEL 21          RETEP          DATE = 79218          16/22/49          PAGE 0001

0001      SUBROUTINE RETEP(I1,W,C11,TX,CUM11)
0002      C***** TRANSMITTANCE FOR NITRIC ACID*****
0003      DIMENSION C11(44),TX(11),W(11)
0004      NABS=0
0005      IF(I1-100,CR,I-GT,278) GO TO 1
0006      IF(I1-GT,116,AND,I-LT,136) GO TO 1
0007      IF(I1-GT,231,AND,I-LT,266) GO TO 1
0008      IF(I1-LF,116) I1=100
0009      IF(I1-LF,186,AND,I-LF,201) I1=170
0010      IF(I1-LF,266) I1=1-234
0011      I1=C11(I1)
0012      COW=I1/5
0013      TX(I1)=NABS*W(I1)
0014      CUM11=CUM11+TX(I1)
0015      IF (TX(I1),LE,0.01) GO TO 4
0016      IF (TX(I1),LE,0.1) GO TO 5
0017      IF (TX(I1),GT,20.1) GO TO 7
0018      TX(I1)=EXP(-TX(I1))
0019      GO TO 4
0020      TX(I1)=1.0-TX(I1)+0.3*TX(I1)*TX(I1)
0021      GO TO 4
0022      TX(I1)=1.0
0023      GO TO 4
0024      TX(I1)=0.3
0025      RETURN
0026      END

```

```

FORTRAN IV G LEVEL 21          SUSEJ          DATE = 79218          16/22/49          PAGE 0001

0001      SUBROUTINE SUSEJ(I,M,C12,TX)
0002      COMMON /W10/ FS(9),S1(9),S2(5)
0003      DIMENSION C12(115),TA(12),WS(12),W(12)
C *****
C      THIS SUBROUTINE CALCULATES THE TRANSMITTANCE BY SO2 ( PPM READ IN
C      THE MAIN PROGRAM).
C *****
0004      IF (W(12).LT.1.0E-20) GO TO 5
0005      IF (1.0E-19.AND.1.1E-54) I1=18
0006      IF (1.0E-182.AND.1.1E-181) I1=18
0007      IF (1.0E-193.AND.1.1E-213) I1=1-104
0008      IF (1.0E-421) I1=1-323
0009      WS(12)=ALOG10(W(12))*C12(I1)
0010      GO 1 J=1-9
0011      IF(WS(12)=FS(J)) 2,2,1
0012      CONTINUE
0013      TX(I2)=EXP(-10*(S1(J)+S2(J)*WS(12)))
0014      RETURN
0015      END

```

```

FOPTAN IV G LEVEL 21      ARZE      DATE = 79218      16/22/49      PAGE 0001

0001      SUBROUTINE ARZE(I,M,C13,TX)
0002      COMMON /M011/ ENO(9),FNI(9),FA2(9)
0003      DIMENSION C13(43),TX(13),WS(13),M(13)
C*****
C      THIS SUBROUTINE CALCULATES THE TRANSMITTANCE BY NO. 1 PPM READ IN
C      THE MAIN PROGRAM).
C*****
      I1=I-242
      IF (M(13)-LT-1.0E-20) GO TO 3
      WS(13)=ALOG10(M(13))+C13(I1)
      DO 1 J=1,9
      IF (WS(13)-ENO(J)) 2,2,1
      CONTINUE
      TX(13)=EXP(-10**((FNI(J)+FA2(J))*WS(13)))
      RETURN
      END
0004
0005
0006
0007
0008
0009
0010
0011
0012

```

```

FORTRAN IV C LEVEL 21          SUTIT          DATE = 79218          16/22/49          PAGE 0001

0001      SUBROUTINE SUTIT(I,M,C14,TX)
0002      COMMON /M012/ FWH3(9),FWH1(9),FWH2(9)
0003      DIMENSION C14(109),TX(14),WS(14),W(14)
0004      *****
0005      C
0006      C THIS SUBROUTINE CALCULATES THE TRANSMITTANCE BY NH3 ( PPM READ IN
0007      C THE MAIN PROGRAM).
0008      C
0009      C *****
0010      I1=I-04
0011      IF (W(I1)-LT-1.0E-20) GO TO 3
0012      WS(I1)=ALOG10(W(I1))+C14(I1)
0013      D7 1 J=1-9
0014      IF (WS(I1)-FWH3(J)) 2,2,1
0015      CONTINUE
0016      TX(I1)=EXP(-10**((FWH1(J)+FWH2(J)+WS(I1)))
0017      4E**J-4.
0018      END

```

```

0001
0002
0003
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0014

FORTRAN IV G LEVEL 21
SUBROUTINE RQJ(I,M,C15,TX)
COMMON /MO13/ FNO2(9),OI(9),C2(9)
DIMENSION C15(45),TX(15),WS(15),M(15)
C*****
C THIS SUBROUTINE CALCULATES THE TRANSMITTANCE BY NO2 ( PPM READ IN
C THE MAIN PROGRAM).
C*****
IF (I.LE.106) II=I-105
IF (I.LE.239.AND.I.LE.265) II=I-192
IF (I.LE.499.AND.I.LE.519) II=I-425
IF (M(15).LT.1.OE-20) GO TO 3
WS(15)=ALOG10(M(15))+C15(11)
DO 1 J=1,9
IF (WS(15)=FNO2(J)) 2,Z,I
C*TIME*
TX(15)=EXP(-10**((C1(J)+C2(J)*WS(15)))
RETURN
END
1
2
3

```

PAGE 0001

16/22/49

DATE = 79218

80J

PROGRAM WILL BE EXECUTED IN THE TRANSMISSION MODE
 1 1 0 0 0 0 0 0 0 0.0 0.0
 0.0 2.500 65.000 5.000 0.0 0.0
 450.000 455.000 5.000

HORIZONTAL PATH, ALTITUDE = 0.0 KM, RANGE = 5.000 KM

MODEL ATMOSPHERE 1 = TROPICAL

HAZE MODEL 1 = 23KM VISUAL RANGE

FREQUENCY RANGE V1 = 450.0 CM-1 TO V2 = 455.0 CM-1 FOR QV = 5.0 CM-1 (21.98 - 22.22 MICRONS)

FREQ WAVELENGTH H2O CO2+ O2+NE MCL SCAT AEROSOL AEROSOL
 CM-1 MICRONS TRANS TRANS TRANS TRANS ARE ARE
 450 22.222 1.0000 1.0000 1.0000 1.0000 0.0331 0.0376
 455 21.780 1.0000 1.0000 1.0000 1.0000 0.4324 0.0376

FREQ WAVELENGTH SO2 NO3 NO2 INTEGRATED TOTAL
 CM-1 MICRONS TRANS TRANS TRANS ARE ARE
 450 22.222 1.0000 1.0000 1.0000 0.0000 0.0000
 455 21.780 1.0000 1.0000 1.0000 0.0000 0.0000
 INTEGRATED AVERAGE FROM 450 TO 455 CM-1 = 5.00E-05 TRANSMITTANCE = 0.0000

FREQUENCY SCALE VIF = 550.0 CM-1 TO V2 = 555.0 CM-1 (VIF = 5.0 CM-1 (18.2 = 18.18 MICRONS))

EQUILAVANT GAS LEVEL AVERAGE AMOUNTS

WATER VAPOR CO2 ETC. OZONE AIR-NO2N (CONT) H2O (CONT) WIL SCAT WIL SCAT
 CM-1 CM-2 CM-2 CM-2 CM-2 CM-2 CM-2 CM-2
 W(1-9)= 0.911E-01 0.440E-01 0.128E-01 0.368E-01 0.246E-01 0.455E-01 0.500E-01 0.131E-01

NIT-1+ ACID SO2 NH3 NO2

W(11-15)= 0.0 0.940E-01 0.102E-01 0.953E-01 0.398E-01

FREQ WAVELENGTH H2O CO2+ OZONE N2 CONT H2O CONT MOL SCAT AEROSOL AEROSOL
 CM-1 MICRONS TRANS TRANS TRANS TRANS TRANS TRANS TRANS TRANS
 550 18.1818 0.0211 0.9365 1.0000 1.0000 1.0000 1.0000 1.0000 0.9332 0.0343
 555 18.0180 0.0232 0.9193 1.0000 1.0000 1.0000 1.0000 1.0000 0.9324 0.0349

FREQ WAVELENGTH SO2 NO NH3 NO2 INTEGRATED TOTAL
 CM-1 MICRONS TRANS TRANS TRANS TRANS ABSORPTION TRANS
 550 18.1818 0.9175 1.0000 1.0000 2.4577 0.0169
 555 18.0180 0.9308 1.0000 1.0000 4.9113 0.0185
 INTEGRATED ABSORPTION FROM 550 TO 555 CM-1 = 4.91 AVERAGE TRANSMITTANCE = 0.0177

FREQUENCY RANGE V1 = 650.0 CM-1 TO V2 = 655.0 CM-1 FOR DV = 5.0 CM-1 (15.27 = 15.38 MICRONS)
 EQUILIVANT SEA LEVEL ABSORBER AMOUNTS

WATER VAPOR CO2 ETC. OZONE NITROGEN (CONT) H2O (CONT) MOL SCAT AEROSOL CZONE(UV-VIS)
 GM CM-2 K4 ATM CM4 KM CM CM-2 KM KM ATM CM
 W(1-9) = 0.911E 01 0.440E 01 0.128E-01 0.348E 01 0.246E 00 0.455E 01 0.500E 01 0.131E-01

NITROIC ACID SO2 NO NH3 NO2
 W(11-15) = 0.0 0.940E-01 0.102E 00 0.953E-01 0.398E-01

FREQ WAVELENGTH H2O CO2+ OZONE N2 CONT H2O CONT NCL SCAT AEROSOL AEROSOL
 CM-1 MICRONS TRANS TRANS TRANS TRANS TRANS TRANS TRANS TRANS
 950 10.5263 0.8800 0.9603 0.9994 1.0000 0.1042 1.0000 0.9731 0.0341
 955 10.4717 0.9681 0.9612 0.9988 1.0000 0.1692 1.0000 0.9226 0.0347

FREQ WAVELENGTH SO2 NO3 N2O INTEGRATED TOTAL
 CM-1 MICRONS TRANS TRANS TRANS TRANS
 950 10.5263 1.0000 1.0000 0.9212 1.0000 2.2052 0.1179
 955 10.4717 1.0000 1.0000 0.8078 1.0000 4.4165 0.1155
 INTEGRATED ABSORPTION FROM 950 TO 955 CM-1 = 4.42 AVERAGE TRANSMITTANCE = 0.1167

FREQUENCY RANGE W1= 1150.0 CM-1 TO V2= 1155.0 CM-1 FOR DV = 5.0 CM-1 (8.66 = 8.75 MICRONS)

TRANSLUCENT SEA LEVEL ABSORBER AMOUNTS

WATER VAPOR CO2 ETC. NITROGEN (COUNT) H2O (COUNT) AEROSOL CZONE(UV-VIS)
 CM CM-2 KM KM CM-2 KM CM-2 KM
 W(1-a)= 0.911E-01 0.440E-01 0.128E-01 0.348E-01 0.246E-00 0.455E-01 0.500E-01 0.131E-01

NITRIC ACID SO2 NO3 NH3 NO2
 W(1-b)= 0.0 0.900E-01 0.102E-00 0.953E-01 0.393E-01

FREQ WAVELENGTH M2O CO2+ OZONE N2 CONT H2O CONT MCL SCAT AEROSOL AEROSOL
 CM-1 MICRONS TRANS TRANS TRANS TRANS TRANS TRANS TRANS TRANS
 750 13.3333 0.4889 0.4739 0.9980 1.0000 0.0084 1.0000 0.9361 0.0261
 755 13.2450 0.5450 0.5962 0.9983 1.0000 0.0037 1.0000 0.9359 0.0260

FREQ WAVELENGTH SO2 NO3 NO2 INTEGRATED TOTAL
 CM-1 MICRONS TRANS TRANS TRANS TRANS TRANS TRANS TRANS TRANS
 750 13.3333 1.0000 1.0000 0.9914 0.9994 2.4956 0.0019
 755 13.2450 1.0000 1.0000 0.9783 0.9995 4.9884 0.0029
 INTEGRATED ABSORPTION FROM 750 TO 755 CM-1 = 4.99-AVERAGE TRANSMITTANCE = 0.0023

FREQUENCY RANGE V1 = 950.0 CM-1 TO V2 = 955.0 CM-1 FREQ DV = 5.0 CM-1 (10.47 - 10.53 MICRONS)

EQUILAVANT SEA LEVEL ABSORBER AMOUNTS

WATER VAPOR CO2 ETC. OZONE NITROGEN (CONT) H2O (CONT) MCL SCAT AEROSOL OZONE(UV-VIS)
 CM CM-2 KM KM CM CM-2 CM CM-2 CM CM-2 KM KM ATM CM
 MCL-9) = 0.911E 01 0.440E 01 0.129E-01 0.348E 01 0.246E 00 0.455E 01 0.500E 01 0.131E-01

NITRIC ACID SO2 NO NH3 NO2

MCL-15) = 0.0 0.990E-01 0.102E 00 0.953E-01 0.398E-01

FREQ	WAVELENGTH	H2O	CO2+	OZONE	N2	CONT	H2O	CONT	MOL	SCAT	AEROSOL	AEROSOL
CM-1	MICRONS	TRANS	TRANS	TRANS	TRANS	TRANS	TRANS	TRANS	TRANS	TRANS	TRANS	ABS
1150	8.6957	0.7275	0.9622	0.9973	1.0000	0.3041	1.0000	0.9055	0.0548			
1155	8.6580	0.7094	0.9612	0.9980	1.0000	0.3060	1.0000	0.9373	0.0560			

FREQ	WAVELENGTH	SO2	NO	NH3	NO2	INTEGRATED	TOTAL
CM-1	MICRONS	TRANS	TRANS	TRANS	TRANS	ABSORPTION	TRANS
1150	8.6957	0.9040	1.0000	0.9768	1.0000	2.0748	0.1701
1155	8.6580	0.8929	1.0000	0.9820	1.0000	4.1606	0.1657

INTEGRATED ABSORPTION FROM 1150 TO 1155 CM-1 = 4.16, AVERAGE TRANSMITTANCE = 0.1679

FREQUENCY RANGE V1 = 1350.0 CM-1 TO V2 = 1355.0 CM-1 FOP'OV = 5.0 CM-1 (7.38 = 7.61 MICRONS)

EQUILIVANT SEA LEVEL ABSORBER AMOUNTS

WATER VAPOR	CO2 ETC.	OZONE	NITROGEN	H2O	AEROSOL	OZONE(UV-VIS)
CM CM-2	KM	ATM CM	KM	GM CM-2	KM	ATM CM
W(1-9)= 0.911E 01	0.440E 01	0.128E-01	0.348E 01	0.246E 00	0.455E 01	0.131E-01
NITRIC ACID	SO2	NO	NH3	NO2		
W(11-15)= 0.0	0.590E-01	0.102E 00	0.953E-01	0.398E-01		

FREQ WAVELENGTH H2O CO2+ OZONE N2 CONT H2O CONT MOL SCAT AEROSOL AEROSOL
 CM-1 MICRONS TRANS TRANS TRANS TRANS TRANS TRANS TRANS TRANS
 1350 7.4074 0.0001 0.6343 1.0000 1.0000 1.0000 1.0000 0.9310 0.0347
 1355 7.3801 0.0001 0.6823 1.0000 1.0000 1.0000 1.0000 0.9302 0.0350

FREQ WAVELENGTH SO2 NO3 INTEGRATED TOTAL
 CM-1 MICRONS TRANS TRANS TRANS TRANS
 1350 7.4074 0.2780 1.0000 1.0000 2.5000 0.0000
 1355 7.3801 0.2728 1.0000 1.0000 5.0000 0.0000
 INTEGRATED ABSORPTION FROM 1350 TO 1355 CM-1 = 5.00, AVERAGE TRANSMITTANCE = 0.0000

FREQUENCY RANGE VIS = 1850.0 CM-1 TO V2 = 1855.0 CM-1 FOR DV = 5.0 CM-1 (5.39 = 5.41 MICRONS)

FOULAVENT SEA LEVEL ABSORBER AMOUNTS

WATER VAPOR CO2 ETC. OZONE NITROGEN (CONT) H2O (CONT) MOL SCAT AEROSOL OZONE (UV-VIS)
 CM CM-2 KM CM CM-2 GM CM-2 GM CM-2 K_v ATM CM
 W(1-R) = 0.911E-01 0.440E-01 0.124E-01 0.348E-01 0.246E-01 0.455E-01 0.500E-01 0.131E-01

NITRIC ACID SO2 NO3 NO2
 W(11-R) = 0.0 0.000E-01 0.102E-01 0.953E-01 0.393E-01

FREQ WAVELENGTH H2O CO2+ OZONE N2 CONT H2O CONT MCL SCAT AEROSOL
CM-1 MICRONS TRANS TRANS TRANS TRANS TRANS TRANS ABS
2450 4.0816 0.9922 0.9617 1.0000 0.7665 0.8288 1.0000 0.9212 0.0119
2455 4.0733 0.9914 0.9645 1.0000 0.7927 0.8320 1.0000 0.9211 0.0119

FREQ WAVELENGTH SO2 NO3 NO2 INTEGRATED TOTAL
CM-1 MICRONS TRANS TRANS TRANS TRANS ABSORPTIV TRANS
2450 4.0816 1.0000 1.0000 1.0000 1.1041 0.5584
2455 4.0733 0.9998 1.0000 1.0000 2.1705 0.5734
INTEGRATED ABSORPTION FROM 2450 TO 2455 CM-1 = 2.17, AVERAGE TRANSMITTANCE = 0.5659

1

FREQUENCY RANGE V1= 3150.0 CM-1 TO V2= 3155.0 CM-1 FOR CV = 5.0 CM-1 (3.17 = 3.17 MICRONS)

EQUILIVANT SEA LEVEL ABSORBER AMOUNTS

WATER VAPOR CO2 ETC. OZONE NITROGEN (CONT) H2O (CONT) MCL SCAT AEROSOL OZONE(UV-VIS)
CM CM-2 KM KM CM-2 GM CM-2 KM KM ATN CM
W11-R1= 0.911E 01 0.440E 01 0.123E-01 0.348E 01 0.246E 00 0.455E 01 0.500E 01 0.131E-01

NITRIC ACID SO2 NO3 NO2

W11-L5)= 0.0 0.990E-01 0.102E 00 0.953E-01 0.398E-01

FREQ WAVELENGTH H2O CO2+ OZONE N2 CONT H2O CONT MOL SCAT AEROSOL AEROSOL
CM-1 MICRONS TRANS TRANS TRANS TRANS TRANS TRANS ABS
1850 5.4054 0.0000 0.9955 1.0000 1.0000 1.0000 0.9283 0.0186
1855 5.3908 0.0000 0.9949 0.9999 1.0000 1.0000 1.0000 0.9282 0.0185

FREQ WAVELENGTH SO2 NO3 NO2 INTEGRATED TOTAL
CM-1 MICRONS TRANS TRANS TRANS TRANS TRANS
1850 5.4054 1.0000 0.8961 1.0000 1.0000 2.5000 0.0000
1855 5.3908 1.0000 0.9034 1.0000 1.0000 5.0000 0.0000
INTEGRATED ABSORPTION FROM 1850 TO 1855 CM-1 = 5.00, AVERAGE TRANSMITTANCE = 0.0000

FREQUENCY RANGE V1= 2450.0 CM-1 TO V2= 2455.0 CM-1 FCP DV = 5.0 CM-1 (4.07 = 4.06 MICRONS)

FOUILLAVENT SEA LEVEL ABSORBER AMOUNTS

W(1-9)=	WATER VAPOR GM CM-2	CO2 ETC. KM	OZONE ATM CM	NITROGEN (CONT) KM	H2O (CONT) GM CM-2	MOL SCAT KM	AEROSOL KM	OZONE(UV-VIS) ATM CM
0.911E 01	0.440E 01	0.128E-01	0.348E 01	0.246E 00	0.455E 01	0.500E 01	0.131E-01	

NITRIC ACID SO2 NO3 NO2

W(11-15)= 0.0 0.590E-01 0.102E 00 0.953E-01 0.398E-01

FREQ WAVELENGTH		H2O		CO2+		OZONE		N2		H2O CONT		MOL SCAT		AEROSOL	
CM-1	MICRONS	TRANS	ABS	TRANS	ABS	TRANS	ABS	TRANS	ABS	TRANS	ABS	TRANS	ABS	TRANS	ABS
3150	3.1746	0.4800	0.9190	0.9998	0.9998	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	0.9116	0.0231
3155	3.1696	0.5021	0.9373	0.9998	0.9998	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	0.9116	0.0233

FREQ WAVELENGTH		SO2		NO		NH3		N2		INTEGRATED		TOTAL	
CM-1	MICRONS	TRANS	ABS	TRANS	ABS	TRANS	ABS	TRANS	ABS	TRANS	ABS	TRANS	ABS
3150	3.1746	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.4951	0.4023	1.4951	0.4023
3155	3.1696	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	2.9229	0.4289	2.9229	0.4289

INTEGRATED ABSORPTION FROM 3150 TO 3155 CM-1 = 2.92, AVERAGE TRANSMITTANCE = 0.4154

0

ADSET V 1-3

EVALUATION OF ABSORBER PARAMETERS AND STANDARD EMPIRICAL AND
PIECEWISE-ANALYTICAL TRANSMISSION FUNCTIONS

THIS CODE USES THE SUBROUTINE SIMQ IN SSP LIBRARY

THIS CODE CONSISTS OF

MAIN: COMPUTATIONS OF BAND PARAMETERS N,M,C'
AND EMPIRICAL STANDARD TRANSMISSION FUNCTION
NMBC: COMPUTATION OF NON-MAJOR BANDS' C-VALUES
INTPL1: COMPUTATION OF THE PIECEWISE-ANALYTICAL
STANDARD TRANSMISSION FUNCTION GIVEN BY
 $\tau = \exp(-10^{**}(A1+A2*X))$
INTPL2: COMPUTATION OF THE PIECEWISE-ANALYTICAL
STANDARD TRANSMISSION FUNCTION GIVEN BY
 $\tau = \exp(-10^{**}(A1+A2*X+A3*X**2))$
SDTAU: COMPUTATION OF THE ERROR STANDARD DERIVATIONS
BETWEEN PIECEWISE ANALYTICAL STANDARD
TRANSMISSION FUNCTION AND THE ORIGINAL DATA
USED IN THE MAIN PROGRAMME

DATA SET-UP

1. 1ST CARD TITLE IN 20A4
(ABSORBER TYPE,ETC)
2. 2ND CARD FOUR CONTROL NUMBERS IN 4I5
MAXRPT MAXIMUM NUMBER OF REPETITION OF
THE COMPUTATION IN MAIN
INDX(1) SUBROUTINE NMBC IS CALLED IF > 0
INDX(2) SUBROUTINE INTPL1 IS CALLED IF > 0
INDX(3) SUBROUTINE INTPL2 IS CALLED IF > 0
3. DATA SET FOR MAIN
CONSISTS OF SEVERAL SUBSETS (MAX.6) OF DATA
CORRESPONDING TO INDIVIDUAL MAJOR BANDS
FIRST CARD FOR EACH SUBSET IS A CONTROL CARD WHICH
CONTAINS BAND#, WAVE NUMBER, # OF CUTS AND # OF LEVELS
IN THIS ORDER BY THE FORMAT (I5,F10.3,2I5)
REFER TO THE READ(5,105) AND FORMAT 105 FOR THE
CONTENTS OF EACH CARD.
END OF DATA IS DEFINED BY A BLANK CONTROL CARD
4. DATA SET FOR NMBC
INDIVIDUAL DATA FORMAT - SAME AS FOR MAIN
END OF EACH DATA SET FOR A BAND IS MARKED BY
A BLANK CARD
END OF ALL DATA IS MARKED BY -1 (I2) IN ADDITION TO
A BLANK CARD
IF NO DATA BUT A BLANK CARD IS SUPPLIED, THEN
THIS SUBROUTINE IS SKIPPED.
5. DATA SET FOR INTPL1
FORMATION OF THE DATA IS THE SAME AS THAT FOR MAIN
DATA (IF SUPPLIED) WILL BE USED FOR S.D. COMPUTATION
ONLY.
IF NO DATA BUT A BLANK CARD IS SUPPLIED, THEN THE
S.D. COMPUTATION IS SKIPPED.
6. DATA SET FOR INTPL2

C FORMATION OF THE DATA IS THE SAME AS THAT FOR MAIN
 C IF NO DATA BUT A BLANK CARD IS SUPPLIED, THEN
 C THIS SUBROUTINE IS SKIPPED.
 C NOTE: DATA SET MUST HAVE A CUT STRUCTURE SUCH THAT EQUAL
 C TRANSMITTANCE DATA ARE GROUPED TOGETHER AND THESE GROUPS
 C ARE QUEUED IN THE DECENDING ORDER IN TAU. THE QUEUING OF
 C THE LEVELS WITHIN EVERY GROUP MUST BE THE SAME.

```

    C
    C      DIMENSION V(19),A(19,19),X(361),B(19),RI(6,12,10)
    C      DIMENSION P(10),WWW(12,10),STANDV(12),TSD(6),NDATA(6),INDX(3)
    C      COMMON /PARM1/ TSTD(12),PW(12),WN(6),CSTD(6),NCUT,NC,NAME(20),
    C      *              AN,AM,CF,ICONST(6),NEL
    C      COMMON /PARM2/ PRES(6,12,10),TEMP(6,12,10),UGAS(6,12,10),
    C      *              TAU(6,12),NTC(6),NLV(6)
    C      CF=1.0
    C      LOOPCT=1
    C      WCRIT=2.
    C      M=0
    C      READ(5,100) (NAME(I),I=1,20)
100  FORMAT(20A4)
    C      READ(5,101) MAXRPT,(INDX(I),I=1,3)
101  FORMAT(4I5)
    C
    C      COMPUTATION OF ABSORBER PARAMETERS N, M & C-VALUES IS REPEATED
    C      MAXRPT TIMES, WHERE 1 < MAXRPT < 10 IS READ IN BY I5 FORMAT
    C      (SUGGESTED VALUE IS 5)
    C
    C      DATA READ-IN ROUTINE
    C
1000 CONTINUE
    C      READ(5,102) IC,W,JM,KM
102  FORMAT(I5,F10.3,2I5)
    C      IF(IC.LE.0) GO TO 2000
    C      IF(M.GT.0) GO TO 10
    C      CALL DATE (MONTH,IDAY,IYEAR)
    C      WRITE(6,111)MONTH,IDAY,IYEAR
111  FORMAT(1H1,T60,I4,' / ',I2,' / ',I2,/)
    C      WRITE(6,200) (NAME(I),I=1,20)
200  FORMAT(1H ,T25,20A4)
    C      GO TO 11
    C      10 CONTINUE
    C      WRITE(6,201)
201  FORMAT(1H1)
    C      11 CONTINUE
    C      M=M+1
    C      WN(M)=W
    C      NTC(M)=JM
    C      NLV(M)=KM
    C      WRITE(6,202) M,WN(M),NTC(M),NLV(M)
202  FORMAT(1H0,T15,'*** BAND',I3,' (WAVE NUMBER =',F10.3,') ***',
    C      * ///,T20,'TOTAL # OF CUTS' =',I3,/,T20,'TOTAL # OF LEVELS =',I3,
    C      * ///)
    C      WRITE(6,203)
203  FORMAT(1H ,T5,'( DATA FORMAT )',/,T9,'GAS#',T15,'WAVE #',T24,
    C      * 'PRESSURE',T36,'TEMP.',T46,'PPM',T58,'RANGE',T70,'UGAS',T78,
    C      * 'TRANSM.',/)
  
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```

DO 12 J=1,JM
WRITE(6,204) J
204 FORMAT(1H0,T5,'< CUT',I3,' >',/)
T=0.
IT=0
DO 13 K=1,KM
READ(5,103) KGAS,FREQ,RPRES,RTEMP,PPM,RANGE,RUGAS,TX
103 FORMAT(I2,F10.3,E11.4,F9.3,E11.4,E13.6,E11.4,F7.4)
RUGAS=RUGAS/CF
WRITE(6,205) KGAS,FREQ,RPRES,RTEMP,PPM,RANGE,RUGAS,TX
205 FORMAT(T10,I2,F10.3,E11.4,F9.3,E11.4,E13.6,E11.4,F8.4)
C
C      PRES, TEMP & UGAS ARE CONVERTED TO THE LOG OF THE NORMALIZED
C      VALUES. IF RPRES=0 (INDICATES NO DATA), THEN UGAS(M,J,K) IS SET
C      AT AN IMPOSSIBLE VALUE , ALSO RI(M,J,K) IS SET TO ZERO.
C
IF(RPRES.GT.0.) GO TO 14
PRES(M,J,K)=0.
TEMP(M,J,K)=0.
UGAS(M,J,K)=10.
RI(M,J,K)=0.
GO TO 15
14 CONTINUE
PRES(M,J,K)=ALOG10(RPRES/1013.)
TEMP(M,J,K)=ALOG10(273.15/RTEMP)
UGAS(M,J,K)=ALOG10(RUGAS)
15 CONTINUE
C
T=T+TX
IT=IT+1
RI(M,J,K)=1.0
13 CONTINUE
TAU(M,J)=T/FLOAT(IT)
12 CONTINUE
GO TO 1000
C
C      END OF DATA INPUT
C
C      CONSTANTS USED IN LATER COMPUTATION ARE INITIALIZED
C      FROM 2000 TO 3000.
C      NCUT = MAXIMUM # OF CUTS USED IN COMPUTATION
C      NDIM = DIMENSION OF THE COEFFICIENT MATRIX
C
2000 CONTINUE
IF(M.GT.0) GO TO 20
WRITE(6,206)
206 FORMAT(1H0,/,T10,'$$$ NO INPUT DATA $$$')
STOP
20 CONTINUE
NC=M
CSTD(1)=0.
NCUT=NTC(1)
NPTS=NTC(1)*NLV(1)
IF(NC.LE.1) GO TO 21
DO 22 I=2,NC
NCUT=MAX0(NCUT,NTC(I))

```

```

      NPTS=NPTS+NTC(I)*NLV(I)
22 CONTINUE
21 CONTINUE
      FNC=FLOAT(NC)
      RIT=FLOAT(NPTS)
      DO 23 J=1,NCUT
      TC=0.
      DO 24 M=1,NC
      TC=TC+TAU(M,J)
24 CONTINUE
      TSTD(J)=TC/FNC
23 CONTINUE
      NDIM=NC+1+NCUT
C
C*****
C      COMPUTATION OF THE ABSORBER PARAMETERS.
C      THIS LOOP WILL BE REPEATED MAXRPT TIMES.
C
C      FORMATION OF THE NORMAL EQUATION  $AX = B$  , A IS SYMMETRIC
C
3000 CONTINUE
      DO 30 I=1,19
      B(I)=0.
      DO 31 J=1,19
      A(I,J)=0.
31 CONTINUE
30 CONTINUE
C
      DO 1 M=1,NC
      JM=NTC(M)
      KM=NLV(M)
      DO 2 J=1,JM
      DO 3 K=1,KM
      IF(RI(M,J,K).LT.0.5.) GO TO 3
      DO 4 IC=1,19
      V(IC)=0.
4 CONTINUE
      V(NDIM-M)=1.
      V(NDIM)=PRES(M,J,K)
      V(NDIM-1)=TEMP(M,J,K)
      VV=-UGAS(M,J,K)
      V(NCUT+1-J)=1.
      DO 5 II=1,NDIM
      DO 6 IJ=1,NDIM
      A(II,IJ)=V(II)*V(IJ)*RI(M,J,K) + A(II,IJ)
6 CONTINUE
      B(II)=V(II)*VV*RI(M,J,K) + B(II)
5 CONTINUE
3 CONTINUE
2 CONTINUE
1 CONTINUE
C
C      IF J-TH ROW OF "A" IS ZERO, A(J,J) IS CHANGED TO -1
C      WHICH IS DONE IN ORDER TO MAKE "A" NON-SINGULAR
C      THIS HAPPENS WHEN ALL OF THE DATA FOR BAND J-1 FAIL TO SATISFY
C      THE CRITERION  $W < WCRIT$ . THE BAND J-1 WILL BE IGNORED IF THIS

```

HAPPENS, AND THE C-VALUE FOR BAND J-1 WILL BE COMPUTED
SEPARATELY.

C
C

```

      ICONST(1)=1
      IF(NC.EQ.1) GO TO 40
      DO 41 M=2,NC
      ICONST(M)=1
      I=NDIM-M
      IF(A(I,I).NE.0.) GO TO 41
      A(I,I)=-1.0
      ICONST(M)=0
41  CONTINUE
40  CONTINUE

```

C
C

```

      NCOL=0
      DO 42 J=1,NDIM
      DO 43 I=1,NDIM
      NCOL=NCOL+1
      X(NCOL)=A(I,J)
43  CONTINUE
42  CONTINUE

```

C
C
C

PRINTING OF THE HEADING FOR EACH TRIAL AND THE NORMAL EQUATION

```

      IF(LOOPCT.GT.1) GO TO 50
      WRITE(6,207) MAXRPT,LOOPCT
207  FORMAT(1H1,T20,'*** ABSORBER PARAMETER COMPUTATION ***',///,
      * T15,'NOTE: THE COMPUTATION WILL BE REPEATED MAXRPT =',I2,
      * ' TIMES.',///,T10,'TRIAL #',I1,5X,'(ALL DATA WERE USED)')
      GO TO 51
50  CONTINUE
      WRITE(6,208) LOOPCT
208  FORMAT(1H1,T10,'TRIAL #',I1,5X,'(PARTIAL DATA WERE USED WITH',
      * ' CUT-OFF CRITERION : W < 2 )')
51  CONTINUE
      WRITE(6,209) NDIM,NDIM
209  FORMAT(//,1H0,'< NORMAL EQUATION : AX = B >',//,T10,'WHERE THE',
      * ' COEFFICIENT MATRIX A(',I3,' ',I3,' ) AND THE CONSTANT VECTOR',
      * ' B ARE',//)
      IF(NDIM.LE.17) GO TO 52
      WRITE(6,210) NDIM
210  FORMAT(1H , '*** WARNING : DIMENSION OF THE MATRIX IS TOO LARGE',
      * ' (',I3,' ) TO BE PRINTED IN A MATRIX FORM ***',/)
52  CONTINUE
      DO 53 I=1,NDIM
      WRITE(6,211) (A(I,J),J=1,NDIM),B(I)
211  FORMAT(1H ,18F7.3)
53  CONTINUE

```

C
C
C

***** MATRIX INVERSION SUBROUTINE SIMQ IN SSP IS CALLED *****

C

CALL SIMQ(X,B,NDIM,KS)

C
C
C

PRINTING OF THE SOLUTION FOR THE NORMAL EQUATION


```

      IF(KS.EQ.1) WRITE(6,212)
212  FORMAT(1H0,T10,'WARNING:  THE COEFFICIENT MATRIX IS SINGULAR.')
```

AN=B(NDIM)
AM=B(NDIM-1)
IF(NC.LE.1) GO TO 54
DO 55 M=2,NC
CSTD(M)=B(NDIM-M)

55 CONTINUE
54 CONTINUE
DO 56 J=1,NCUT
PW(J)=-B(NCUT+1-J)

56 CONTINUE
WRITE(6,213) AN,AM,(CSTD(M),M=1,NC)

213 FORMAT(/,1H0,' < RESULTS >',///,T7,'N',T17,'M',T27,'C1',T37,'C2',
* T47,'C3',T57,'C4',T67,'C5',T77,'C6',//,2F10.5,6F10.3)
WRITE(6,214) (PW(I),I=1,NCUT)

214 FORMAT(/,1H0,T7,'X*1',T17,'X*2',T27,'X*3',T37,'X*4',T47,'X*5',
* T57,'X*6',T67,'X*7',T77,'X*8',T87,'X*9',T97,'X*10',T107,'X*11',
* T117,'X*12',//,12F10.3)
NEL=NPTS-INT(RIT)
WRITE(6,215) NEL

215 FORMAT(/,1H0,T4,'# OF ELIMINATED POINTS =',I5)

C
C
C
C
C
C

CHECKING OF THE CRITERION (W < WCRIT) AND THE COMPUTATION
OF C-VALUES FOR THE IGNORED BANDS.
RI(M,J,K) = 0 IF W IS GREATER THAN OR EQUAL TO WCRIT
RI(M,J,K) = 1 IF W IS LESS THAN WCRIT

RIT=0.
DO 60 M=1,NC
JM=NTC(M)
KM=NLV(M)
CAVG=0.0
DO 61 J=1,JM
DO 62 K=1,KM
W=AN*PRES(M,J,K)+AM*TEMP(M,J,K)+UGAS(M,J,K)
IF(W.GE.WCRIT) RI(M,J,K)=0.
RIT=RIT+RI(M,J,K)
CAVG=CAVG+(PW(J)-W)

62 CONTINUE
61 CONTINUE
IF(ICONST(M).EQ.1) GO TO 60
CSTD(M)=CAVG/FLOAT(JM*KM)
WRITE(6,216) M,M,M,CSTD(M)

216 FORMAT(/,1H ,T7,'** WARNING **',T25,'NO DATA FOR BAND',I2,
* ' SATISFIES THE CRITERION (W < 2).',//,T25,'THE C',I1,
* ' VALUE IS SEPARATELY COMPUTED BY AVERAGING.',//,T30,'C',I1,
* ' =',F10.3)

60 CONTINUE

C
C
C

COMPUTATIONS OF STANDARD DEVIATIONS IN X

NGDATA=0
GTSD=0.
ICST=NC
DO 70 M=1,NC

```

JM=NTC(M)
KM=NLV(M)
NDATA(M)=0
TSD(M)=0.
WRITE(6,201)
WRITE(6,202) M,WN(M),NTC(M),NLV(M)
WRITE(6,217) AN,AM,M,CSTD(M)
217 FORMAT(1H ,T10,'N' =',F10.5,/,T10,'M' =',F10.5,/,T10,'C',I1,
* ' =',F10.5)
WRITE(6,218)
218 FORMAT(/,1H0,T7,'RECOMPUTED X-VALUES AND STANDARD DEVIATIONS',
* ' IN X-VALUES',/,1H0,T2,'CUT',T11,'TAU',T20,'X*',T30,'X1',T39,
* 'X2',T48,'X3',T57,'X4',T66,'X5',T75,'X6',T84,'X7',T93,'X8',
* T102,'X9',T111,'X10',T121,'CUTWISE-SD',/)

```

C
C
C

COMPUTATION OF THE CUTWISE STANDARD DEVIATIONS IN X

```

DO 71 J=1,JM
DN=0.
WW=0.
DO 72 K=1,KM
P(K)=CSTD(M)+AN*PRES(M,J,K)+AM*TEMP(M,J,K)+UGAS(M,J,K)
WWW(J,K)=(PW(J)-P(K))*2*RI(M,J,K)
WW=WW+WWW(J,K)
DN=DN+RI(M,J,K)
72 CONTINUE
WW=SQRT(WW/DN)
NDATA(M)=NDATA(M)+IFIX(DN)
WRITE(6,219) J,TAU(M,J),PW(J),(P(K),K=1,KM)
219 FORMAT(1H ,I5,F9.3,F9.4,1X,10F9.4)
WRITE(6,220) WW
220 FORMAT(1H+,T121,F10.5)
71 CONTINUE

```

C
C
C

COMPUTATION OF THE LEVELWISE STANDARD DEVIATIONS IN X

```

DO 73 K=1,KM
WW=0.
DN=0.
DO 74 J=1,JM
WW=WW+WWW(J,K)
DN=DN+RI(M,J,K)
74 CONTINUE
TSD(M)=TSD(M)+WW
STANDV(K)=SQRT(WW/DN)
73 CONTINUE
WRITE(6,221) (STANDV(K),K=1,KM)
221 FORMAT(1H0,T4,'LEVELWISE-SD :',T26,10F9.5)
NGDATA=NGDATA+NDATA(M)*ICONST(M)
GTSD=GTSD+TSD(M)*FLOAT(ICONST(M))
ICST=ICST-ICONST(M)
TSD(M)=SQRT(TSD(M)/FLOAT(NDATA(M)))
WRITE(6,222) TSD(M)
222 FORMAT(/,1H0,T4,'TOTAL STANDARD DEVIATION FOR THIS BAND :',
* F15.6)
70 CONTINUE

```

C
C
C
C
C
C

PRINTOUT OF THE SUMMARY.
ALL VITAL INFORMATIONS ARE PRINTED OUT HERE.

```

GTSD=SQRT(GTSD/FLOAT(NGDATA))
WRITE(6,223) LOOPCT,AN,AM
223 FORMAT(1H1,T15,'***' SUMMARY OF THE ABSORBER PARAMETER',
* ' COMPUTATION FOR TRIAL #',I2,' ***',///,T20,
* 'PRESSURE EXPONENT      N =',F10.5,///,T20,
* 'TEMPERATURE EXPONENT M =',F10.5,///,T5,'CASE #',3X,
* 'WAVE NUMBER',5X,'C-VALUE',5X,'TOTAL # OF DATA',3X,
* 'CASEWISE S.D. IN P')
WRITE(6,224) (M,WN(M),CSTD(M),NDATA(M),TSD(M),M=1,NC)
224 FORMAT(1H0,T6,I3,6X,F9.2,5X,F8.3,10X,I3,12X,F12.6)
WRITE(6,225) NGDATA,NEL,GTSD
225 FORMAT(//,1H0,T15,'GRAND TOTAL # OF DATA =',I5,///,T15,'# OF',
* ' ELIMINATED DATA =',I5,///,T15,'GLOBAL STANDARD DEVIATION IN P',
* ' =',F12.6,/)
IF(ICST.LE.0) GO TO 75
DO 76 M=1,NC
IF(ICONST(M).EQ.1) GO TO 76
WRITE(6,226) M
226 FORMAT(1H ,T15,'NOTE: THE BAND',I3,' IS NOT INCLUDED IN THE',
* ' FINAL STANDARD DEVIATION')
76 CONTINUE
75 CONTINUE
WRITE(6,227) LOOPCT,(TSTD(J),PW(J),J=1,NCUT)
227 FORMAT(///,1H0,T15,'***' STANDARD EMPIRICAL TRANSMISSION',
* ' FUNCTION FOR TRIAL #',I2,' ***',///,T20,'TAU',T35,'X*',/,
* (1H0,T17,F7.3,T30,F8.4))

C
C
IF(RIT.GT.0.) GO TO 80

C
C
IF NO INPUT DATA SATISFIES THE CRITERION, THE COMPUTATION IS
TERMINATED. THE MOST RECENT RESULTS WILL BE USED IN THE SEQUAL.

C
WRITE(6,228)
228 FORMAT(1H1,///,T15,'$$$ NO INPUT DATA SATISFIES THE CRITERION OF',
* ' ( W < 2 ) $$$',///,T15,'$$$ THE COMPUTATION FOR THIS STEP IS',
* ' TERMINATED $$$')
GO TO 4000
80 CONTINUE
LOOPCT=LOOPCT+1
IF(LOOPCT.GT.MAXRPT) GO TO 4000
GO TO 3000

C
4000 CONTINUE

C
C
SUBROUTINE COMPUTATIONS FOLLOW

C
IF(INDX(1).LE.0) GO TO 90

C
CALL NMBC

```

```

C
90 CONTINUE
  IF(INDX(2).LE.0) GO TO 91
C
  CALL INTPL1
C
91 CONTINUE
  IF(INDX(3).LE.0) GO TO 92
C
  CALL INTPL2
C
92 CONTINUE
  STOP
  END
  SUBROUTINE NMBC
C
C      COMPUTATION OF C'-VALUES FOR NON-MAJOR BANDS
C
  DIMENSION B(15),CS(15),FS(15)
  COMMON /PARM1/ TSTD(12),PW(12),WN(6),CSTD(6),NCUT,NC,NAME(20),
  *           AN,AM,CF,ICONST(6),NEL
  WRITE(6,5) (NAME(I),I=1,20)
5  FORMAT(1H1,T15,20A4)
  WRITE(6,10)
10 FORMAT(1H0,T15,' *** CALCULATION OF THE SPECTRAL PARAMETERS',
  * 'FOR NON-MAJOR BANDS ***'///)
  DF=1.E30
11 CONTINUE
  NFREQ=0
12 CONTINUE
  C=0.
  I=0
15 CONTINUE
  READ(5,20) KGAS,FREQ,P,T,UGAS,TX
20 FORMAT(I2,F10.3,E11.4,F9.3,24X,E11.4,F7.4)
  IF(KGAS.EQ.0) GO TO 25
  IF (KGAS.LT.0) GO TO 35
C
C      THE FOLLOWING IF-STATEMENT IS INSERTED TO DETECT
C      AND TO IGNORE THE INVALID DATA POINTS.
C
  IF(UGAS.GE.DF) GO TO 15
  I=I+1
  WX=FREQ
  UGAS=UGAS/CF
  C=C+(PW(I)-AN*ALOG10(P/1013.)-AM*ALOG10(273.15/T)-ALOG10(UGAS))
  GO TO 15
25 C=C/FLOAT(I)
  NFREQ=NFREQ+1
  CS(NFREQ)=C
  FS(NFREQ)=WX
  DO 27 M=1,NC
  IF(ABS(WX-WN(M)).LE.0.1) CS(NFREQ)=CSTD(M)
27 CONTINUE
  IF(NFREQ.EQ.10) GO TO 30
  GO TO 12

```

```

30 CONTINUE
  WRITE(6,31) (FS(K),K=1,NFREQ)
31 FORMAT(1H0,2X,'WAVE NUMBER',2X,10F11.0)
  WRITE(6,32) (CS(K),K=1,NFREQ)
32 FORMAT(1H0,5X,'C VALUES',2X,10F11.3//)
  GO TO 11
35 CONTINUE
  IF(NFREQ.EQ.0) GO TO 40
  WRITE(6,31) (FS(K),K=1,NFREQ)
  WRITE(6,32) (CS(K),K=1,NFREQ)
40 CONTINUE
  RETURN
  END

```

```

C
SUBROUTINE INTPL1
C
C      COMPUTATION OF THE STANDARD PIECEWISE-ANALYTICAL TRANSMISSION
C      FUNCTION
C
C      VERSION 1 - 1  ** A3(I) = 0 **
C      TAU = EXP(-10** ( A1(I)+A2(I)*X ))
C
C      DIMENSION SDCUT(15),ICUT(15),SDTCUT(15),ITCUT(15)
C      COMMON /PARM1/ TSTD(12),PW(12),WN(6),CSTD(6),NCUT,NC,NAME(20),
C      *              AN,AM,CF,ICONST(6),NEL
C      COMMON /PARM3/ A1(11),A2(11),A3(11)
C      SSD=0.
C      ITOTAL=0
C      IM=NCUT-1
C      JM=NCUT-2
C
C      COMPUTATION OF THE COEFFICIENTS A1(I), A2(I) AND A3(I)
C
C      CTX1=ALOG10(-ALOG(TSTD(1)))
C      DO 50 I=1,IM
C      PDIF=PW(I)-PW(I+1)
C      CTX2=ALOG10(-ALOG(TSTD(I+1)))
C      A1(I)=(PW(I)*CTX2-PW(I+1)*CTX1)/PDIF
C      A2(I)=(CTX1-CTX2)/PDIF
C      A3(I)=0.
C      CTX1=CTX2
C
C      SDTCUT(I)=0.
50 ITCUT(I)=0
C
C      THE FIRST AND LAST VALUES OF TSTD AND PW ARE CHANGED
C      FOR THE TABLE OUTPUT. TRUE VALUES ARE TEMPORARY STORED
C      IN THE RESERVE.
C
C      TRES1=TSTD(1)
C      TRES2=TSTD(NCUT)
C      PWRES1=PW(1)
C      PWRES2=PW(NCUT)
C      TSTD(1)=1.0
C      TSTD(NCUT)=0.0

```

PW(1)=-1.E70
PW(NCUT)=1.E70

C
C
C

PRINT OUT OF THE RESULTS

WRITE(6,2) (NAME(I),I=1,20)
2 FORMAT(1H1,T25,20A4,/,T15,'PIECEWISE-ANALYTICAL STANDARD',
* 'TRANSMISSION FUNCTION',/,T20,'TAU(X) =',
* 'EXP(-10** (A1 + A2*X))',/,T15,'DATA:',T23,'FROM (TAU ,',
* 'X-VALUE) TO (TAU ,X-VALUE) WITH (A1 , A2)')
WRITE(6,3) (TSTD(I),PW(I),TSTD(I+1),PW(I+1),A1(I),A2(I),I=1,IM)
3 FORMAT(1H0,T28,(' ',F6.3,' ',',F7.3,') (' ',F6.3,' ',',F7.3,')',T74,
* '(',F7.4,' ',',F7.4,')')
WRITE(6,4) (I,WN(I),CSTD(I),I=1,NC)
4 FORMAT(1H0,/,T15,'ABSORPTION BANDS:',T40,
* '# WAVENUMBER C-VALUE'/(1H0,T39,I2,5X,F7.1,F11.5))

C
C
C
C
C
C
C

CHECK IF ANY DATA IS AVAILABLE FOR S.D. COMPUTATION
DATA FORMAT IS THE SAME AS THAT FOR MAIN PROGRAMME
ONE CONTROL CARD IS READ-IN FIRST FOR BRANCHING
IFQ > 0 DATA SET FOLLOWS, READ-IN DATA
IFQ = 0 END OF DATA, GO TO THE FINAL PRINTING

READ(5,11,END=42) FQ,IFQ
11 FORMAT(5X,F10.3,T41,I4)
IF(IFQ.GT.0) GO TO 18
42 WRITE(6,41)
41 FORMAT(///,1H0,T5,'\$\$\$ NO DATA FOR STANDARD DEVIATION COMPUTATION
* \$\$\$')
GO TO 40
8 READ(5,11,END=30) FQ,IFQ
IF(IFQ.LE.0) GO TO 30
18 CONTINUE
ST=0.
DO 51 I=1,IM
SDCUT(I)=0.
51 ICUT(I)=0
CLOG=100.
DO 52 I=1,NC
52 IF(ABS(FQ-WN(I)).LT.1.) CLOG=CSTD(I)
IF(CLOG.LT.99.) GO TO 13

C
C
C
C

THE READ-IN WAVENUMBER DOES NOT MATCH THE MAJOR BAND
WAVENUMBER (WN(I)).THE DATA IN THIS BAND ARE IGNORED.

WRITE(6,12) FQ
12 FORMAT(1H0,T10,'** ERROR IN WAVENUMBER **',
* ' (READ-IN WAVENUMBER =',F10.5,')')
DO 61 IDUM=1,IFQ
READ(5,60) DUMMY
60 FORMAT(F1.0)
61 CONTINUE
GO TO 8

C
C
C

VALID DATA INPUTS, READ-IN OF THE DATA AND STANDARD
DEVIATION COMPUTATION ARE PERFORMED SIMULTANEOUSLY.

```

C
13 CONTINUE
  WRITE(6,17) FQ
17 FORMAT(1H1,T15,'( WAVE NUMBER =',F8.1,' )',///,6X,'WAVEN.',3X,
  * 'PRESS.',4X,'TEMP.',7X,'U',8X,'TRANSM. - T(COMP) = DIFF',6X,
  * 'DIFF**2',4X,'X-VALUE',/)
  DO 9 M=1,NDATA
    READ(5,10) KGAS,FQ,PRES,TEMP,UG,TX
10 FORMAT(I2,F10.3,E11.4,F9.3,24X,E11.4,F7.4)
    UG=UG/CF
    X=CLOG+AN*ALOG10(PRES/1013.)+AM*ALOG10(273.15/TEMP)+ALOG10(UG)
    DO 14 J=1,JM
      IF(X.LE.PW(J+1)) GO TO 15
14 CONTINUE
    J=IM
C
15 TC=EXP(-10**(A1(J)+A2(J)*X))
C
    D=TX-TC
    SD=D*D
    ST=ST+SD
    SDCUT(J)=SDCUT(J)+SD
    ICUT(J)=ICUT(J)+1
    WRITE(6,16) FQ,PRES,TEMP,UG,TX,TC,D,SD,X
16 FORMAT(1H ,3X,F8.1,F10.2,F9.2,E13.4,F9.4,F12.4,F13.6,E12.3,F9.3)
    9 CONTINUE
C
    END OF DATA READ-IN FOR THIS BAND.
    TOTAL STANDARD DEVIATIONS ARE COMPUTED AND PRINTED.
C
20 SSD=SSD+ST
    ITOTAL=ITOTAL+IFQ
    ST=SQRT(ST/FLOAT(IFQ))
    DO 21 I=1,IM
      SDTCUT(I)=SDTCUT(I)+SDCUT(I)
      ITCUT(I)=ITCUT(I)+ICUT(I)
21 SDCUT(I)=SQRT(SDCUT(I)/FLOAT(ICUT(I)))
    WRITE(6,22) (I,TSTD(I),TSTD(I+1),'CUT(I),SDCUT(I),I=1,IM)
22 FORMAT(1H0,///,T10,'CUTWISE STANDARD DEVIATION',//,T15,'#',T20,
  * '( FROM, TO ) ',T40,'# OF DATA',T53,'CUTWISE SD',//,(T14,I2,
  * T20,'(',F5.2,',',F5.2,')',T43,I4,T52,F10.6,/)
    WRITE(6,23) IFQ,ST
23 FORMAT(1H0,T10,'TOTAL # OF DATA FOR THIS BAND =',I5,9X,
  * ' STANDARD DEVIATION =',F12.6,/)
    GO TO 8
C
    END OF THE STANDARD DEVIATION COMPUTATION FOR ALL DATA.
    GRAND TOTAL STANDARD DEVIATION IS COMPUTED AND PRINTED OUT
    TOGETHER WITH VITAL INFORMATIONS.
C
30 SSD=SQRT(SSD/FLOAT(ITOTAL))
    DO 31 I=1,IM
      SDTCUT(I)=SQRT(SDTCUT(I)/FLOAT(ITCUT(I)))
31 WRITE(6,32) (I,TSTD(I),PW(I),TSTD(I+1),PW(I+1),A1(I),A2(I),
  * ITCUT(I),SDTCUT(I),I=1,IM)
32 FORMAT(1H1,T20,'*** PIECEWISE-ANALYTICAL STANDARD TRANSMISSION',

```

```

* ' FUNCTION ***',///,T10,'TOTAL CUTWISE STANDARD DEVIATION',//,
* T15,'CURVE #',3X,'FROM ( TAU ,X-VALUE) TO ( TAU ,X-VALUE)',
* ' WITH ( A1 , A2 )',3X,'# OF DATA',4X,'CUTWISE SD',//,
* (T18,I2,T30,'(,F6.3,' ,',F7.3,') (,F6.3,' ,',F7.3,')',T76,
* '(,F7.4,' ,',F7.4,')',7X,I3,5X,F10.6,/)
WRITE(6,33) ITOTAL,SSD
33 FORMAT(1H0,T10,'GLOBAL RESULTS',//,T15,'TOTAL NUMBER OF DATA',
* ' USED',I5,///,T15,'GLOBAL STANDARD DEVIATION',F12.6)

C
40 CONTINUE

C
C      END OF ALL COMPUTATION.
C      RESERVED TRUE VALUES OF THE FIRST AND LAST TSTD
C      AND PW ARE RETURNED.
C

TSTD(1)=TRES1
TSTD(NCUT)=TRES2
PW(1)=PWRES1
PW(NCUT)=PWRES2

C
CALL SDTAU

C
RETURN
END
SUBROUTINE INTPL2

C
C      COMPUTATION OF THE PIECEWISE-ANALYTICAL STANDARD TRANSMISSION
C      FUNCTION
C
C      VERSION 2 - 1
C      TAU=EXP(-10**((A1+A2*X+A3*X**2)))

COMMON /PARM1/ TSTD(12),PW(12),WN(6),CSTD(6),NCUT,NC,NAME(20),
* AN,AM,CF,ICONST(6),NEL
COMMON /PARM3/ A1(11),A2(11),A3(11)
DIMENSION T(10),TD(6,74),PD(6,74),JI(6,10),
* SDK(7),SDE(7,9),SUME(2,9),DE(6,9)
NWC=0
K=0
READ(5,2,END=80) FREQ,MAXDAT
IF(MAXDAT.GT.0) GO TO 3
80 CONTINUE
WRITE(6,99)
99 FORMAT(///,1H0,T5,'$$$ NO DATA FOR STANDARD DEVIATION COMPUTATION
* $$$')
GO TO 77
1 CONTINUE
READ(5,2,END=21) FREQ,MAXDAT
2 FORMAT(5X,F10.5,T41,I4)
IF(MAXDAT.EQ.0) GO TO 21
3 CLOG=1.E 10
DO 5 L=1,NC
IF(ABS(FREQ-WN(L)).LE. .01) CLOG=CSTD(L)
5 CONTINUE
IF(ABS(CLOG-1.E10).GE..01) GO TO 9
WRITE(6,100) FREQ

```



```

100 FORMAT('1',////////,' ERROR IN INPUT DATA ; WAVE NUMBER ',F10.3,
* ' NOT USED IN COMPUTATION OF CONSTANTS.')
DO 6 J=1,MAXDAT
  READ(5,101) KGAS,FREQ,PRES,TEMP,PPM,RANGE,UGAS,TX
6 CONTINUE
  GO TO 1
9 CONTINUE
  K=K+1
  NWC=NWC+1
  JI(K,1)=0
  JI(K,NCUT)=MAXDAT
  J=2
  DO 20 I=1,MAXDAT
    READ(5,101) KGAS,FREQ,PRES,TEMP,PPM,RANGE,UGAS,TX
101 FORMAT(I2,F10.3,E11.4,F9.3,E11.4,E13.6,E11.4,F7.4)
    TD(K,I)=TX
    PD(K,I)= AN *ALOG10(PRES/1013.)+ AM *ALOG10(273.15/TEMP)+ALOG10
    * (UGAS/CF)+CLOG
    IF(TD(K,I).GE.TSTD(J)) GO TO 20
    IF(J.EQ.NCUT) GO TO 20
    JI(K,J)=I-1
    J=J+1
20 CONTINUE
  GO TO 1
21 CONTINUE
  IF(NWC.LE.0) RETURN
  DO 30 J=1,NCUT
    T(J)=ALOG10(-ALOG(TSTD(J)))
30 CONTINUE
  SUMT=0.
  DT=0.0
  NCC=NCUT-1
  DO 45 I=1,NCC
    SA=0.
    TA=0.
    UA=0.
    DO 41 K=1,NWC
      SUME(K,I)=0.0
      M=JI(K,I)+1
      N=JI(K,I+1)
      DO 40 J=M,N
        TC=ALOG10(-ALOG(TD(K,J)))
        SA=SA+ TC *PW(I)*PW(I+1)*(PD(K,J)-PW(I))*(PD(K,J)-PW(I+1))
        TA=TA+((PD(K,J)-PW(I))*(PD(K,J)-PW(I+1))*((PD(K,J)**2)*(PW(I+1)
* *T(I)-PW(I)*T(I+1))+PD(K,J)*((PW(I)**2)*T(I+1)-(PW(I+1)**2)*T(I)
* )))/(PW(I)-PW(I+1))
        UA=UA+((PD(K,J)-PW(I))*(PD(K,J)-PW(I+1)))**2
40 CONTINUE
41 CONTINUE
    A1(I)=(SA-TA)/UA
    A3(I)=(T(I)-T(I+1))/(PW(I+1)*(PW(I)-PW(I+1)))-(T(I)-A1(I))/(PW(I)*
* PW(I+1))
    A2(I)=(T(I)-T(I+1))/(PW(I)-PW(I+1))-A3(I)*(PW(I)+PW(I+1))
    DI=0.
    SUMI=0.
    DO 44 K=1,NWC

```

```

M=JI(K,I)+1
N=JI(K,I+1)
DE(K,I)=FLOAT(1+N-M)
DO 43 J=M,N
  SUME(K,I)=SUME(K,I)+(TD(K,J)-EXP(-10.**(A3(I)*PD(K,J)*PD(K,J)+
*   A2(I)*PD(K,J)+A1(I))))**2
43 CONTINUE
  SDE(K,I)=SQRT(SUME(K,I)/DE(K,I))
  SUMI=SUMI+SUME(K,I)*FLOAT(ICONST(K))
  DI=DI+DE(K,I)*FLOAT(ICONST(K))
44 CONTINUE
  SUMT=SUMT+SUMI
  DT=DT+DI
  SDE(NWC+1,I)=SQRT(SUMI/DI)
45 CONTINUE
  DO 51 K=1,NWC
    SUMK=0.0
    DK=0.0
    DO 50 I=1,NCC
      SUMK=SUMK+SUME(K,I)
      DK=DK+DE(K,I)
50 CONTINUE
    SDK(K)=SQRT(SUMK/DK)
51 CONTINUE
    SDK(NWC+1)=SQRT(SUMT/DT)
    DUM1=PW(1)
    DUM2=PW(NCUT)
    DUM3=TSTD(1)
    DUM4=TSTD(NCUT)
    PW(1)=-1000000.
    PW(NCUT)=1000000.
    TSTD(1)=1.0
    TSTD(NCUT)=0.0
    DO 60 K=1,NWC
      WRITE(6,102)(NAME(J),J=1,20),WN(K),NCC,(I,TSTD(I),TSTD(I+1),PW(I),
* PW(I+1),A1(I),A2(I),A3(I),SDE(K,I),I=1,NCC)
102 FORMAT ('1',/,35X,'RENDITION OF EMPIRICAL TRANSMITTANCE FUNCTION
*FOR : ',/,20A4,/,40X,'WAVE NUMBER : ',F15.4,/,20X,'THE TRANSMI
*SSION CURVE IS DIVIDED INTO',I3,' SEPARATE CURVES.',/20X,'EACH CU
*RVE IS EXPRESSED BY A FUNCTION OF THE FORM " TAU = EXP(-10**(A3*P
*#*P+A2*P+A1)) ".',/20X, 'THE FUNCTION COEFFI
*CIENTS AND RESULTING STANDARD DEVIATION FOR EACH CURVE ARE AS FOL
*LOWS:',/,22X,'TAU',20X,'P',24X,'A1',13X,'A2',13X,'A3',11X,'STAND
*ARD DEVIATION',/, (5X,'CURVE #',I3,3X,'(',F4.2,'-',F4.2,')',5X,
* '(',F9.5,'-',F9.5,')',5X,3F15.6,6X,F15.6 /))
      WRITE(6,401) SDK(K)
401 FORMAT(1X,/,87X,'TOTAL STANDARD DEVIATION',F15.6)
60 CONTINUE
    K=K+1
    WRITE(6,104) (NAME(J),J=1,20),NCC, (I,TSTD(I),TSTD(I+1),PW(I),
* PW(I+1),A1(I),A2(I),A3(I),SDE(K,I),I=1,NCC)
104 FORMAT ('1',/,35X,'RENDITION OF EMPIRICAL TRANSMITTANCE FUNCTION
*FOR : ',/,20A4,/,40X,'TOTAL PROFILE AVERAGED OVER ALL WAVE NUMBER
*S',/,20X,'THE TRANSMI
*SSION CURVE IS DIVIDED INTO',I3,' SEPARATE CURVES.',/20X,'EACH CU
*RVE IS EXPRESSED BY A FUNCTION OF THE FORM " TAU = EXP(-10**(A3*P

```

```

      #*P+A2*P+A1)) ".',20X,          'THE FUNCTION COEFFI
      *CIENTS AND RESULTING STANDARD DEVIATION FOR EACH CURVE ARE AS FOL
      *LOWS:',///,22X,'TAU',20X,'P',24X,'A1',13X,'A2',13X,'A3',11X,'STAND
      *ARD DEVIATION',///, (5X,'CURVE #',I3,3X,'(',F4.2,'-',F4.2,')',5X,
      *(' ',F9.5,'-',F9.5,')',5X,3F15.6, 6X,F15.6 /))
      WRITE(6,402) SDK(K)
402  FORMAT(1X,/,81X,'GRAND TOTAL STANDARD DEVIATION',F15.6)
C   WRITE(7,201)(A1(I),A2(I),A3(I),I=1,NCC)
C 201  FORMAT(3F10.6)
C
      IDT=IFIX(DT)
      WRITE(6,225)IDT,NEL,SDK(K)
225  FORMAT(//,1H0,T15,'GRAND TOTAL # OF DATA =',I5,/,T15,'# OF',
      * ' ELIMINATED DATA =',I5,/,T15,'GLOBAL STANDARD DEVIATION IN',
      * ' TAU =',F12.6,/)
      DO 76 M=1,NWC
      IF(ICONST(M).EQ.1) GO TO 76
      WRITE(6,226) M
226  FORMAT(1H ,T15,'NOTE: THE BAND',I3,' IS NOT INCLUDED IN THE',
      * ' FINAL STANDARD DEVIATION')
76  CONTINUE
      PW(1)=DUM1
      PW(NCUT)=DUM2
      TSTD(1)=DUM3
      TSTD(NCUT)=DUM4
C
      CALL SDTAU
C
277  CONTINUE
      RETURN
      END
      SUBROUTINE SDTAU
C
C      COMPUTATIONS OF STANDARD DEVIATIONS IN TAU USING THE ORIGINAL
C      DATA USED IN MAIN
C
      DIMENSION NDATA(6),TSD(6),WWW(12,10),STANDV(12),P(10),T(10)
      COMMON /PARM1/ TSTD(12),PW(12),WN(6),CSTD(6),NCUT,NC,NAME(20),
      *              AN,AM,CF,ICONST(6),NEL
      COMMON /PARM2/ PRES(6,12,10),TEMP(6,12,10),UGAS(6,12,10),
      *              TAU(6,12),NTC(6),NLV(6)
      COMMON /PARM3/ A1(11),A2(11),A3(11)
C
      NGDATA=0
      GTSD=0.
      ICST=NC
      DO 70 M=1,NC
      JM=NTC(M)
      KM=NLV(M)
      NDATA(M)=JM*KM
      NGDATA=NGDATA+NDATA(M)*ICONST(M)
      TSD(M)=0.
      WRITE(6,214)
214  FORMAT('1',///// ,45X,'RECOMPUTATION OF TAU',///// )
      IF(M.GT.1) GO TO 77
      WRITE(6,215)

```

```

215 FORMAT(20X,'A TAU VALUE , T , IS RECOMPUTED FOR THE ORIGINAL DATA
* USING THE PIECEWISE-ANALITICAL TRANSMISSION FUNCTION.'//20X,
* 'STANDARD DEVIATIONS BETWEEN THE ACTUAL TAU AND THE RECOMPUTED',
* 'TAU VALUES ARE COMPUTED.'////)
77 CONTINUE
WRITE(6,202) M,WN(M),NTC(M),NLV(M)
202 FORMAT(1H0,T15,'*** CASE',I3,' (WAVE NUMBER =',F10.3,') ***',
* ///,T20,'TOTAL # OF CUTS' =',I3,///,T20,'TOTAL # OF LEVELS' =',I3,
* ///)
WRITE(6,216) AN,AM,M,CSTD(M)
216 FORMAT(10X,'N' =',F10.5,///10X,'M' =',F10.5,///,10X,'C',I1,' =',
* F10.5,////)
WRITE(6,217)
217 FORMAT(//,1H0,T7,'RECOMPUTED TAU AND STANDARD DEVIATIONS',
* ' IN TAU ',/,1H0,T2,'CUT',T11,'TAU',T20,'X*',T30,'X1',T39,
* 'X2',T48,'X3',T57,'X4',T66,'X5',T75,'X6',T84,'X7',T93,'X8',
* T102,'X9',T111,'X10',T121,'CUTWISE-SD',/)

```

C
C
C

COMPUTATION OF THE CUTWISE STANDARD DEVIATIONS IN X

```

DO 71 J=1,JM
WW=0.
DO 72 K=1,KM
P(K)=CSTD(M)+AN*PRES(M,J,K)+AM*TEMP(M,J,K)+UGAS(M,J,K)
IM=JM-1
DO 75 I=1,IM
IF(PW(I+1).GT.P(K)) GO TO 76
75 CONTINUE
I=IM
76 CONTINUE
T(K)=EXP(-10**(A3(I)*P(K)*P(K)+A2(I)*P(K)+A1(I)))
WWW(J,K)=(TAU(M,J)-T(K))**2
WW=WW+WWW(J,K)
72 CONTINUE
WW=SQRT(WW/FLOAT(KM))
WRITE(6,218) J,PW(J),TAU(M,J),(T(K),K=1,KM)
218 FORMAT(1H ,I5,F9.4,F9.4,1X,10F9.4)
WRITE(6,219) WW
219 FORMAT(1H+,T121,F10.5)
71 CONTINUE

```

C
C
C

COMPUTATION OF THE LEVELWISE STANDARD DEVIATIONS IN X

```

DO 73 K=1,KM
WW=0.
DO 74 J=1,JM
WW=WW+WWW(J,K)
74 CONTINUE
TSD(M)=TSD(M)+WW
STANDV(K)=SQRT(WW/FLOAT(JM))
73 CONTINUE
WRITE(6,220) (STANDV(K),K=1,KM)
220 FORMAT(1H0,T4,'LEVELWISE-SD :',T26,10F9.5)
GTSD=GTSD+TSD(M)*FLOAT(ICONST(M))
ICST=ICST-ICONST(M)
TSD(M)=SQRT(TSD(M)/FLOAT(NDATA(M)))

```

```

WRITE(6,221) TSD(M)
221 FORMAT(1H0,/,T15,'TOTAL STANDARD DEVIATION FOR THIS CASE  :',
* F15.6)
70 CONTINUE
GTSD=SQRT(GTSD/FLOAT(NGDATA))
WRITE(6,223) AN,AM
223 FORMAT('1',T15,'*** SUMMARY OF THE TRANSMITTANCE RECOMPUTATION *
* **',/,T20,'PRESSURE EXPONENT      N =',F10.5,/,T20,
* 'TEMPERATURE EXPONENT M =',F10.5,/,T5,'CASE #',3X,
* 'WAVE NUMBER',5X,'C-VALUE',5X,'TOTAL # OF DATA',3X,
* 'CASEWISE S.D. IN TAU')
WRITE(6,224) (M,WN(M),CSTD(M),NDATA(M),TSD(M),M=1,NC)
224 FORMAT(1H0,T6,I3,6X,F9.2,5X,F8.3,10X,I3,12X,F12.6)
WRITE(6,225) NGDATA,NEL,GTSD
225 FORMAT(/,1H0,T15,'GRAND TOTAL # OF DATA =',I5,/,T15,'# OF',
* ' ELIMINATED DATA =',I5,/,T15,'GLOBAL STANDARD DEVIATION IN',
* ' TAU =',F12.6,/)
IF(ICST.LE.0) RETURN
DO 78 M=1,NC
IF(ICONST(M).EQ.1) GO TO 78
WRITE(6,226) M
226 FORMAT(1H ,T15,'NOTE:  THE BAND',I3,' IS NOT INCLUDED IN THE',
* ' FINAL STANDARD DEVIATION')
78 CONTINUE
RETURN
END

```

```

C
C*****  COMPUTER CODE  SIMMIN  *****
C      VERSION ( 6 - 3 ) TRACE GASSES
C
C      COMPUTATION OF ABSORBER PARAMETERS AND ANALYTICAL STANDARD
C      TRANSMISSION FUNCTION
C
C      THIS CODE USES THE SUBROUTINE FMCG IN SSP LIBRARY
C
C      THIS CODE CONSISTS OF
C      MAIN:  DATA READ-IN AND CONTROL OF COMPUTATION
C      FUNCT:  COMPUTATION OF THE COST AND ITS DERIVATIVES
C      TITLE:  PRINTING OF HEADINGS AND INITIAL CONDITIONS
C      PRINT1: PRINTOUT OF RESULTS AND COMPUTATION/PRINTING OF S.D.S
C      NMBC:  COMPUTATION OF NON-MAJOR BANDS' C-VALUES
C
C      DATA SET-UP
C      1. INITIAL GUESSES  X(I)  (9 CARDS WITH T12,F10.7)
C          X(1)=A1, X(2)=A2, X(3)=A3, X(4)=N, X(5)=M, X(5+I)=LOG(C(I))
C          (NEED DUMMY INPUTS FOR PROBLEMS WITH DIMENSION < 9)
C      2. SIGNAL VARIABLES  S(I)  (9 CARDS WITH T12,F10.7)
C          S(I) = 0 ... X(I) IS KEPT CONSTANT
C          S(I) = 1 ... X(I) IS VARIED
C          (NEED DUMMY INPUTS FOR PROBLEMS WITH DIMENSION < 9)
C      3. COMMENT CARD  (20A4)  FOR TITLE AND ABSORBER TYPE ETC.
C      4. DATA SETS (MAX. 4 SETS) - ONE FOR EACH ABSORPTION BAND
C          EACH SET CONSISTS OF
C              1ST(CONTROL) CARD: WAVENUMBER, # OF DATA AND COMMENTS
C                                  (SEE FORMAT 101)
C              DATA CARDS: P, T, U, TAU ETC.
C                                  (SEE FORMAT 102)
C              (TOTAL # OF DATA SHOULD NOT EXCEED 900)
C      5. BLANK CARD - FOR THE TERMINATION OF DATA INPUT FOR MAIN
C      6. DATA SETS FOR NMBC - ONE FOR EACH ABSORPTION BAND
C          EACH SET CONSISTS OF
C              DATA CARDS:  SAME AS MAIN
C              FINAL CARD:  BLANK
C          TERMINATION  A CONTROL CARD WITH -1 IN FIRST TWO COLUMNS
C                      THIS COMES AFTER THE FINAL BLANK CARD
C                      (IF NO DATA BUT A BLANK CARD IS SUPPLIED, NMBC IS SKIPPED)
C
C      DIMENSION X(9),G(9),Y(9),H(72),WN(4)
C      COMMON /PARM1/ NC,ND(5),RW(4)
C      COMMON /PARM2/ IC,PLOG(900),TLOG(900),ULOG(900),TAU(900),S(9)
C      COMMON /PARM3/ P(900),T(900),U(900),L(20)
C      COMMON /PARM4/ PO,TO,NDIM,ID(5,9)
C      EXTERNAL FUNCT
C
C      CONSTANTS
C      PO=1.013E+03
C      TO=273.15
C      CF=2.69E+19
C      N=9
C      V=0.
C      IC=0
C      MAXNC=4

```

```

C
C      DATA INPUT
C
      READ(5,100) (X(I),I=1,N)
      READ(5,100) (S(I),I=1,N)
100  FORMAT (T12,F10.7)
C
C      COMMENT CARD (THIS INCLUDES THE ABSORBER TYPE)
C      READ(5,500) (L(I),I=1,20)
500  FORMAT(20A4)
C
C      NC = # OF MAJOR ABSORPTION BANDS
C      ND(1)=0, ND(2)=N1, ND(3)=N1+N2, ND(4)=N1+N2+N3, ...
C      WHERE N1, N2, N3, ... ARE #S OF DATA IN BANDS 1, 2, 3, ...
C      ND(NC+1)= TOTAL # OF DATA
C
      NC=0
      ND(1)=0
      DO 10 M=1,MAXNC
      READ(5,101) WN(M),IX,(ID(NC+1,I),I=1,9)
101  FORMAT(5X,F10.3,T41,I4,9A4)
      IF(IX.LE.0) GO TO 11
      NC=NC+1
      IM=ND(NC)+1
      IN=ND(NC)+IX
      ND(NC+1)=IN
      DO 12 I=IM,IN
      READ(5,102) P(I),T(I),U(I),TAU(I)
102  FORMAT (12X,E11.4,F9.3,24X,E11.4,F7.4)
      U(I)=U(I)/CF
C
C      DATA ARE CONVERTED TO THE LOG OF THE NORMALIZED VALUES
C
      PLOG(I)=ALOG10(P(I)/PO)
      TLOG(I)=ALOG10(TO/T(I))
      ULOG(I)=ALOG10(U(I))
C
      12 CONTINUE
      10 CONTINUE
      11 CONTINUE
C
C      END OF DATA INPUT
C
      IF(NC.GT.0) GO TO 13
      WRITE(6,110)
110  FORMAT (1H0,'ERROR IN DATA INPUT')
      GO TO 1000
      13 CONTINUE
C
      NDIM=0
      N=5+NC
      DO 14 I=1,N
      IF(S(I).NE.0.) NDIM=NDIM+1
14  CONTINUE
      DO 15 I=1,NC
      RW(I)=FLOAT(ND(NC+1))/(FLOAT(ND(I+1)-ND(I))*FLOAT(NC))

```

```

      RW(I)=1.0
15  CONTINUE
C
      DO 16 I=1,N
      Y(I)=X(I)
16  CONTINUE
C
      EST=1.E-6
      EPS=1.E-6
      LIMIT=1
      IER=0
C
C***** FMCG SEARCH ***** START *****
C
      CALL FMCG(FUNCT,N,X,V,G,EST,EPS,LIMIT,IER,H)
C
C***** FMCG SEARCH ***** END *****
C
      CALL TITLE(N,Y,LIMIT,EPS)
C
      CALL PRINT1(N,X,V,G,IER)
C
      CALL NMBC(X,L,NC,WN,CF,PO,TO)
C
1000 CONTINUE
      STOP
      END
      SUBROUTINE FUNCT(N,X,V,G)
C
C      COMPUTATION OF THE FUNCTION VALUE AND DERIVATIVES
C
C      (DOUBLE EXPONENTIAL FUNCTION)
C
      DIMENSION X(9),G(9),F(9)
      COMMON /PARM1/ NC,ND(5),RW(4)
      COMMON /PARM2/ IC,PLOG(900),TLOG(900),ULOG(900),TAU(900),S(9)
C
      IC=IC+1
      V=0.
      DO 20 K=1,N
      G(K)=0.
20  CONTINUE
C
      DO 21 J=1,NC
      JJ=J+5
      SQER=0.
      DO 22 L=1,5
      F(L)=0.
22  CONTINUE
      F(JJ)=0.
      IM=ND(J)+1
      IN=ND(J+1)
      DO 23 I=IM,IN
      W1=X(JJ)+X(4)*PLOG(I)+X(5)*TLOG(I)+ULOG(I)
      R=X(1)+X(2)*W1+X(3)*W1*W1
      R=10.**R

```



```

      IF(R.LE.70.) GO TO 24
      TC=0.
      GO TO 25
24  CONTINUE
      TC=EXP(-R)
25  CONTINUE
      E=TAU(I)-TC
      R=R*E*TC
      SQER=SQER+E**2
      F(1)=F(1)+R
      F(2)=F(2)+R*W1
      F(3)=F(3)+R*W1*W1
      R=R*(X(2)+2.*X(3)*W1)
      F(4)=F(4)+R*PLOG(I)
      F(5)=F(5)+R*TLOG(I)
      F(JJ)=F(JJ)+R
23  CONTINUE
      V=V+SQER*RW(J)
      DO 26 K=1,5
      G(K)=G(K)+F(K)*RW(J)
26  CONTINUE
      G(JJ)=F(JJ)*RW(J)
21  CONTINUE
C
      DO 27 I=1,N
      G(I)=4.60517*G(I)*S(I)
27  CONTINUE
C
      RETURN
      END
      SUBROUTINE TITLE(N,X,LIMIT,EPS)
C
C      PRINTING OF THE TITLE AND INITIAL VALUES
C
      DIMENSION X(9),L(4)
      COMMON /PARM1/ NC,ND(5),RW(4)
      COMMON /PARM4/ PO,TO,NDIM,ID(5,9)
C
      DO 40 I=1,NC
      L(I)=ND(I+1)-ND(I)
40  CONTINUE
C
      CALL DATE (MONTH,IDAY,IYEAR)
      WRITE(6,111)MONTH,IDAY,IYEAR
111  FORMAT(1H1,T60,I4,' / ',I2,' / ',I2,/)
      WRITE(6,400) NC,NDIM
400  FORMAT (1H ,T14,'*** SIMULTANEOUS PARAMETER EVALUATION ***',///,
* ' PARAMETERS : ( N , M , A1 , A2 , A3 , C(I), I=1,',I2,' )',
* 8X,'( DIMENSION =',I3,' )',///,' DATA :')
      WRITE(6,401) ((ID(K,J),J=1,9),L(K),K=1,NC)
401  FORMAT(1H+,T11,'(',9A4,' )',5X,'# OF POINTS =',I5,/)
C
      WRITE(6,402) ND(NC+1),PO,TO,LIMIT,EPS
402  FORMAT (1H+,T51,'TOTAL # OF DATA =',I5,///,
* ' FUNCTION : TAU ( W ) = EXP ( -10 ** ( A1 + A2 * W +',
* ' A3 * W**2 + A4 * W**3 ) )',//,T15,'WHERE, ',

```

```

* ' W = LOG(C) + LOG( U * (P/PO)**N * (TO/T)**M ) ',
* ' , A4 = 0. ', ///,
* ' CONSTANTS : PO = ',F8.2,7X,'TO = ',F8.2,7X,
* ' LIMIT = ',I5,7X,'EPS = ',1PE10.1,/)

```

C

```

IF(NC.EQ.1) WRITE(6,403) X(1),X(6),X(2),X(3),X(4),X(5)
IF(NC.EQ.2) WRITE(6,404) X(1),X(6),RW(1),X(2),X(7),RW(2),X(3),
* X(4),X(5)
IF(NC.EQ.3) WRITE(6,405) X(1),X(6),RW(1),X(2),X(7),RW(2),X(3),
* X(8),RW(3),X(4),X(5)
IF(NC.EQ.4) WRITE(6,406) X(1),X(6),RW(1),X(2),X(7),RW(2),X(3),
* X(8),RW(3),X(4),X(9),RW(4),X(5)
403 FORMAT (1H0,'INITIAL VALUES : ',T22,'A1 = ',F12.7,9X,'LOG(C1) = ',
* F12.7,/,T22,'A2 = ',F12.7,/,T22,'A3 = ',F12.7,/,T22,'N = ',
* F12.7,/,T22,'M = ',F12.7,/)
404 FORMAT (1H0,'INITIAL VALUES : ',T22,'A1 = ',F12.7,9X,'LOG(C1) = ',
* F12.7,4X,'( WEIGHT = ',F8.4,' )',/,T22,'A2 = ',F12.7,9X,
* 'LOG(C2) = ',F12.7,4X,'( WEIGHT = ',F8.4,' )',/,T22,'A3 = ',
* F12.7,/,T22,'N = ',F12.7,/,T22,'M = ',F12.7,/)
405 FORMAT (1H0,'INITIAL VALUES : ',T22,'A1 = ',F12.7,9X,'LOG(C1) = ',
* F12.7,4X,'( WEIGHT = ',F8.4,' )',/,T22,'A2 = ',F12.7,9X,
* 'LOG(C2) = ',F12.7,4X,'( WEIGHT = ',F8.4,' )',/,T22,'A3 = ',
* F12.7,9X,'LOG(C3) = ',F12.7,4X,'( WEIGHT = ',F8.4,' )',/,T22,
* 'N = ',F12.7,/,T22,'M = ',F12.7,/)
406 FORMAT (1H0,'INITIAL VALUES : ',T22,'A1 = ',F12.7,9X,'LOG(C1) = ',
* F12.7,4X,'( WEIGHT = ',F8.4,' )',/,T22,'A2 = ',F12.7,9X,
* 'LOG(C2) = ',F12.7,4X,'( WEIGHT = ',F8.4,' )',/,T22,'A3 = ',
* F12.7,9X,'LOG(C3) = ',F12.7,4X,'( WEIGHT = ',F8.4,' )',/,T22,
* 'N = ',F12.7,9X,'LOG(C4) = ',F12.7,4X,'( WEIGHT = ',F8.4,' )',/,
* T22,'M = ',F12.7,/)

```

C

```

RETURN
END
SUBROUTINE PRINT1(N,X,V,G,IER)

```

C

C

C

C

```

PRINTING OF THE RESULTS AND COMPUTATION/PRINTING OF ERRORS
AND STANDARD DEVIATIONS

```

```

DIMENSION X(9),G(9),E(900),PD(900),TC(900),W(900)
COMMON /PARM1/ NC,ND(5),RW(4)
COMMON /PARM2/ IC,PLOG(900),TLOG(900),ULOG(900),TAU(900),S(9)
COMMON /PARM3/ P(900),T(900),U(900),L(20)
COMMON /PARM4/ PO,TO,NDIM,ID(5,9)
EQUIVALENCE (E,PLOG),(PD,TLOG),(TC,ULOG)

```

C

C

C

```

EQUIVALENCE IS FOR SPACE CONSERVATION

```

```

IT=0
TTD=0.
TV=0.
V=SQRT(V/FLOAT(ND(NC+1)))

```

C

```

WRITE(6,510) IER,IC,(X(I),G(I),I=1,5)
510 FORMAT (1H0,'** RESULTS OF COMPUTATION : IER = ',I3,4X,
* 'SUBROUTINE FUNCT WAS CALLED',I6,' TIMES **',
* '///, ' FINAL VALUES AND GRADIENTS : ',

```

```

* T35,'A1      =',F12.7,T65,'D/D(A1)      =',E15.6,/,/,
* T35,'A2      =',F12.7,T65,'D/D(A2)      =',E15.6,/,/,
* T35,'A3      =',F12.7,T65,'D/D(A3)      =',E15.6,/,/,
* T35,'N       =',F12.7,T65,'D/D(N)       =',E15.6,/,/,
* T35,'M       =',F12.7,T65,'D/D(M)       =',E15.6)
WRITE(6,511) (I,X(I+5),I,G(I+5),I=1,NC)
511 FORMAT(1H0,T35,'LOG(C',I1,')=',F12.7,T65,'D/D(LOG(C',I1,'))=',
* E15.6)
WRITE(6,512) V
512 FORMAT(/,1H0,'FINAL STANDARD DEVIATION  : ',F15.7)
C
WRITE(6,513) (L(I),I=1,20)
513 FORMAT(1H0,T5,'( COMMENT : ',20A4,' )')
C
DO 50 J=1,NC
JJ=J+5
V=0.
TD=0.
IM=ND(J)+1
IN=ND(J+1)
K=ND(J+1)-ND(J)
RK=FLOAT(K)
C
DO 51 I=IM,IN
W(I)=X(JJ)+X(4)*PLOG(I)+X(5)*TLOG(I)+ULOG(I)
R=10.**((X(1)+X(2)*W(I)+X(3)*W(I)**2)
IF(R.LE.70) GO TO 52
TC(I)=0.
GO TO 53
52 CONTINUE
TC(I)=EXP(-R)
53 CONTINUE
E(I)=TAU(I)-TC(I)
PD(I)=100.*E(I)/TAU(I)
TD=TD+ABS(E(I))
V=V+E(I)**2
51 CONTINUE
C
TTD=TTD+TD
TV=TV+V
TD=TD/RK
V=V/RK
SF=SQRT(V)
WRITE(6,514) (ID(J,I),I=1,9),K,(X(I),I=1,5),J,X(JJ),TD,V,SF
514 FORMAT (1H1,T15,'ACTUAL/COMPUTED TRANSMITTANCES',/,/,/,
* T10,'DATA  : ',9A4,5X,'# OF POINTS =',I4,/,/,/,T10,
* 'A1 =',F12.7,8X,'A2 =',F12.7,8X,'A3 =',F12.7,/,/,T10,'N  =',F12.7,
* 8X,'M  =',F12.7,8X,'LOG(C',I1,') =',F12.7,/,/,/,
* T15,'AVERAGE DISCREPANCY =',F12.7,/,/,
* T15,'MEAN SQUARE ERROR   =',F12.7,/,/,
* T15,'STANDARD DEVIATION  =',F12.7,/,/,/,
* T5,'# ',T11,'U =',T26,'P =',T36,'T =',T46,'X =',T56,'ACTUAL',
* T65,'COMPUTED',T76,'DIFFERENCE',T90,'% DIFF.',/)
WRITE(6,515) (I,U(I),P(I),T(I),W(I),TAU(I),TC(I),E(I),PD(I),
* I=IM,IN)
515 FORMAT (1H ,I5,T10,E11.4,T24,F8.2,T34,F8.2,T43,F9.4,T53,F9.4,T63,

```

```

      * F9.4,T74,F11.6,T87,F10.4)
50 CONTINUE
C
      FK=FLOAT(ND(NC+1))
      TTD=TTD/FK
      TV=TV/FK
      TSD=SQRT(TV)
      WRITE(6,516) ND(NC+1),TTD,TV,TSD
516 FORMAT (1H1,///,T10,'TOTAL # OF POINTS USED           =',I6,///,T10,
      * 'GLOBAL AVERAGE DISCREPANCY      =',F12.7,///,T10,
      * 'GLOBAL MEAN SQUARE ERROR        =',F12.7,///,T10,
      * 'GLOBAL STANDARD DEVIATION       =',F12.7)
      RETURN
      END
      SUBROUTINE NMBC(X,NAME,NC,WN,CF,PO,TO)
C
C      COMPUTATION OF THE C'-VALUES FOR NON-MAJOR BANDS
C
      DIMENSION X(9),NAME(20),WN(4)
      DIMENSION CS(10),FS(10)
      DF=1.E30
      SGN=1.
      IF(X(3).LT.0.) SGN=-1.
C
C      IF THE QUADRATIC TERM IS TOO SMALL, THEN IT WILL BE IGNORED
C
      SMI=-2.*X(3)/X(2)
      IF(ABS(SMI).LE.1.E-6) GO TO 50
      SYM=1./SMI
50 CONTINUE
C
      WRITE(6.5)(NAME(I),I=1,20)
5  FORMAT(1H1,T15,20A4)
      WRITE(6,10)
10 FORMAT(1H0,T15,' *** CALCULATION OF THE SPECTRAL PARAMETER FOR',
      * ' NON-MAJOR BANDS ***',///)
C
11 CONTINUE
      NFREQ=0
12 CONTINUE
      C=0.
      I=0
15 CONTINUE
      READ(5,20,END=40) KGAS,FREQ,P,T,UGAS,TX
20 FORMAT(I2,F10.3,E11.4,F9.3,24X,E11.4,F7.4)
      IF(KGAS.EQ.0) GO TO 25
      IF(KGAS.LT.0) GO TO 35
      IF(UGAS.GE.DF) GO TO 15
C
      I=I+1
      WX=FREQ
      UGAS=UGAS/CF
      IF(SMI.LE.1.E-6) GO TO 51
C
C      CASE 1 QUADRATIC TERM IS LARGE AND USED
C

```

AD-A081 789

TEXAS UNIV AT EL PASO SCHELLENGER RESEARCH LABS

F/8 7/4

COMPUTERIZED METHOD FOR THE GENERATION OF MOLECULAR TRANSMITTAN--ETC(U)

DEC 79 J H PIERLUISSI, K TOMIYAMA

DAA629-79-C-0067

UNCLASSIFIED

FR1-79-UA-72

ARO-16641.1-65

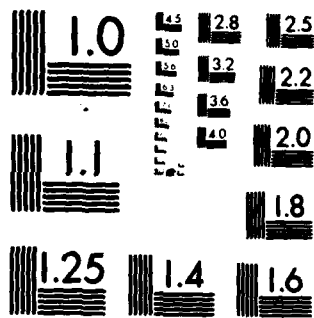
NL

3 - 3

2-10-79



END	END
DATE	DATE
FORMED	FORMED
4 80	4 80
DTIC	DTIC



MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS-1963-A

```

XS=SYM+SGN*ABS(SQRT(X(2)**2-4.*X(3)*(X(1)-ALOG10(-ALOG(TX))))
* /(2.*X(3)))
GO TO 52
51 CONTINUE

```

C
C
C

CASE 2 QUADRATIC TERM IS SMALL AND IGNORED

```

XS=(ALOG10(-ALOG(TX))-X(1))/X(2)
52 CONTINUE
XC=X(4)*ALOG10(P/P0)+X(5)*ALOG10(T0/T)+ALOG10(UGAS)
C=C+(XS-XC)
GO TO 15

```

C

```

25 C=C/FLOAT(I)
NFREQ=NFREQ+1
CS(NFREQ)=C
FS(NFREQ)=WX
DO 27 M=1,NC
IF(ABS(WX-WN(M)).LE.0.1) CS(NFREQ)=X(5+M)
27 CONTINUE
IF(NFREQ.EQ.10) GO TO 30
GO TO 12
30 CONTINUE
WRITE(6,31)(FS(K),K=1,NFREQ)
31 FORMAT(1H0,2X,'WAVE NUMBER',2X,10F11.0)
WRITE(6,32)(CS(K),K=1,NFREQ)
32 FORMAT(1H0,5X,'C VALUES',2X,10F11.3//)
GO TO 11

```

C

```

35 CONTINUE
IF(NFREQ.EQ.0) GO TO 40
WRITE(6,31)(FS(K),K=1,NFREQ)
WRITE(6,32)(CS(K),K=1,NFREQ)
40 CONTINUE
RETURN
END

```