AN INVESTIGATION OF A MATHEMATICAL MODEL FOR ATMOSPHERIC ABSORPTION SPECTRA

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ABSTRACT

A computer program that calculates absorption spectra for slant paths through the atmosphere is described. The program uses an efficient convolution technique (Romberg integration) to simulate instrument resolution effects. A brief information analysis is performed on a set of calculated spectra to illustrate how such techniques may be used to explore the quality of the information in a spectrum.
I. INTRODUCTION

Radiation which has passed through and been modified by the atmosphere contains a wealth of information about atmospheric conditions. This includes information about the temperature and density structure of the atmosphere as well as the abundance and distribution of constituent gases and aerosols. In order to retrieve this information, however, an accurate model is needed which describes the dependence of absorption spectra on the atmospheric conditions and on the instrument characteristics. The first dependence has received considerable attention, both theoretical and computational, but the second has received much less. Equivalent width techniques and transmittance averaging are common ways of extracting information from spectra when instrument effects are unknown or poorly understood. However, because these effects mask underlying atmospheric effects, knowledge of the instrument behavior, when properly included in the data analysis, allows extraction of more detailed information than can be obtained in the absence of such knowledge.

Nonlinear least-squares is one data analysis technique which can include all relevant influences on the data. It involves a great deal of computation, however, so efficient computer codes must be developed in order to take advantage of the least-squares techniques. This report describes a program for calculating absorption spectra that was specifically written to efficiently include instrument effects. It is therefore suitable for use in least-squares analysis.

In constructing a model for any experiment it is important to know what type of information the experimental data are likely to contain. Such knowledge allows the level of sophistication for the model to be balanced between computational complexity and interpretative accuracy. The third chapter of this report addresses this question and illustrates a variety of simple techniques for information analysis with a set of atmospheric absorption spectra.
II. FUNDAMENTALS OF ATMOSPHERIC TRANSMITTANCE

A beam of radiation propagating through the atmosphere is modified through the action of many different processes. Among these are scattering, reflection, refraction, polarization changes, atmospheric emission, and absorption. This report is only concerned with the modifications due to refraction and absorption by gas molecules in the atmosphere, and, in particular, that portion of the absorption due to rotational and vibrational transitions of the molecules. Each transition has associated with it a frequency position, width, intensity and profile. The Voigt profile\(^2,3,4\) is assumed throughout this report, although other shapes can be incorporated if desired.

A. HOMOGENEOUS PATHS

If radiation with a spectral irradiance \(E(\nu)\) is incident on a homogeneous gas sample, the spectral radiant exitance \(M(\nu)\) is given by

\[
M(\nu) = E(\nu) \cdot \tau(\nu) ,
\]

where \(\nu\) is the frequency of the radiation measured in \(\text{cm}^{-1}\). The modifying factor, \(\tau(\nu)\), in Eq. (1) is called the spectral transmittance, which is referred to simply as transmittance in this report, it being understood that the transmittance is a function of frequency.

For a narrow homogeneous sample of thickness \(d\xi\), Bouguer's law\(^5\) states that the radiation lost in the sample is linear in \(E(\nu)\) and \(d\xi\). Beer's law\(^6\) states that the radiation lost is also linear in the concentration \(N\) of the absorber, so that

\[
dE(\nu,\xi) = -k(\nu) E(\nu,\xi) N d\xi ,
\]

where \(k(\nu)\) is called the absorption coefficient. When \(N\) is measured in molecules/cm\(^3\) and \(d\xi\) in cm, \(k(\nu)\) is measured in cm\(^2\)/molecule. When \(N\) is independent of path length, Eq. (2) can be integrated over the entire path length, \(L\), through the sample to give

\[
M(\nu) = E(\nu,L) = E(\nu,0) \exp[-k(\nu) NL] .
\]

Consequently, the transmittance is given by

\[
\tau(\nu) = \exp[-k(\nu) NL] .
\]

Equation (2) is based on independent absorption by each absorbing molecule. It does not apply to self-broadening absorption, therefore, in which \(k\) can also depend on \(N\). The factor in the exponential of Eq. (4) is called the absorbance.

If there are \(M\) different absorbers with concentrations \(N_1, N_2, \ldots, N_M\) independently absorbing in the sample, the total absorbance \(A(\nu)\) is
A(\nu) = \sum_{m=1}^{M} N_m k_m(\nu) L , \quad (5)

where \( k_m(\nu) \) is the absorption coefficient for the \( m \)th absorber. As stated above, this report assumes that the absorption is due to many individual absorption lines, each with absorption coefficient \( k_{mj}(\nu) \). Consequently Eq. (5) becomes

\[
A(\nu) = L \cdot \sum_{m=1}^{M} N_m \cdot \sum_{j=1}^{J_m} k_{mj}(\nu) , \quad (5b)
\]

where \( J_m \) is the total number of lines for the \( m \)th absorber.

B. ATMOSPHERIC PATHS

Radiation paths in the atmosphere are usually not homogeneous. For such paths, Eq. (2) can still be integrated to give \( E \) as a function of path length, provided the variation of \( k \) and \( N \) with path length is known. The analog of Eq. (5) for atmospheric paths is

\[
A(\nu) = \int_0^L \sum_{m=1}^{M} N_m(\ell) \sum_{j=1}^{J_m} k_{mj}(\nu, \ell) \, d\ell . \quad (6)
\]

It is convenient to define the mixing ratio \( a_m(\ell) \) for the \( m \)th absorber as

\[
a_m(\ell) = \frac{N_m(\ell)}{\bar{N}(\ell)} ,
\]

where \( \bar{N}(\ell) \) is the mean density of the atmosphere as a function of path length.

Defining a new variable \( u(\ell) \), the so-called airmass along the path, by

\[
du \equiv \bar{N}(\ell) \, d\ell ,
\]

Eq. (6) becomes

\[
A(\nu) = \int_0^U \sum_{m=1}^{M} a_m(u) \sum_{j=1}^{J_m} k_{mj}(\nu, u) \, du , \quad (7)
\]

where

\[
U = \int_0^L \bar{N}(\ell) \, d\ell
\]

is the total airmass of the path.
C. REFRACTION EFFECTS

This report uses a program written by Treve\textsuperscript{7,8} and Snider\textsuperscript{9} to determine the path of radiation through the atmosphere. The necessary geometry is shown in Fig. 1, assuming that the sun is the radiation source. The observer is at a height $H_0$ above the surface of the earth at latitude $\phi$. The direction of propagation of the radiation makes an angle $\theta'$ with the observer's local zenith. A straight line drawn from the observer to the source makes an angle $\theta$ with the local zenith and has a minimum height $H_{\text{min}}$ above the surface of the earth. Because of refraction, the true radiation path is not straight and has a different minimum height $H'_{\text{min}}$. The actual path taken by the radiation depends on the density profile of the atmosphere as a function of height. This profile is calculated by the program from an input temperature profile and base level pressure by integrating the hydrostatic equation and assuming an ideal gas law for the relationship between pressure, temperature, and density.\textsuperscript{10} The input profile is in the form of many thin atmospheric layers. The program uses Snell's law and the Lorentz-Lorenz relation to perform a ray-tracing through the layers. The output consists of a series of airmass values, effective temperatures, and pressures, one for each layer crossed by the ray.

In order to use these to calculate the spectrum, the integral in Eq. (7) is approximated by a sum according to

$$A(v) = \int_0^U \sum_{m=1}^M \sum_{j=1}^{J_m} a_m(u) k_{mj}(v,u) \, du$$

$$= \sum_{i=1}^{I_L} \sum_{m=1}^{M} \sum_{j=1}^{J_m} \left[ a_m k_{mj}(v) \right]_i \Delta u_i ,$$

where $I_L$ is the number of terms in the sum which replaces the integral in Eq. (7).

The form of $[a_m k_{mj}(v)]_i$ is determined by assuming that the product $a_m(u) k_{mj}(v,u)$ for fixed $v$ can be written as a function of the pressure $P(u)$ and temperature $T(u)$ along the path. We therefore write

$$\int a_m(u) k_{mj}(v,u) \, du = \int f[P(u), T(u)] \, du .$$

Expanding $f$ in a Taylor series about some value, $P_0, T_0$,

$$f(P,T) = f(P_0, T_0) + \frac{\partial f}{\partial P} \bigg|_{P_0, T_0} (P - P_0) + \frac{\partial f}{\partial T} \bigg|_{P_0, T_0} (T - T_0) + \text{[second-order terms]} .$$

Substituting this expression into the integral
θ = "true" or astronomical zenith angle
θ' = apparent zenith angle
$H_{ob}$ = observer height
$H'_{min}$ = unrefracted minimum height
$H_{min}$ = true minimum height
$R(\phi)$ = radius of earth at latitude $\phi$

Fig. 1 - Observer-source geometry
\[
\int f[P(u), T(u)] \, du = f(P_0, T_0) \int du \\
+ \frac{\partial f}{\partial P} \left\{ \int (P - P_0) \, du \right\} + \frac{\partial f}{\partial T} \left\{ \int [T(u) - T_0] \, du \right\} \\
+ \{ \text{second-order terms} \} \\
= \left[ f(P_0, T_0) + \right. \\
\left. \frac{\partial f}{\partial P} \left( \bar{P} - P_0 \right) + \frac{\partial f}{\partial T} \left( \bar{T} - T_0 \right) \right] \\
+ \{ \text{second-order terms} \} \int du ,
\]

where

\[
\bar{P} = \int P(u) \, du / \int du \\
\bar{T} = \int T(u) \, du / \int du .
\]

But the expression in the brackets, to first-order, is just \( f(\bar{P}, \bar{T}) \). Consequently, provided the variation of \( P(u) \) and \( T(u) \) is sufficiently small that the first-order terms in the Taylor series are adequate, we may write

\[
\int f[P(u), T(u)] \, du \approx f(\bar{P}, \bar{T}) \Delta u ,
\]

where \( \bar{P} \) and \( \bar{T} \) are defined as in Eq. (9).

If the atmospheric layers are sufficiently thin, we are therefore justified in replacing the integral in Eq. (7) with the sum in Eq. (8) provided

\[
\left[ a_n k_m (\nu) \right] = a_m (\bar{P}_1, \bar{T}_1) k_m (\bar{P}_1, \bar{T}_1, \nu) ,
\]

where

\[
\bar{P}_1 = \int P(u) \, du / \Delta u_i \\
\text{layer } 1
\]

and

\[
\bar{T}_1 = \int T(u) \, du / \Delta u_i .
\]

layer 1
Equations (11) and (12) are close to the familiar scaling approximations. The same argument applies to any other variables that effect the $a \cdot k$ product (such as mixing ratio dependence in $k$). One can therefore approximate the inhomogeneous atmosphere with a series of homogeneous layers whose properties are given by averages over the true inhomogeneous variation.

D. LINE SHAPE

As stated above, this report assumes that the absorption coefficient $k_{mj}(v)$ follows the Voigt profile. This profile combines the effects of collision broadening (which is dominant in the troposphere) and Doppler broadening (which is dominant in the upper stratosphere). It is given by

$$k_{mj}(v,P,T) = k_{0mj} \frac{y}{\pi} \int_{-\infty}^{\infty} \frac{\exp(-t^2)}{y^2 + (x - t)^2} dt,$$

where

$$k_{0mj} = \frac{S_{im}}{\alpha_D} \frac{\sqrt{n_j^2/\pi}}{n},$$

$$y = \frac{\alpha_D}{\alpha_D} \sqrt{n_j^2},$$ and

$$x = \frac{v - v_{0mj}}{\alpha_D} \sqrt{n_j^2}.$$

The line intensity $S_{jm}$ is defined as $S_{jm} = \int_0^\infty k_{jm}(v) \, dv$.

From Quantum Mechanics, this quantity is given by

$$S_{jm} = \frac{g \alpha^2 v_{0jm}}{3hc} \frac{g''(1 - e^{-hcv_{0jm}/kT})}{Q_m(T)} \exp\left(-\frac{E_m}{kT}\right) \cdot |\langle \psi_j^m | \bar{n} | \psi_j^m \rangle|^2.$$ 

In this expression, $v_{0jm}$ is the line center frequency for the $mj$th line with lower state energy $E_m^j$ and upper state energy $E_m^u = hc\nu_{0jm} + F_m^u$. $g''$ is the degeneracy of the lower state and $Q_m(T)$ is the partition function. In the infrared, the expression $\frac{1 - \exp(-hcv_{0jm}/kT)}{Q_m(T)}$ can usually be approximated by $1/Q_{rot}(T)$ where $Q_{rot}(T)$, the rotational partition function, is proportional to $T^{3/2}$ for linear molecules such as CO, N$_2$O, CO$_2$, and NO. It is proportional to $T^3$ for molecules like O$_3$, H$_2$O, and CH$_4$. The term $|\langle \psi_j^m | \bar{n} | \psi_j^m \rangle|^2$ is the square of the dipole matrix element.
The temperature dependence of \( S_{jm} \) is made explicit by writing it as

\[
S_{jm} = S_{0jm} \left( \frac{T_0}{T} \right)^\beta \exp\left[-\frac{E_{nm}}{kT_0} (T_0 - T) / 0.6946TT_0 \right],
\]

(15)

where \( \beta = 1 \) or \( 3/2 \) depending on the molecular structure. The above expression assumes that \( E \) is measured in cm\(^{-1} \) and \( T \) in Kelvin. \( S_{0jm} \) is the value of \( S_{jm} \) at some standard temperature, \( T_0 \).

The quantities \( \alpha_L \) and \( \alpha_D \) in Eq. (13) are the Lorentz width and Doppler width of the line, respectively. These are given by

\[
\alpha_D = \frac{\nu_{0m1}}{\epsilon} \sqrt{\frac{2kT \ln^2 e}{M_m}},
\]

and

\[
\alpha_L = \frac{\nu_{0m1}}{\epsilon} \frac{T_0}{T} \left( \frac{P_0}{P} \right)^\gamma.
\]

\( M_m \) is the mass of molecular species \( m \); \( \omega_{0m1} \) is the Lorentz width at some standard temperature and pressure, \( T_0 \) and \( P_0 \); and \( \gamma \) is an empirical term describing the temperature dependence of \( \alpha_L \). This report makes the standard assumption that \( \gamma = 1/2 \) although other values are often more accurate for bands of specific molecules. The necessary line parameters were taken from the AFGL line listing.

E. INSTRUMENT EFFECTS

When Eq. (13) and (8) are combined, they constitute a mathematical model for the frequency make-up of a beam of radiation as it propagates through the atmosphere. Since real spectrometers have finite resolution, the signal observed at frequency setting \( \nu \) is a weighted sum of the radiation incident on the instrument. This is described by writing

\[
\tau_{\text{con}}(\nu) = \int_0^\infty \sigma(\nu, \nu') \tau_{\text{mon}}(\nu') \, d\nu',
\]

(17)

where \( \tau_{\text{con}}(\nu) \) is the observed transmittance, \( \tau_{\text{mon}}(\nu') \) is the monochromatic transmittance, and \( \sigma(\nu, \nu') \) is the instrument spectral response function (or "slit" function) with

\[
\int_0^\infty \sigma(\nu, \nu') \, d\nu' = 1.
\]

It is often assumed that \( \sigma \) can be written as a function of \( (\nu - \nu') \), and many different forms are used. For grating instruments, triangular and Gaussian shapes are common, and for interferometers sinc, sinc\(^2\), and various Bessel functions have been tried, depending upon the apodization.

When calculated and observed spectra are to be compared visually, the exact form of \( \sigma \) is often unimportant. However, when more sensitive
techniques, such as least-squares analysis, are used, instrument effects must be modeled with a precision at least better than the precision of the observed spectral values. This imposes an additional set of computational restrictions on spectrum calculation routines, especially when the convolution integral in Eq. (17) must be evaluated numerically, as is usually the case. While considerable effort has gone into devising efficient algorithms for calculating monochromatic transmittances, little work seems to have been done on the special problems associated with calculating convolved transmittances.

Since one of the problems this report seeks to address is the applicability of least-squares data analysis to atmospheric transmission spectra, the precision of convolved transmittances has been a central concern from the start. To see how this concern dictates the overall calculation strategy, consider how Eq. (17) is evaluated in practice. Because of the complex frequency dependence of \( \tau(v') \), the integral must be evaluated numerically; i.e., replaced by a weighted sum. Each term in the sum requires a value of \( \tau_{\text{mon}} \) and one of \( \sigma \). If \( N_C \) is the number of terms in the sum and \( N_S \) is the number of observed spectral values, then \( N_C \times N_S \) monochromatic transmittance values are needed to calculate the convolved transmittance, \( \tau_{\text{con}} \).

A typical frequency position may have contributions from 20 different lines and require 20 atmospheric layers to model the atmosphere (Mankin\(^{17}\) used \( \sim 1000 \) lines over a 10 cm\(^{-1} \) region; Snider and Goldman\(^{10}\) used 197 layers). In addition, if the resolution is \( \delta v_R \) a typical frequency spacing for observed spectra is \( \delta v_R/2 \). Consequently for a 200 cm\(^{-1} \)-long spectrum at moderate resolution, \( \delta v_R = 0.10 \text{ cm}^{-1} \) (some interferometers have 10 times better resolution), a total of 4000 observed points must be calculated. Assuming that the most time-consuming part of the calculation is the evaluation of the Voigt profile, a total of \( N_C \times 20 \times 20 \times 4000 = 1.6 \times 10^8 N_C \) Voigt evaluations must be performed. Running time is dependent on machine characteristics, but Pierluissi and Vanderwood\(^{18}\) quote a time of \( \sim 3 \) seconds for 100 evaluations on an IBM 360/65. This gives \( 4.8 \times 10^4 \times N_C \) seconds of CPU time in the Voigt routine alone. Clearly \( N_C \) must be made as small as possible.

1. Convolution Strategies

The numerical evaluation of the integral in Eq. (17) is represented schematically in Fig. 2. To each observed frequency position \( v_i \) there corresponds a set of frequency positions \( \{v'\}_i \) at which monochromatic transmittances must be calculated. Clearly the number of points \( v' \) can be reduced by making some of the \( \{v'\}_{i+1} \) points overlap some of the \( \{v'\}_i \) points. However, because the number of \( \{v'\}_i \) values needed for a given level of accuracy \( \epsilon \) in \( \tau_{\text{con}}(v_i) \) depends upon the form of the monochromatic transmittance, the density of \( \{v'\}_i \) points will be a function of \( v_i \) for a given \( \epsilon \). The exact density depends on the numerical integration rule employed, but usually this takes the form of bounds on the magnitude of high-order derivatives of \( \tau_{\text{mon}} \) over the convolution frequency range. The use of an iterative quadrature routine can often eliminate the need for
Fig. 2 - Schematic representation of Eq. (17)
evaluating these derivatives. Also, if the $\tau_{\text{con}}(v_i)$ values are calculated in order of increasing [or decreasing] frequency position, values of $\tau_{\text{mon}}$ at frequencies lower [higher] than the $i$th range of $v'$ values need not be saved. This reduces storage requirements.

Of the many available iterative routines, an equally spaced abscissa Romberg integration algorithm was selected. Gaussian rules require fewer [$v'$] points for a given $\epsilon$, but are not well adapted to iterative evaluation. Neither are they well suited for overlapping [$v'$] positions for successive $v_i$ values. Adaptive Simpson's rule techniques are good at varying the $v'$-density to meet the accuracy requirements and could be written so as to use overlapping [$v'$] positions. Unfortunately they are much more complicated than Romberg schemes, which proved to be complicated enough. Better programmers than the author of this report may wish to use them, however.

2. Romberg Integration

To use classical Romberg integration to evaluate the integral

$$I = \int_a^b f(x)dx$$

the interval $[a, b]$ is divided into $2^{k_0}$ equal pieces. The function $f$ is evaluated at each of the $2^{k_0} + 1$ points,

$$x_i = a + (i - 1)(b - a)/2^{k_0} \quad i = 1, \ldots, 2^{k_0} + 1,$$

and the sum,

$$T_0^{(k_0)} = \frac{(b - a)}{2^{k_0}} [f(x_1 = a) + f(x_2) + \ldots + f(x_{2^{k_0}}) + 1/2 f(x_{2^{k_0} + 1} = b)], \quad (18)$$

forms the first element of a table of approximations to $I$ called the Romberg T-table. Equation (18) is easily recognized as the trapezoidal rule. Next, $k_0$ is replaced by $k_1 = k_0 + 1$ and $T_0^{(k_1)}$ is calculated from Eq. (18) with $k_0$ replaced by $k_1$. This value forms a second estimate for $I$ and is written next to $T_0^{(k_0)}$ in the top-most row of the table, as shown in Fig. 3. From these two estimates a third estimate, $T_1^{(k_0)}$, is formed according to

$$T_m^{(k)} = \frac{T_m^{(k+1)} - T_m^{(k)}}{\frac{\text{error}}{T_m^{(k+1)}} - 1}. \quad (19)$$
\begin{align*}
&\begin{array}{ccc}
T_0^{(k_0)} & T_0^{(k_1)} & T_0^{(k_2)} \\
T_1^{(k_0)} & T_1^{(k_1)} & T_1^{(k_2)} \\
T_2^{(k_0)} & T_2^{(k_1)} & \ldots \\
\ddots & \ddots & \ddots \\
\end{array}
\end{align*}

\textbf{Fig. 3 - The Romberg T-table}
The values of $T_0^{(k_0)}$ and $T_1^{(k_0)}$ are then compared, and if
\[
\left| T_1^{(k_0)} - T_0^{(k_0)} \right| < \epsilon ,
\] (20)
the process stops and outputs $T_1^{(k_0)}$ as the final approximation to $I$. If the convergence criterion in Eq. (20) is not satisfied, the table construction continues with $T_0^{(k_2)}$, $T_1^{(k_2)}$ and so on until two successive elements along the diagonal of the table do satisfy the convergence criterion.

Davis and Rabinowitz\(^\text{19}\) discuss a modification of the classical Romberg scheme which requires calculation of a second table, the Romberg M-table. In this scheme, after $T_0^{(k_0)}$ is calculated, the quantity
\[
M_0^{(k_0)} = \frac{b - a}{2^{k_0}} \sum_{j=1}^{2^{k_0}} f \left[ a + \left( j - \frac{1}{2} \right) \frac{b - a}{2} \right]
\] (21)
is calculated. Equation (21) is easily recognized as the midpoint rule. The values of $T_0^{(k_0)}$ and $M_0^{(k_0)}$ are then compared and if
\[
\left| M_0^{(k_0)} - T_0^{(k_0)} \right| < \epsilon ,
\] (22)
the process stops and outputs
\[
T_0^{(k_1)} = \frac{1}{2} \left( T_0^{(k_0)} + M_0^{(k_0)} \right)
\] (23)
as the final approximation to $I$. If the new convergence criterion [Eq. (22)] is not met, the next diagonal element of the T-table is calculated from
\[
T_m^{(k)} = M_m^{(k)} + \frac{2 \cdot 4^{m-1} - 1}{4^m - 1} \left( T_{m-1}^{(k)} - M_{m-1}^{(k)} \right).
\] (24)
The next element of the M-table, $M_1^{(k_1)}$, is calculated from Eq. (21) with $k_0$ replaced by $k_1 = k_0 + 1$. The two M values are then combined as in Eq. (19) to form $M_1^{(k_0)}$. The convergence criterion is then applied to $M_1^{(k_0)}$ and $T_1^{(k_0)}$. If the criterion is satisfied, these two are combined as in Eq. (23) and output. Otherwise the process continues halving the interval $[a,b]$ and recursively generating the T- and M-tables until two corresponding diagonal elements satisfy the convergence criterion.

Those referring to Davis and Rabinowitz\(^\text{19}\) should note that Eq. (6.3.9) in their book is incorrect in some editions, as can be verified from their
Eq. (6.3.8) and the equation below (6.3.2). Also, the FORTRAN version of this technique, incorporated into the program in Appendix A, has a maximum number of interval halvings in the search for convergence. When this limit is exceeded, the output is taken from Eq. (24) rather than Eq. (23).

Incorporating the Romberg Table evaluation in the spectrum calculation routine required less than 15 FORTRAN statements. The logic needed to save $T_{\text{mon}}$ values required nearly 10 times as many statements. The details are given in Appendix A.

F. VERIFYING CALCULATION BEHAVIOR

The program which evaluates Eq. (17), described in Appendix A, is composed of three basic parts: (1) evaluation of the atmospheric path (subroutine SNIDER), (2) setting up approximate layer parameters (subroutine PATHST), and (3) spectrum calculation (subroutine NSPEC). These were first checked individually and then as a whole.

A specific observer-source geometry was selected. This had an observer at 45° N latitude, 45-km height, and an observed zenith angle ($\theta'$ in Fig. 1) of 95.2°. The source was assumed to be above the atmosphere. Unfortunately, the atmospheric model used by Snider and Goldman could not be obtained so the January reference atmosphere of Cole and Kantor was used instead. The program's analysis of the path is shown in Table 1 along with the associated results taken from Ref. (10). Also shown are the results using a 190-layer atmosphere taken from the U.S. Standard Atmosphere, 1976. The agreement shown in the table and the proper behavior of the subroutine to changes in zenith angle, observer height, and ground-level pressure indicated that the subroutine was functioning properly.

The output for the 190-layer model included 198 sets of $(u_i, \bar{P}_i, \bar{P}_j)$ values; 59 values for layers crossed in the portion of the path going from the observer in layer #99 to the minimum height in layer #1, and 139 values for layers crossed in the portion from the minimum height to the top of the atmosphere. The average layer thickness in this model is ~4.4 km. Examination of these 198 sets showed that of the $2.00099 \times 10^{26}$ mol/cm² in the path, $1.341 \times 10^{26}$, or 26%, were in the 0.35 km thick portion of layer #1 that contains the lowest segment of the path. This demonstrates the height selective nature of the limb geometry.

Compare this to the result obtained by Schmidt that a uniform error of 0.5 km in the minimum height of a limb emission spectrum produced a 21% rms error in retrieved mixing ratios (using simulated balloon data).

The next highest layer, #42, contained $1.4154 \times 10^{25}$ mol/cm², or 11.8%. A full 60% of the air mass lay between 18.45 and 20.49 km.

Next the Voigt function evaluation routine, due to Hui, Armstrong, and Wray, was checked against the tables of Young. It gave good agreement over the tabulated range of $x$ and $y$ values. A set of sample
Table 1. Comparison of path characteristics.

<table>
<thead>
<tr>
<th></th>
<th>Ref. (20)</th>
<th>Ref. (10)</th>
<th>Ref. (21)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Apparent Zenith angle</td>
<td>95.2</td>
<td>95.2</td>
<td>95.2</td>
</tr>
<tr>
<td>(degrees)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Lower height (m)</td>
<td>45000.0</td>
<td>45000.0</td>
<td>45000.0</td>
</tr>
<tr>
<td>Upper height (m)</td>
<td>89999.9</td>
<td>99000.0</td>
<td>82000.0</td>
</tr>
<tr>
<td>Minimum height (m)</td>
<td>18454.5</td>
<td>18434.1</td>
<td>18450.0</td>
</tr>
<tr>
<td>Chapman airmass</td>
<td>5.168</td>
<td>7.098</td>
<td>6.385</td>
</tr>
<tr>
<td>Optical airmass</td>
<td>5.422</td>
<td>6.085</td>
<td>5.573</td>
</tr>
<tr>
<td>HDIFF (m)</td>
<td>1000.5</td>
<td>1138.5</td>
<td>1030.0</td>
</tr>
<tr>
<td>Refraction (degrees)</td>
<td>0.11255</td>
<td>0.12788</td>
<td>0.11579</td>
</tr>
<tr>
<td>Astronomical Zenith angle</td>
<td>95.31</td>
<td>95.33</td>
<td>95.32</td>
</tr>
<tr>
<td>angle (degrees)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>P(EFF) (N/m²)</td>
<td>4518.41</td>
<td>5494.93</td>
<td>4999.92</td>
</tr>
<tr>
<td>T(EFF) (K)</td>
<td>216.26</td>
<td>219.54</td>
<td>218.93</td>
</tr>
<tr>
<td>P(TAN) (N/m²)</td>
<td>7890.17</td>
<td>9066.33</td>
<td></td>
</tr>
</tbody>
</table>
line parameters were then chosen. These are shown in Table 2. A uniform mixing ratio of 0.1 ppm was used to calculate the absorbance in each layer.

The total absorbance was $1.231378$ at $v = v_0 = 2090.796$ cm$^{-1}$, corresponding to a transmittance (no convolution) of 0.29189. The absorbance in layer 41 was 0.197407, or $\sim 16\%$, and the absorbance between 18.45 and 20.49 km was 0.456708, or $37\%$. These values show that the absorbance at line center is less peaked with height than the airmass. For Lorentz-like lines, the absorbance at $v_0$ is $S_u/\alpha$. Consequently the decrease in $u$ with height is offset by the decrease in $\alpha$ (because of decreasing pressure) and the absorbance is "smared out" with height. The degree of Lorentz-like behavior for Voigt lines is determined by $y$ in Eq. (13). Large $y$ implies a high degree of Lorentz-like behavior; small $y$ implies mainly Doppler-like behavior. The Lorentz-Doppler crossover point, $y = 1$, occurs at layer 63 for the sample line and atmospheric profile used; consequently, the observed "smearing" is reasonable.

The above observations suggest that high-resolution spectra should have better height sensitivity than low-resolution spectra because the same effect which "smears" the line center absorbance sharpens the wing absorbance, which goes as $S_u \alpha$. In low-resolution spectra the observed signal is a mix of the two and has intermediate height sensitivity. High-resolution spectra are better to use to study the height-sensitive wing absorbance.

A second consequence of the "smearing" is found when the fine layers are combined into thicker layers. Let consecutive layers $l_1, l_2, \ldots, l_n$ with parameters $(u_1, T_1, P_1), \ldots, (u_n, T_n, P_n)$ be combined into one layer with parameters

$$u = \sum_{i=1}^{n} u_i,$$

$$\bar{T} = \sum_{i=1}^{n} \frac{u_i T_i}{u}, \text{ and}$$

$$\bar{P} = \sum_{i=1}^{n} \frac{u_i P_i}{u}.$$  \hspace{1cm} (25)

The new layer represents a less accurate approximation to the atmosphere than the original layers. In order to save computation time, it is desirable to use the minimum number of layers to calculate the spectrum. Subroutine SNIDER is sufficiently fast, however, that no such concerns apply to it. To test the sensitivity of the calculated spectrum to the layer coarseness, the original 139 sets of $(u, T, P)$, one for each layer crossed, were combined into segments of approximately equal airmass. Each new layer had an airmass as close to, but less than, $U/N_{ge}$ as possible, where $N_{ge}$ is some integer. The calculated absorbances at three different frequencies for several different values of $N_{ge}$ are shown in Table 3. It is clear from these results that more layers are required at line center than in the wings. This is because the result of decreasing $N_{ge}$ is to
Table 2. Sample line parameters*

\[ \nu_0 = 2090.796 \text{ cm}^{-1} \]
\[ S_0 = 0.189 \times 10^{-20} \text{ mol}^{-1} \text{ cm} \]
\[ \alpha_0 = 0.110 \text{ cm}^{-1} \]
\[ E'' = 272.220 \text{ cm}^{-1} \]
\[ m = 48 \text{ amu} \]

*corresponding to the (6,13)-(6,14) line of the \( \nu_1 + \nu_3 \) band of \(^{16}\text{O}_3\).

Table 3. Effect of different layer thicknesses.

<table>
<thead>
<tr>
<th>( \nu(\text{cm}^{-1}) )</th>
<th>Nge</th>
<th># Layers</th>
<th>A((\nu))</th>
</tr>
</thead>
<tbody>
<tr>
<td>2090.796</td>
<td>3</td>
<td>3</td>
<td>1.2296698</td>
</tr>
<tr>
<td>2090.796</td>
<td>9</td>
<td>7</td>
<td>1.20571646</td>
</tr>
<tr>
<td>2090.796</td>
<td>35</td>
<td>18</td>
<td>1.22967891</td>
</tr>
<tr>
<td>2090.796</td>
<td>-</td>
<td>139</td>
<td>1.231378</td>
</tr>
<tr>
<td>2090.806</td>
<td>3</td>
<td>3</td>
<td>0.204556963</td>
</tr>
<tr>
<td>2090.806</td>
<td>9</td>
<td>7</td>
<td>0.202129669</td>
</tr>
<tr>
<td>2090.806</td>
<td>35</td>
<td>18</td>
<td>0.20184368</td>
</tr>
<tr>
<td>2090.806</td>
<td>-</td>
<td>139</td>
<td>0.201829374</td>
</tr>
<tr>
<td>2090.816</td>
<td>3</td>
<td>3</td>
<td>0.0613707937</td>
</tr>
<tr>
<td>2090.816</td>
<td>9</td>
<td>7</td>
<td>0.0616293664</td>
</tr>
<tr>
<td>2090.816</td>
<td>35</td>
<td>18</td>
<td>0.0614016373</td>
</tr>
<tr>
<td>2090.816</td>
<td>-</td>
<td>139</td>
<td>0.0613723083</td>
</tr>
</tbody>
</table>
produce thicker layers in the upper portions of the atmosphere where the \( u_1 \) values are small. Since the line center absorbance is more sensitive to these upper layers, the loss of detail has more effect on it than wing absorbance values.

The program in Appendix A includes a subroutine called PATHST which performs the layer combination. The parameter \( N_{ge} \) is used to set the fineness of the layers used to calculate the spectrum. As written, however, the subroutine combines the layers in such a way that each has an airmass at least as great as \( U/N_{ge} \) but as close to \( U/N_{ge} \) as possible. For the spectra in the next section, a value of \( N_{ge} = 15 \) was found to be acceptable, but Table 3 indicates that different values may be required for different types of spectra.

The convolution portion of the program was tested on a flat \((\partial v/\partial v = 0)\) spectral region with a Gaussian slit function of the form

\[
\sigma_{\text{Gauss}}(v - v') = \frac{\sqrt{2\pi}}{H\sqrt{\pi}} \exp\left( -\frac{(v' - v)^2}{2H^2} \right).
\] (26)

A five-point initial trapezoidal evaluation was used to start the Romberg iterations with a frequency extent of \( 8H \). The \( T \) and \( M \) table entries calculated for one run are shown in Table 4. A convergence criterion corresponding to 1% between the respective \( T \) and \( M \) table elements [see Eq. (22)] was used. Only the diagonal of the \( T \)-table is shown since the other elements are not calculated in the modified routine. The table elements must be multiplied by 2 to get the corresponding transmittance values. In this example, the routine went two iterations beyond the initial trapezoidal and midpoint evaluations before converging. The final value shows excellent agreement with the true value.

The routine was also tried on a Voigt line with parameters

\[
\begin{align*}
\nu_0 &= 2875.90 \text{ cm}^{-1} \\
S_0 &= 0.0668 \text{ atm}^{-1} \text{ cm}^{-1}/\text{cm} \\
\alpha_{\nu_0} &= 0.023176 \text{ cm}^{-1} \\
E'' &= 400.00 \text{ cm}^{-1} \\
m &= 36 \text{ amu}
\end{align*}
\]

at a uniform pressure of 1 atm and temperature of 300 K. The total airmass was \( u = 200 \text{ atm cm} \). Table 5 shows the results for 10 different observed frequency positions spaced 0.2 cm\(^{-1}\) apart. The second column gives the calculated transmittance values with \( \epsilon = 0.01 \), \( H = 0.083819 \text{ cm}^{-1} \), and an initial five-point trapezoidal evaluation that extended 2-1/2 \( H \) on either side of the central position. By comparing values equally spaced around 2875.90 cm\(^{-1}\) the consistency is seen to be ~0.001, which is \( \epsilon/10 \). The
Table 4. A sample T and M table for convolution routine. (Table values must be multiplied by 2 to give transmittance value.)

<table>
<thead>
<tr>
<th>TRAP</th>
<th>MID</th>
<th>Iteration</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>1</td>
</tr>
<tr>
<td>0.5284401</td>
<td>0.471553</td>
<td>0.4999984</td>
</tr>
<tr>
<td>0.4905153</td>
<td>0.5094798</td>
<td>0.4999971</td>
</tr>
<tr>
<td>0.5006297</td>
<td></td>
<td>0.4993649</td>
</tr>
</tbody>
</table>

\[ \tau = 0.9999946 \text{ (exact = 1.0000000)} \]

Table 5. Convolution results for a sample Voigt line convolved with a Gaussian slit function.

<table>
<thead>
<tr>
<th>( \nu \text{ (cm}^{-1})</th>
<th>( \tau_{\text{con}} )</th>
<th>Iterations</th>
<th>Total Points</th>
<th>New Points</th>
</tr>
</thead>
<tbody>
<tr>
<td>2875.00</td>
<td>0.9984500</td>
<td>1</td>
<td>9</td>
<td>9</td>
</tr>
<tr>
<td>2875.20</td>
<td>0.9952382</td>
<td>1</td>
<td>9</td>
<td>3</td>
</tr>
<tr>
<td>2875.40</td>
<td>0.9944796</td>
<td>1</td>
<td>9</td>
<td>4</td>
</tr>
<tr>
<td>2875.60</td>
<td>0.9885907</td>
<td>1</td>
<td>9</td>
<td>4</td>
</tr>
<tr>
<td>2875.80</td>
<td>0.8511999</td>
<td>3</td>
<td>33</td>
<td>29</td>
</tr>
<tr>
<td>2876.00</td>
<td>0.8508019</td>
<td>2</td>
<td>17</td>
<td>8</td>
</tr>
<tr>
<td>2876.20</td>
<td>0.9872358</td>
<td>1</td>
<td>9</td>
<td>3</td>
</tr>
<tr>
<td>2876.40</td>
<td>0.9942334</td>
<td>1</td>
<td>9</td>
<td>4</td>
</tr>
<tr>
<td>2876.60</td>
<td>0.9960335</td>
<td>1</td>
<td>9</td>
<td>4</td>
</tr>
<tr>
<td>2876.80</td>
<td>0.9964244</td>
<td>1</td>
<td>9</td>
<td>4</td>
</tr>
</tbody>
</table>

TOTAL 72
third column lists the number of iterations required for convergence of the convolution integral. A value of 1 means that the convergence criterion was satisfied on the first try. The fourth column lists the number of monochromatic transmittances required for the convolution, and the fifth column lists the number of new monochromatic transmittance values calculated at each observed frequency. The increased density of points around line center, where the monochromatic transmittance changes most rapidly, is apparent.

Table 6 shows similar results for the identical spectrum except with a smaller frequency spacing. The fifth column shows the larger savings in calculations for more closely spaced observed frequencies. For reference, the 10 points in Table 6 took 0.09 second of cpu time to execute. This corresponds to 1.7 ms per monochromatic transmittance calculation. A later sample spectrum including 55 atmospheric layers and 13 lines, averaged 0.15 ms per monochromatic transmittance calculation on the OSU Amdahl Computer.

Sample spectra for other sets of line parameters produced similar results. It was found that extremely narrow and strong lines required considerably more iterations than broad lines. This can lead to unreasonably high numbers of iterations unless some maximum number of iterations is specified; usually a value of 7 was used. When convergence does not occur on the seventh iteration, the program outputs the most recent element of the T-table, sets an error flag, and proceeds to the next frequency position.

A variety of other tests were performed on the program, including the effect of different convergence criterion values. More is said about this in the next chapter. Overall the behavior was found to be satisfactory but one persistent problem did arise; it was found that the convolution routine would often converge prematurely. An example is shown in Table 7. The rapid decrease in the number of iterations, in a spectral region where the transmittance is not changing much, indicates a premature convergence. This is verified in the T- and M-tables for these two points shown in Table 8. The boxed portions correspond to the values in Table 7 where the convergence criterion was 0.005 (or 0.5%). The larger values in Table 8 correspond to a convergence criterion of 0.0001 (or 0.01%). The premature convergence at 1900.05 cm⁻¹ is seen to be due to a misleading resemblance between the first T- and M-values. Subsequent iterations show the true value to be considerably lower than these, which the more stringent convergence criterion has picked up. This type of behavior is often encountered in iterative procedures. This problem was only detected when the slit function width was much larger than the line widths, though in principle it could occur in other situations. It was found that the problem could usually be avoided by adjusting the convergence criterion and the number of points in the first trapezoidal evaluation. The parameters can only be set based on experience and knowledge of the spectral region, and those lacking both these should indicate some caution.
Table 6. Convolution results for sample line with smaller frequency spacing.

<table>
<thead>
<tr>
<th>$\nu$ (cm$^{-1}$)</th>
<th>$\tau_{\text{con}}$</th>
<th>Iterations</th>
<th>Total Points</th>
<th>New Points</th>
</tr>
</thead>
<tbody>
<tr>
<td>2875.70</td>
<td>0.9694133</td>
<td>1</td>
<td>9</td>
<td>9</td>
</tr>
<tr>
<td>2875.74</td>
<td>0.9396371</td>
<td>1</td>
<td>9</td>
<td>0</td>
</tr>
<tr>
<td>2875.78</td>
<td>0.8870856</td>
<td>2</td>
<td>17</td>
<td>10</td>
</tr>
<tr>
<td>2875.82</td>
<td>0.8118306</td>
<td>3</td>
<td>33</td>
<td>18</td>
</tr>
<tr>
<td>2875.86</td>
<td>0.7381039</td>
<td>3</td>
<td>33</td>
<td>3</td>
</tr>
<tr>
<td>2875.90</td>
<td>0.7074896</td>
<td>3</td>
<td>33</td>
<td>3</td>
</tr>
<tr>
<td>2875.94</td>
<td>0.7380002</td>
<td>3</td>
<td>33</td>
<td>3</td>
</tr>
<tr>
<td>2875.98</td>
<td>0.8117288</td>
<td>3</td>
<td>33</td>
<td>3</td>
</tr>
<tr>
<td>2876.02</td>
<td>0.8863926</td>
<td>3</td>
<td>33</td>
<td>3</td>
</tr>
<tr>
<td>2876.06</td>
<td>0.9391911</td>
<td>2</td>
<td>17</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>TOTAL 53</td>
<td></td>
</tr>
</tbody>
</table>

Table 7. An example of a premature convergence.

<table>
<thead>
<tr>
<th>$\nu$ (cm$^{-1}$)</th>
<th>$\tau_{\text{con}}$</th>
<th>Iterations</th>
</tr>
</thead>
<tbody>
<tr>
<td>1900.00</td>
<td>0.96867</td>
<td>5</td>
</tr>
<tr>
<td>1900.05</td>
<td>0.99230</td>
<td>1</td>
</tr>
</tbody>
</table>
Table 8. The T- and M-tables for convolutions in Table 7. (Boxed portions correspond to a convergence criterion of 0.005. Entire tables for convergence criterion of 0.0001. Multiply table values by 0.0625 to get transmittance.)

<table>
<thead>
<tr>
<th>TRAP</th>
<th>MID</th>
<th>( \nu = 1900.00 \text{ cm}^{-1} )</th>
<th>( \nu = 1900.05 \text{ cm}^{-1} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>15.85111</td>
<td>15.72414</td>
<td>14.90784</td>
<td>15.61850</td>
</tr>
<tr>
<td>15.77746</td>
<td>14.63574</td>
<td>15.85539</td>
<td>15.49529</td>
</tr>
<tr>
<td>15.16341</td>
<td>15.93670</td>
<td>15.47128</td>
<td>15.48721</td>
</tr>
<tr>
<td>15.55619</td>
<td>15.46389</td>
<td>15.49771</td>
<td></td>
</tr>
<tr>
<td>15.50986</td>
<td>15.48755</td>
<td>15.49775</td>
<td></td>
</tr>
<tr>
<td>15.49869</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
As a final check on the entire calculation routine, two sample spectra were calculated under conditions similar to those used by Kyle and Goldman. The observer was at a height of 4 km with the sun overhead. The spectra for the 1900-1902 cm\(^{-1}\) and 1930-1935 cm\(^{-1}\) regions are shown in Figs. 4 and 5, respectively. There are some differences in the conditions between these spectra and the corresponding high-resolution spectra of Kyle. Both have an instrument resolution of 0.1 cm\(^{-1}\) but Kyle used a triangular slit function and we used a Gaussian. Also, the values of the CO\(_2\) and H\(_2\)O mixing ratios are somewhat different. The calculation routine is currently set up for only constant mixing ratios, whereas Kyle used a decreasing H\(_2\)O mixing ratio with height. An attempt was made to fix the CO\(_2\):H\(_2\)O ratio in the lowest level. With a CO\(_2\) mixing ratio of 322 ppm (volume), this gave a H\(_2\)O = 1080 ppm (volume). Also, it was found that SNIDER will not work with a zenith angle of 0°. In spite of these differences, the spectra show good agreement, indicating the two routines are consistent.

In the next chapter, the spectrum calculation routine is used in a brief study that illustrates some information analysis techniques for experimental design.
Fig. 4 - Comparison with Kyle²₅ spectrum
III. SOME INFORMATION ANALYSIS TECHNIQUES

A. IDENTIFYING "BAD" PARAMETERS

The equations in the previous chapter describe how the appearance of an atmospheric absorption spectrum depends on the physical characteristics of the atmosphere and the molecular properties of the absorbing gases. Assuming that the molecular parameters (line intensity, broadening coefficient, line position, lower state term value) are known, the equations predict what the spectrum will look like, given the atmospheric conditions. This report is concerned with the inverse problem (i.e., inferring the atmospheric conditions given the spectrum). It is clear that those aspects of the atmosphere which have no effect on the spectrum cannot be determined from the spectrum. Similarly, those aspects which have only a slight influence on the spectrum will be harder to determine than those aspects with a large influence. For example, consider the calculated spectrum in Fig. 6. This 200-point spectrum corresponds to the same observer-source geometry as in Chapter II-F with the 190-layer model and \( N_{m} \) equal to 15 in Eq. (25). The CO\(_2\) mixing ratio was 322 ppm, and the H\(_2\)O mixing ratio was 3.889 ppm. Both were assumed independent of height. The slit function was Gaussian, with a full width at half height of 0.02 cm\(^{-1}\). This particular region contains contributions from nearly 150 CO\(_2\) lines and about a dozen H\(_2\)O lines, so it should be sensitive to the mixing ratios of CO\(_2\) and H\(_2\)O. It contains no information, however, about the O\(_3\) mixing ratio. A convergence criterion of 0.5% was used with an extent of 0.05 cm\(^{-1}\) in the convolution. A more stringent criterion of 0.1% produced an rms change in the transmittance values of 2.89 \( \times \) 10\(^{-4}\) with a maximum of 0.003, indicating that the accuracy of the convolution is consistent with the convergence criterion. A frequency spacing of 2 points per full width at half height of the slit function was used.

Several atmospheric parameters were selected for investigation. These are listed in Table 9 along with the two different values used to study the influence of the parameter on the spectrum. The spectrum in Fig. 6 corresponds to the upper value for each parameter and is referred to as the reference spectrum. Eight new spectra were then calculated by changing the values of the parameters one at a time. Figure 7 shows the effect on the spectrum of increasing the zenith angle from 95.2° to 95.4°. The difference spectrum is shown in Fig. 8. The sum of the squares of the differences for this pair is 0.44482, which is listed in column 3 of Table 9. The corresponding values are also shown for the other seven parameters. These numbers are one indicator of how much influence a particular parameter has on the spectrum. Of course larger parameter changes produce larger squared differences so the only valid comparisons between parameters are conditioned on specific parameter changes; e.g., a 0.2° change in zenith angle is more influential than a 2 K change in the temperature at layer 41 (18.38 - 18.80 km). It is reasonable, therefore, to scale the difference spectrum by dividing it by the size of the parameter change or step before squaring. Let \( \Delta \theta \) denote the ith parameter with step \( \Delta \theta \). The procedure above produces a set of 8 quantities \( W_{i} \), \( i = 1, \ldots, 8 \).
Table 9. Parameter values used to compute sample spectra.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values</th>
<th>$\sum (\Delta y)^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. CO$_2$ mixing ratio</td>
<td>322 ppm</td>
<td>0.011773</td>
</tr>
<tr>
<td></td>
<td>354.2 ppm</td>
<td></td>
</tr>
<tr>
<td>2. Resolution</td>
<td>0.02 cm$^{-1}$</td>
<td>0.062913</td>
</tr>
<tr>
<td></td>
<td>0.028 cm$^{-1}$</td>
<td></td>
</tr>
<tr>
<td>3. Zenith angle</td>
<td>95.2°</td>
<td>0.44482</td>
</tr>
<tr>
<td></td>
<td>95.4°</td>
<td></td>
</tr>
<tr>
<td>4. Temperature in layer 41</td>
<td>216.65 K</td>
<td>8.4118 x $10^{-5}$</td>
</tr>
<tr>
<td></td>
<td>218.65 K</td>
<td></td>
</tr>
<tr>
<td>5. Temperature in layer 42</td>
<td>216.65 K</td>
<td>5.4798 x $10^{-5}$</td>
</tr>
<tr>
<td></td>
<td>218.65 K</td>
<td></td>
</tr>
<tr>
<td>6. Temperature in layer 40</td>
<td>216.65 K</td>
<td>4.888 x $10^{-7}$</td>
</tr>
<tr>
<td></td>
<td>218.65 K</td>
<td></td>
</tr>
<tr>
<td>7. Ground-level pressure</td>
<td>1013 mb</td>
<td>0.008109</td>
</tr>
<tr>
<td></td>
<td>1063 mb</td>
<td></td>
</tr>
<tr>
<td>8. Background value</td>
<td>1.0</td>
<td>0.10954</td>
</tr>
<tr>
<td></td>
<td>1.025</td>
<td></td>
</tr>
</tbody>
</table>
Fig. 7 - Spectrum for increased zenith angle — 95.4°, ---- 95.2° (reference spectrum)
where

\[ W_{ik} = \sum_{j=1}^{N} \left( y_j^{(0)} - y_j^{(i)} \right)^2/\Delta \theta_i^2, \]

with \( N \) the number of points in the spectrum, \( y^{(0)} = (y_1^{(0)}, \ldots, y_N^{(0)}) \) the reference spectrum, and \( y^{(i)} = (y_1^{(i)}, \ldots, y_N^{(i)}) \) the spectrum with the \( i \)th parameter stepped by \( \Delta \theta_i \).

These scaled and summed square difference values alone, however, are insufficient to indicate how well groups of parameters can be determined simultaneously. This is illustrated by Fig. 9. It shows the difference spectra for changes in the temperature values \( T(1) \) and \( T(2) \) for layers 41 and 42. From the similarity of these spectra and the assumption that the change in the spectrum \( \Delta y \) is linear in \( \Delta \theta \), it is clear that a simultaneous increase of 2 K in \( T(41) \) and a 2 K decrease in \( T(42) \) will produce a much smaller difference spectrum than either one in Fig. 9. Each change tends to cancel out the other. This corresponds to a 2 K change in \( [T(41) - T(42)]/2 \), with the average temperature \( [T(41) + T(42)]/2 \) held constant. Similarly, a simultaneous 2 K increase in \( T(41) \) and \( T(42) \) will produce a much larger difference spectrum than either in Fig. 9. This corresponds to a 2 K change in the average temperature, with the difference temperature held constant, and indicates that changes in different linear combinations of the parameters can have significantly different amounts of influence on the spectrum. That, in turn, implies that some combinations are harder to determine from a spectrum than others. Similar observations apply to linear combinations of all 8 different parameters.

The question arises as to whether there exists some linear combination

\[ \phi = \sum_{j=1}^{8} u_j \theta_j \]

which has the least influence on the spectrum and hence is the hardest to determine. Lees\textsuperscript{28} addressed this question in connection with attempts to analyze methyl alcohol spectra. He found that changes in a particular linear combination of the unknown parameters produced no change in the spectrum, which he called a linear dependence, and he proposed a technique for identifying these as well as "near" linear dependences. In order to adapt this technique to the present problem, form the quantities

\[ W_{ik} = \sum_{j=1}^{N} \frac{(y_j^{(0)} - y_j^{(i)}) \cdot (y_j^{(0)} - y_j^{(k)})}{\Delta \theta_i \Delta \theta_k}, \]

(28)
Fig. 9 - Difference spectra for 2 K changes in the temperature in layers 41 and 42. — $\Delta T(41) = 2$ K, $\Delta T(42) = 0$, ---- $\Delta T(41) = 0$, $\Delta T(42) = 2$ K.
and place these in a matrix $\mathbf{W}$, where the $i$th diagonal element is $W_{ii}$ from Eq. (27) and the $i$th $k$th and $k$th element is $W_{ik}$. This matrix is often referred to as the information matrix or the curvature matrix.

To be more precise, $\mathbf{W}$ becomes the information matrix in the limit as $\Delta \theta \to 0$ and the quantities $y(0) - y(1)/\Delta \theta$ become the partial derivative of $y$ with respect to $\theta_i$ evaluated at $\theta_0$. $\mathbf{W}$ is therefore a function of $\theta_0$.

For small simultaneous changes in the parameters $\Delta \theta = \begin{pmatrix} \Delta \theta_1 \\ \vdots \\ \Delta \theta_8 \end{pmatrix}$ the summed squared difference spectrum is given by

$$Q(\Delta \theta) = \sum_{i,j} W_{ij} \Delta \theta_i \Delta \theta_j = \sum_k \left[ y_k(0) - y_k(\Delta \theta) \right]^2$$

or, in matrix notation,

$$Q(\Delta \theta) = \Delta \theta' \mathbf{W} \Delta \theta,$$

where $'$ denotes transpose. Lees proposes examining the eigenvalues and eigenvectors of a modified information matrix $\mathbf{W}^*$ given by

$$W_{ik}^* = W_{ik}/\sqrt{W_{ii}W_{kk}}.$$ 

Let the eigenvector $\lambda^*_i$ with elements $\lambda^*_i$ correspond to the smallest eigenvalue of $\mathbf{W}^*$. The corresponding linear combination of parameters is given by

$$\phi = \sum_{j=1}^8 \lambda^*_i \cdot \theta_i \cdot \sqrt{W_{ii}}.$$ 

When this eigenvalue is much smaller than the others, he says that it indicates a "near" or exact linear dependence. Table 10 lists the information matrix $\mathbf{W}$ and modified matrix $\mathbf{W}^*$ for the set of 9 spectra already introduced. The eigenvalues and eigenvectors of $\mathbf{W}^*$ were calculated in SPEAKEASY with the command EIGENVALS. These are listed in Table 11. None of the eigenvalues is significantly lower than the rest, indicating that there are no exact linear dependences among the 8 parameters in Table 9. It is still possible to deduce the "worst" linear combination from these results with the following restriction:

For each of the 8 parameters $\theta_i$ define a parameter step $\Delta \theta_i$ such that $Q(\Delta \theta_i) = 1$. Assuming that Eq. (29) holds, these steps are given by $\Delta \theta_i = 1/\sqrt{W_{ii}}$. The appropriate steps are listed in Table 12. Define new parameters $\{\psi\}$ according to

$$\psi_i = \theta_i/\Delta \theta_i.$$
Table 10. Information matrices

<table>
<thead>
<tr>
<th>ROW</th>
<th>1.1355E-5</th>
<th>0.034772</th>
<th>0.010634</th>
<th>1.2303E-5</th>
<th>1.0215E-5</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.034772</td>
<td>3932</td>
<td>-1.6132</td>
<td>-0.090516</td>
<td>-0.072398</td>
</tr>
<tr>
<td>3</td>
<td>0.010634</td>
<td>-1.6132</td>
<td>11.12</td>
<td>0.012685</td>
<td>0.010461</td>
</tr>
<tr>
<td>4</td>
<td>1.2303E-5</td>
<td>-0.090516</td>
<td>0.012685</td>
<td>2.1029E-5</td>
<td>1.6957E-5</td>
</tr>
<tr>
<td>5</td>
<td>1.0215E-5</td>
<td>-0.72398</td>
<td>0.010461</td>
<td>1.6957E-5</td>
<td>1.3699E-5</td>
</tr>
<tr>
<td>6</td>
<td>1.0832E-6</td>
<td>-1.3576E-4</td>
<td>0.0011462</td>
<td>1.3054E-6</td>
<td>1.0741E-6</td>
</tr>
<tr>
<td>7</td>
<td>5.7883E-6</td>
<td>-0.0091847</td>
<td>0.0059693</td>
<td>7.0995E-6</td>
<td>5.8427E-6</td>
</tr>
<tr>
<td>8</td>
<td>-0.020427</td>
<td>-70.879</td>
<td>-22.043</td>
<td>-0.021157</td>
<td>-0.017702</td>
</tr>
</tbody>
</table>

W*: 

<table>
<thead>
<tr>
<th></th>
<th>0.946</th>
<th>0.796</th>
<th>0.819</th>
<th>0.920</th>
<th>0.954</th>
<th>-0.458</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-0.165</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>-0.0077</td>
<td>-0.315</td>
<td>-0.312</td>
<td>-0.0084</td>
<td>-0.081</td>
<td>-0.085</td>
</tr>
<tr>
<td>1</td>
<td>0.829</td>
<td>0.848</td>
<td>0.983</td>
<td>0.994</td>
<td>-0.499</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>0.999</td>
<td>0.814</td>
<td>0.860</td>
<td>-0.348</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>0.830</td>
<td>0.876</td>
<td>-0.361</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

[SYMMETRIC] 

<table>
<thead>
<tr>
<th></th>
<th>0.987</th>
<th>-0.451</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
<td>-0.465</td>
</tr>
</tbody>
</table>

1
Table 11. Eigenvalues and associated eigenvectors of $W^*$ from Table 10.

<table>
<thead>
<tr>
<th>ROW</th>
<th>Eigenvectors of $W^*$ (as columns):</th>
<th>Eigenvalues of $W^*$:</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-0.02216 0.069408 -0.25559 0.74657 0.46191</td>
<td></td>
</tr>
<tr>
<td></td>
<td>-0.043359 0.015821 -0.39562</td>
<td>(1) $1.0655 \times 10^{-4}$</td>
</tr>
<tr>
<td>2</td>
<td>0.0038524 -0.032105 -0.052676 0.18343 -0.32712</td>
<td></td>
</tr>
<tr>
<td></td>
<td>-0.39618 0.83294 0.06913</td>
<td>(2) 0.0016232</td>
</tr>
<tr>
<td>3</td>
<td>-0.008285 0.48954 0.71662 -0.13348 0.17436</td>
<td></td>
</tr>
<tr>
<td></td>
<td>-0.11331 0.14197 -0.40684</td>
<td>(3) 0.010273</td>
</tr>
<tr>
<td>4</td>
<td>-0.67639 0.08705 -0.093432 0.087113 -0.56248</td>
<td></td>
</tr>
<tr>
<td></td>
<td>-0.048948 -0.23103 -0.38268</td>
<td>(4) 0.064734</td>
</tr>
<tr>
<td>5</td>
<td>0.7281 -0.032767 -0.0074687 0.12842 -0.50117</td>
<td></td>
</tr>
<tr>
<td></td>
<td>-0.045501 -0.21962 -0.38829</td>
<td>(5) 0.29085</td>
</tr>
<tr>
<td>6</td>
<td>0.062616 0.23679 -0.59867 -0.57696 0.20514</td>
<td></td>
</tr>
<tr>
<td></td>
<td>-0.17077 0.13061 -0.40051</td>
<td>(6) 0.68626</td>
</tr>
<tr>
<td>7</td>
<td>-0.088656 -0.83043 0.22346 -0.18346 0.17485</td>
<td></td>
</tr>
<tr>
<td></td>
<td>-0.1211 0.068128 -0.41116</td>
<td>(7) 1.1985</td>
</tr>
<tr>
<td>8</td>
<td>4.471E-4 0.013133 0.034914 0.023464 0.095041</td>
<td></td>
</tr>
<tr>
<td></td>
<td>-0.88319 -0.40311 0.21564</td>
<td>(8) 5.7477</td>
</tr>
</tbody>
</table>

36
Table 12. Parameter steps producing a summed squared difference spectrum equal to 1, assuming Eq. (29) holds.

<table>
<thead>
<tr>
<th></th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>296.76 ppm (CO₂ mixing ratio)</td>
</tr>
<tr>
<td>2</td>
<td>0.015948 cm⁻¹ (resolution)</td>
</tr>
<tr>
<td>3</td>
<td>0.29988° (zenith angle)</td>
</tr>
<tr>
<td>4</td>
<td>218.07 K ΔT(41)</td>
</tr>
<tr>
<td>5</td>
<td>270.18 K ΔT(42)</td>
</tr>
<tr>
<td>6</td>
<td>2860.6 K ΔT(40)</td>
</tr>
<tr>
<td>7</td>
<td>555.25 mb ΔP(0)</td>
</tr>
<tr>
<td>8</td>
<td>0.075535 (background)</td>
</tr>
</tbody>
</table>
For these new parameters, a unit step in $\psi_i$ produces a $Q(\Delta \psi_i) = 1$. Now consider the set of all linear combinations of steps in the $(\psi_i)$ of the form

$$\Delta \psi = \begin{pmatrix} c_1 \Delta \psi_1 \\ c_2 \Delta \psi_2 \\ \vdots \\ c_g \Delta \psi_g \end{pmatrix}$$

such that

$$\sum_k c_i^2 = 1 . \quad (31)$$

The set of steps $\Delta \psi_i$, with

$$c_i = 1$$

and

$$c_j = 0 \; \; ; \; \; i \neq j ,$$

belongs to this set of $\Delta \psi$ satisfying Eq. (31), and for each $\Delta \psi_i$, $Q(\Delta \psi_i) = 1$. In a sense, steps $\Delta \psi$ satisfying Eq. (31) are all the steps of the same "size," in terms of parameter changes. From the theorems on quadratic forms it can be shown that the extremal values of $Q(\Delta \psi)$ for all $\Delta \psi$ correspond to $\Delta \psi$'s whose $\{c_i\}$ values are the elements of the eigenvalues of $\mathbf{W}^\phi$. Consequently the smallest $Q(\Delta \psi)$, and hence smallest change in the spectrum, for all parameter changes of the same "size" as those in Table 12 results from:
The most significant aspect of this set of parameter changes is the temperature steps. The temperature in level $4_l$ is decreased by $147.5$ K while the temperatures in the two adjacent layers are increased by approximately the same amount. This zigzagging of the temperature profile is a problem that often occurs in profile retrievals. The summed squared difference spectrum corresponding to this "worst" set of parameter changes is given by the corresponding eigenvalue from Table 11, i.e., $1.0655 \times 10^{-4}$. It is seen that this is smaller than most of the values in the third column of Table 9.

The same quadratic forms theorem allows the identification of the set of parameter changes $\Delta \Phi_{\text{max}}$ leading to the largest change in the spectrum. It is given by the eigenvector associated with the largest eigenvalue of $\mathbf{W}$. From the eighth column in Table 12 it is seen that $\Delta \Phi_{\text{max}}$ corresponds to simultaneous decreases in CO$_2$ mixing ratio, zenith angle, ground level pressure, and all three temperature values. All of these changes tend to decrease the amount of absorption in the spectrum and hence add together to increase the summed squared difference spectrum. The net change in the spectrum is more than 50,000 times larger than for $\Delta \Phi_{\text{min}}$.

**B. ESTIMATED PARAMETER UNCERTAINTIES**

Another useful property of the information matrix $\mathbf{W}$ is related to the uncertainties in estimates for the values of the unknown parameters to be determined from an observed spectrum $\mathbf{y}_{\text{obs}}$. If $\mathbf{y}(\hat{\theta})$ is the calculated
spectrum for the set of parameter values \( \tilde{\theta} \), then one estimate for the true parameter values corresponding to \( y_{\text{obs}} \) is the well-known least-squares estimate \( \hat{\theta} \). This is given by the value of \( \hat{\theta} \) which minimizes

\[
\sum_{i=1}^{N} \left[ y_{\text{obs},i} - y(\hat{\theta})_i \right]^2 .
\]

If the rms noise value is \( \sigma \), then the asymptotic variance-covariance matrix for \( \hat{\theta} \) is

\[
\hat{\Sigma} = \sigma^2 \hat{W}^{-1},
\]

where \( \hat{W} \) is evaluated at \( \hat{\theta} \).

The matrix in Table 10 can therefore be used to estimate, for a given noise level, how precisely the eight parameters in Table 9 could be obtained from a spectrum similar to that in Fig. 6. Attempts to invert \( \hat{W} \) however, led to warnings by the inversion routine that the matrix is nearly singular and the calculated inverse may not be significant. This implies that numerical difficulties would be encountered while trying to retrieve all eight parameters. If several of the parameters are constrained to given values, this eliminates the corresponding row and column from \( \hat{W} \). In general this makes retrieval of the other parameters easier. The effect of various sets of constrained parameters were studied by eliminating selected rows and columns and then trying to invert the resulting reduced matrix. Some of the results obtained are listed in Table 13. It is seen from the column labeled 3, that if only the CO\(_2\) mixing ratio, resolution, and zenith angle are determined from a spectrum like Fig. 6 with 1\% noise, the respective uncertainties are 10.5 ppm, 0.00018 cm\(^{-1}\), and 0.0105°. If the noise is 2\%, the uncertainties would be twice as large. Any attempts to determine more than one temperature value always led to very large uncertainties, as compared to the cases where only one temperature was determined. This is consistent with the conclusions in the previous section. Trying to determine \( T(41) \) and \( T(42) \) is the same as trying to determine their difference and average. Yet the temperature difference is very hard to determine, and this gives rise to increased uncertainties in \( T(41) \) and \( T(42) \).

Another way to think of this problem is to consider the addition of a constraint as an injection of information into the analysis. The additional information spreads out over the variance-covariance matrix and leads to smaller uncertainties in the unconstrained parameters. The extent to which the constraint of \( a:j \) improves the retrieval of \( \theta_j \) is determined by the correlation coefficient between \( \theta_i \) and \( \theta_j \). This is given by \( S_{ij}/\sqrt{S_{ii}S_{jj}} \).

It is also seen in Table 13 that attempts to retrieve the zenith angle and the ground level pressure \( P(0) \) produced inversion problems and increased uncertainties. From Table 11 it is seen that this corresponds to the second "worst" parameter combination (column 2 of eigenvectors). Its
Table 13. Parameter uncertainties for various sets of parameter constraints, assuming an rms noise of 1%.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>1</th>
<th>3</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO₂ mix. r.</td>
<td>14.2* ppm</td>
<td>10.5</td>
<td>10.97</td>
<td>10.87</td>
<td>10.87*</td>
<td>10.54*</td>
</tr>
<tr>
<td>resolution</td>
<td>0.00026* cm⁻¹</td>
<td>0.00018</td>
<td>0.00023</td>
<td>0.00023</td>
<td>0.00018*</td>
<td>0.00023*</td>
</tr>
<tr>
<td>zenith angle</td>
<td>0.042°*</td>
<td>0.0105</td>
<td>0.0137</td>
<td>0.0138</td>
<td>0.023*</td>
<td>0.040*</td>
</tr>
<tr>
<td>T(41)</td>
<td>119.5 K*</td>
<td>-</td>
<td>4.91</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>T(42)</td>
<td>157.1 K*</td>
<td>-</td>
<td>-</td>
<td>6.47</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>T(40)</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>166.2°K*</td>
<td>-</td>
</tr>
<tr>
<td>P(0)</td>
<td>78.4 mb*</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>72.8*</td>
</tr>
<tr>
<td>background</td>
<td>0.00094*</td>
<td>-</td>
<td>0.00088</td>
<td>0.00088</td>
<td>0.00091*</td>
<td>0.00094*</td>
</tr>
</tbody>
</table>

*indicates inversion of nearly singular matrix
corresponding eigenvalue, though larger than the smallest, is still 5,000 times smaller than the largest eigenvalue and therefore corresponds to a set of parameter steps having a small effect on the spectrum.

The above techniques of information analysis explore the quality of the information in a proposed set of data. They can be used, therefore, to compare different experimental designs by comparisons of the information in the data produced by the different designs. This function of the techniques was employed to study the effect of decreased instrument resolution on the information in the spectra analyzed above.

C. LOW RESOLUTION INFORMATION ANALYSIS

The calculation steps of the previous two sections were repeated with the parameter values in Table 14. The new reference spectrum is shown in Fig. 10. This spectrum contains 40 points from 1900 - 1902 cm\(^{-1}\) which is 2 points per full width at half height of the slit function. Clearly, since there are five times more points in the high-resolution spectra, the summed squared difference spectra should be correspondingly higher. Any deviation from a five-fold change is an indication of differences in the influence of the parameters on the spectrum. The ratios of the summed squared difference spectra are listed in column 4 of Table 14. Only the value for the resolution is less than the expected value of 5. Since both resolution changes were +4%, this implies that the low-resolution spectrum is more sensitive to percent changes in instrument resolution than the high-resolution spectrum. Similarly, the large value (9.23) for T(41) indicates that the low-resolution spectrum is less sensitive to changes in the temperature in layer 41 and hence should yield considerably larger uncertainties in this parameter. Table 15 shows some typical standard deviations for the low-resolution spectrum. It is seen that the uncertainties are larger than for the high-resolution spectrum, especially the temperature uncertainties.

Table 16 shows some of the results of a Lees-type search for the "bad" parameters. The lowest eigenvalue of the modified information matrix corresponds to the zenith angle and P(O) values and the second lowest corresponds to the zigzagging temperature values. This is a reverse in order from the high-resolution case for the two "worst" combinations. Once again, however, the best combination is a simultaneous decrease in CO\(_2\) mixing ratio, zenith angle, ground-level pressure, and all three temperatures. The variation from worst to best corresponds to a change in summed squared difference of better than 100,000.
Table 14. Parameter values used to calculate low-resolution sample spectra. (The fourth column gives the ratio of the $\Sigma (\Delta y)^2$ values from Table 9 and those in column 3 for each parameter.)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values</th>
<th>$\Sigma (\Delta y)^2$</th>
<th>Ratio of $\Sigma (\Delta y)^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) CO$_2$ mixing ratio</td>
<td>322 ppm</td>
<td>0.0016442</td>
<td>7.16</td>
</tr>
<tr>
<td></td>
<td>354.2 ppm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(2) Resolution</td>
<td>0.10 cm$^{-1}$</td>
<td>0.014764</td>
<td>4.26</td>
</tr>
<tr>
<td></td>
<td>0.14 cm$^{-1}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(3) Zenith angle</td>
<td>95.2°</td>
<td>0.070241</td>
<td>6.33</td>
</tr>
<tr>
<td></td>
<td>95.4°</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(4) Temperature in layer 41</td>
<td>216.65 K</td>
<td>9.1177 x $10^{-6}$</td>
<td>9.23</td>
</tr>
<tr>
<td></td>
<td>218.65 K</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(5) Temperature in layer 42</td>
<td>216.65 K</td>
<td>6.147 x $10^{-6}$</td>
<td>8.91</td>
</tr>
<tr>
<td></td>
<td>218.65 K</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(6) Temperature in layer 40</td>
<td>216.65 K</td>
<td>7.6 x $10^{-8}$</td>
<td>6.43</td>
</tr>
<tr>
<td></td>
<td>218.65 K</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(7) Ground-level pressure</td>
<td>1013 mb</td>
<td>0.0012427</td>
<td>6.53</td>
</tr>
<tr>
<td></td>
<td>1063 mb</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(8) Background value</td>
<td>1.0</td>
<td>0.021652</td>
<td>5.06</td>
</tr>
<tr>
<td></td>
<td>1.025</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table 15. Parameter uncertainties for various sets of parameter constraints for low-resolution spectra, assuming an rms noise of 1%.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>2</th>
<th>3</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 CO₂ mix. r.</td>
<td>61.01 ppm</td>
<td>60.43</td>
<td>61.54</td>
<td>61.93</td>
<td>63.41</td>
<td>64.02*</td>
</tr>
<tr>
<td>2 resolution</td>
<td>0.0036 cm⁻¹</td>
<td>0.0034</td>
<td>0.0042</td>
<td>0.0041</td>
<td>0.0038</td>
<td>0.012*</td>
</tr>
<tr>
<td>3 zenith angle</td>
<td>0.057°</td>
<td>0.057</td>
<td>0.059</td>
<td>0.059</td>
<td>0.092</td>
<td>0.702*</td>
</tr>
<tr>
<td>4 T(41)</td>
<td>-</td>
<td>-</td>
<td>23.03 K</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>5 T(42)</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>29.97 K</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>6 T(40)</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>531.3 K</td>
</tr>
<tr>
<td>7 P(0)</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>1286* mb</td>
</tr>
<tr>
<td>8 background</td>
<td>0.0022</td>
<td>-</td>
<td>0.0023</td>
<td>0.0023</td>
<td>0.0023</td>
<td>0.0027*</td>
</tr>
</tbody>
</table>

*indicates inversion of nearly singular matrix
Table 16. Some eigenvectors and associated eigenvalues of modified information matrix for low-resolution spectra.

<table>
<thead>
<tr>
<th></th>
<th>Eigenvectors:</th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>(1)</td>
<td>0.0083607</td>
<td>0.05296</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(2)</td>
<td>0.025936</td>
<td>0.0074088</td>
<td>0.11675</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(3)</td>
<td>-0.70477</td>
<td>-0.13512</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(4)</td>
<td>-0.16379</td>
<td>0.65338</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(5)</td>
<td>-0.17926</td>
<td>-0.70975</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(6)</td>
<td>-0.016959</td>
<td>-0.06559</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(7)</td>
<td>0.66577</td>
<td>0.20956</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(8)</td>
<td>-0.0071575</td>
<td>0.0028461</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.25133</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Eigenvalues:</th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>(1)</td>
<td>$5.3967 \times 10^{-5}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(2)</td>
<td>$1.4169 \times 10^{-4}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(3)</td>
<td>0.0062167</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(4)</td>
<td>0.020332</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(5)</td>
<td>0.12136</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(6)</td>
<td>0.45162</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(7)</td>
<td>1.134</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(8)</td>
<td>6.2663</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
IV. CONCLUSIONS

This report has described the operation of a computer program for calculating atmospheric absorption spectra for slant paths through the atmosphere, using as input the AFGL line parameter listing. This program, unlike many others, was specifically written to employ an efficient means of including the effects of instrument spectral response functions. In addition the routine is written so that the precision of the convolved or degraded spectral values can be varied to match the noise level of observed spectra. The program was tested and compared to calculated spectra from another source and found to be working correctly.

Some information analysis techniques were then applied to a particular example of slant path spectra. The analysis included an identification of the "bad" parameters and estimated uncertainties for possible sets of unknown parameters. All that was required was a set of spectra and the corresponding conditions for each spectrum. With the aid of a few simple matrix operations the character of the information in the spectra was quickly determined. These techniques are simple and versatile and could be used on many different types of data, both simulated (as in this study) or observed.

The analysis indicated that trying to retrieve closely spaced temperature profile values can lead to large uncertainties in the temperature difference. Problems were also found with simultaneous retrieval of the base level pressure and apparent zenith angle. By analyzing a second set of spectra at a lower spectral resolution, the loss of information with loss of resolution was investigated. In particular, the loss of temperature information was found to be more pronounced than that for the other spectral parameters considered.
APPENDIX A

THE SPECTRUM CALCULATION PROGRAM

The basic layout of the program is shown in the flow chart (Fig. A-1). The four basic parts are (1) a main program controlling input and output and calculation order; (2) the Snider-Goldman slant path program (subroutine SNIDER and associated subroutines called within SNIDER) for calculating the path of radiation in an inhomogeneous atmosphere; (3) subroutine PATHST for converting the output of SNIDER into a series of layers with specific airmass, temperature, and pressure values; and (4) subroutine NSPEC for calculating the spectrum. All of the source statements for these parts are listed at the end of this appendix.

I. MAIN PROGRAM

There are three basic sets of inputs needed by the main or controlling program; these are listed in Table A-1. The first consists of the input parameters for the Snider-Goldman routine; these specify the observer-source geometry (ALAT, Z, HOBS) and the atmospheric profile (LEVELS, H, T, P). Since SNIDER produces its own pressure profile by integrating the hydrostatic equation and using P(0) and the temperature profile, only the first pressure value is used.

The second set consists of parameters needed by PATHST. These are a value for Nge, which determines the smallest airmass in a layer of [total airmass/Nge], and a set of values, R(1), R(2), ..., R(5), for calculating the mixing ratios in the layers. As currently written, only constant mixing ratios are allowed, but other types can be easily included by suitably modifying subroutine RMIX. Also, provision has been made for only five absorbing species but others could be included.

The third set of inputs are values needed to control NSPEC. These include the upper and lower frequency positions, VU and VL; the number of observed frequency values, NVO; and the parameters which control the convolution routine. These latter are discussed more fully in Chapter III describing subroutine NSPEC. Also included in this set is the unit number for the line parameters. This parameter must be passed to NSPEC which controls the input of the line parameter data for the spectrum calculation.

The output from the main program is in two parts. First is the calculated transmittance values starting from \( \tau(\text{VL}) \) up to \( \tau(\text{VU}) \). Second is a series of error codes. The subroutine ERROR called in the last statement of the controlling program dumps the stored error code numbers for any errors which may have occurred during execution of previous steps. These code numbers are in the order in which the errors occurred, and may be interpreted by referring to Table A2. No claims for completeness are made for this list of errors. An attempt was made to write self-correcting routines into the program for some of the more simple errors, but there are undoubtedly many which have not been corrected for. The first output
START

Input observer-source geometry

Read atmospheric profile

Calculate ray path, including refraction

Subroutine SNIDER and associated subroutines

Set-up airmass, temperature, pressure values for layers (combining thin layers if so needed)

Subroutines PATHST, RMIX

Input spectral parameters

Calculate spectrum

Subroutine NSPEC

STOP

Fig. A1 - Overall program logic
Table A1. Inputs to main program.

<table>
<thead>
<tr>
<th>Input</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>LEVELS</td>
<td>Number of levels in atmospheric profile (must be less than 190)</td>
</tr>
<tr>
<td>ALAT</td>
<td>Latitude of the observer (in degrees)</td>
</tr>
<tr>
<td>Z</td>
<td>Apparent zenith angle of incoming ray (in degrees)</td>
</tr>
<tr>
<td>HOBS</td>
<td>Observer height (in kilometers)</td>
</tr>
<tr>
<td>NGE</td>
<td>Integer for structuring layers for input to spectrum calculation routine</td>
</tr>
<tr>
<td>LUNIT</td>
<td>Unit number of file containing line parameters. This must be the same number as in a JCL DD card; e.g., if LUNIT = 11 then there is a DD card of the form //GO.FT11POOL DD . . . identifying the line parameter file.</td>
</tr>
<tr>
<td>H, T, P</td>
<td>Atmospheric profile where H is the height in kilometers, T is the temperature in Kelvin, and P is the pressure in mb. These are on unit 10 (see above).</td>
</tr>
<tr>
<td>R</td>
<td>An array of mixing ratio values. As currently written it requires five values ( R(l), \ldots, R(5) ) for the volume mixing ratio of each species; i.e., ( \frac{\text{molecules of absorber}}{\text{total molecules}} ).</td>
</tr>
<tr>
<td>( \tilde{\nu}_L )</td>
<td>Lower frequency position in ( \text{cm}^{-1} )</td>
</tr>
<tr>
<td>( \tilde{\nu}_U )</td>
<td>Upper frequency position in ( \text{cm}^{-1} )</td>
</tr>
<tr>
<td>NVO</td>
<td>Number of observed frequency values</td>
</tr>
<tr>
<td>NM</td>
<td>Set convolution iteration limits (see write-up for subroutine NSPEC)</td>
</tr>
<tr>
<td>NO</td>
<td></td>
</tr>
<tr>
<td>EPA</td>
<td>Convergence criterion. This corresponds to the estimated uncertainty in the transmittance values.</td>
</tr>
<tr>
<td>EXTNT</td>
<td>Sets the integration limits for the convolution. It is given as the number of B values (see below) in the integral.</td>
</tr>
<tr>
<td>B</td>
<td>Resolution width in ( \text{cm}^{-1} ). As currently written this value is half of the full width at half max of a Gaussian slit function.</td>
</tr>
<tr>
<td>LINTOP</td>
<td>Sets the maximum number of lines contributing to any one spectral value (must be less than 200)</td>
</tr>
</tbody>
</table>
Table Al (continued)

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>TTOP</td>
<td>Sets the maximum value of the absorption coefficient. When a calculated absorption coefficient exceeds TTOP, the corresponding monochromatic transmittance is set to zero.</td>
</tr>
<tr>
<td>NTST</td>
<td>Integer debug flag used to output intermediate convolution results.</td>
</tr>
<tr>
<td></td>
<td>NTST = 0</td>
</tr>
<tr>
<td></td>
<td>NTST = 1</td>
</tr>
<tr>
<td></td>
<td>NTST = 2</td>
</tr>
</tbody>
</table>

The NTST = 2 function has been removed from the version listed in this appendix.

All input is done with unformatted READ statements so that there are no specific format requirements for the input cards.
<table>
<thead>
<tr>
<th>Code No.</th>
<th>Description of Error and Action Taken</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>LEVELS value is greater than 190. LEVELS is set to minimum of 190 and LEVELS.</td>
</tr>
<tr>
<td>2</td>
<td>SNIDER could not find index of atmospheric layer containing the observer. Execution terminated.</td>
</tr>
<tr>
<td>3</td>
<td>SNIDER could not find index of atmospheric layer containing the source. JHT is set equal to LEVELS, where JHT is the variable labeling the index of the source layer. This is equivalent to assuming the source is at the top of the atmosphere.</td>
</tr>
<tr>
<td>4</td>
<td>Zenith angle is incorrect for specified observer-source geometry; e.g., Z &gt; 90 but HOBG &gt; Hsource. Execution terminated.</td>
</tr>
<tr>
<td>5</td>
<td>SNIDER has looped 10 times trying to find astronomical zenith angle without success to 0.001. Execution terminated [see Ref. (10)].</td>
</tr>
<tr>
<td>6</td>
<td>GAMMA = 0 in subroutine OM. Execution continues; results may be in error.</td>
</tr>
<tr>
<td>7</td>
<td>Error in OM, not #6 above. Execution continues; results may be in error.</td>
</tr>
<tr>
<td>8</td>
<td>Error in subroutine OPT1. Execution continues, results may be in error.</td>
</tr>
<tr>
<td>9</td>
<td>FTOT in subroutine PATHST is less than or equal to 0.001, indicating that essentially no airmass is in the path. Execution continues; results may be in error.</td>
</tr>
<tr>
<td>10</td>
<td>NM in subroutine NSPEC was specified too large. NM is set to minimum of 7 and NM.</td>
</tr>
<tr>
<td>11</td>
<td>Failure to converge in convolution routine of subroutine NSPEC for current value of frequency position and specified maximum number of iterations. Execution continues; current value on T-table main diagonal is used as transmittance value.</td>
</tr>
<tr>
<td>Code No.</td>
<td>Description of Error and Action Taken</td>
</tr>
<tr>
<td>---------</td>
<td>-------------------------------------</td>
</tr>
<tr>
<td>12</td>
<td>NLINES equals zero in subroutine NSPEC, indicating that there are no active lines at the current frequency position. Execution continues; transmittance value is set equal to 1.</td>
</tr>
<tr>
<td>13</td>
<td>The number of active lines, NLINES, is greater than LINTOP, the capacity of array IACTV. Execution continues; enough lines are kicked out so that NLINES equals LINTOP.</td>
</tr>
<tr>
<td>14</td>
<td>VU &lt; VL. Execution terminates.</td>
</tr>
</tbody>
</table>
value from ERROR is the number of type II errors which occurred. Since
this is a common error and may occur many times, only the number is kept
and not the sequence. Use of NTST = 1 may be used to check specific fre-
quency positions.

II. SUBROUTINE SNIDER

Questions about the operation of this part of the program can be
answered by referring to Ref. (10). A few minor changes were made in the
program listed in that reference in order to run it as a subroutine.

The most important change involved collecting all the error correc-
tions into the error code listing (Table A-2). Also the profile input
section was modified.

In addition to these changes, statements were inserted to cause
SNIDER to output the individual layer parameters (T, P, u) as it traced the
ray through the atmosphere. This is done by calls to subroutine POUT.
The layer parameters are stored in the array UED, PED, and TED kept in
blank COMMON.

An attempt was made to preserve as much of the flexibility of the
Snider-Goldman program as possible. This includes the option of specifying
the astronomical zenith angle and having the program find the corresponding
apparent zenith angle by an iterative search. To use this facility, the
input to SNIDER must be changed so that LSTOP, the 4th input value passed
to SNIDER, is equal to 1; see Ref. (10) before using this option.

One minor problem encountered with SNIDER during debugging is that
it will not run with an input zenith angle of zero. The associated sub-
routines are OM, OPT1, ASINX, ZCOMP, QUAD, GETT, and POUT.

III. SUBROUTINE PATHST

This subroutine takes the individual layer parameters stored in UED,
PED, and TED and rearranges them into a set of layers with nearly the same
airmass values stretching from the lowest layer crossed by the ray up to
the highest level.

First it sums all the airmass values to get FTOT, the total airmass.
It then folds the parameter arrays to combine contributions from the same
layer that occurred during the descending and ascending portions of the
path, if the zenith angle is greater than 90°. It next starts from the
lowest layer and combines the contributions of the next highest layers
until the summed airmass exceeds FTOT/Nge. A call to subroutine RMIX re-
turns a set of mixing ratio values for this composite layer and then the
program begins combining the next layers until the airmass again exceeds
FTOT/Nge. The recombination continues throughout the entire path. The
resulting modified set of atmospheric path parameters is stored in U,
PRES, TMP, and RMIXR in blank COMMON.
IV. SUBROUTINE NSPEC

This subroutine takes the path parameters from PATHST, the line parameters from unit LIMIT, and the frequency and convolution parameters from the SUBROUTINE call and calculates the transmittance. The file of line parameters has been created by a separate program BOB listed in Appendix B. These consist of (1) the lowest frequency at which the line has significant absorption, (2) the line intensity, (3) the pressure-broadening coefficient, (4) the lower state term value, (5) the molecule code number, and (6) 1/2 the frequency range of significant absorption by the line. The program has a set of arrays in which the parameter values of the active lines are stored. The input file is sorted on the lowest contributing frequency values and NSPEC proceeds from the lowest observed frequency value, VL, to highest value, VU. The input file is processed in sequence and the active lines are sorted by NSPEC according to the highest frequency at which they have significant absorption. Because of this double sorting (i.e., sorted input file and sorted active list), when the transmittance at a new frequency position is to be calculated, the program needs to check only the first active line to see if any lines need to be removed from the active file. If the first line is still active at the new frequency, all the other lines are also still active. This eliminates the need to check every active line at every frequency position. If the first line is no longer active it is deactivated and the next line is checked. This continues until all lines which are not active at the new frequency position have been removed. The program then checks the next line in the input file. If it is not active at the new frequency, none of the lines below it in the file will be, and the program proceeds to calculate the transmittance. If the new line is active, it is inserted into the active list in the proper sequence and then the next input line is checked. This minimizes the number of checking operations required to maintain a correct list of active lines. Also, by not storing the parameters of inactive lines in core, the overall storage requirements of the program are reduced considerably.

In addition to the input parameters, the program stores the molecular masses (in amu) in the array MAS. This value is needed to calculate the Doppler width. The active line parameters are stored in the arrays VO, SO, AMAS, ALL, EPP, MOLNM, and CENTW. Instead of sorting the elements of these seven arrays, an array of indices is kept, called IACTV, and these are kept in such a way that the order of the elements in IACTV determines the order in which the lines have to be checked for possible deactivation.

In order to calculate the convolved transmittance, \( \tau_{\text{con}} \), at observed frequency position, \( v_1 \), the program must calculate the monochromatic transmittance, \( \tau_{\text{mon}} \), at frequency positions \( v_1, \ldots, v_n \) (refer to Fig. 2). These are then multiplied by an instrument response (or slit) function value and summed to give \( \tau_{\text{con}} \). The storage of the \( \tau_{\text{mon}} \) values in array \( T \) proved to be the most logically involved aspect of the calculation. The actual values are calculated quite simply using the Hui et al. 23 Voigt routine and summing absorption coefficients by layers and then by active lines in two nested DO-loops. The slit function value, called WT,
is evaluated, multiplied by the $\tau_{\text{mon}}$ values, and summed in another loop. The problem is how to store the $\tau_{\text{mon}}$ values so as to be able to retrieve them efficiently. This is all done by proper arrangement of the values in the array $T$.

First, the maximum number of $\tau_{\text{mon}}$ values is determined from $NO$ and $NM$ according to $NTOT = 2 \cdot 2^NM + 1$. The $\tau_{\text{mon}}$ values will then be stored in the first $NTOT$ elements of $T$ as if each position in $T$ were a frequency position with a spacing between elements of $\text{DELVC} = \text{EXTNT} \times H/2^{NM+1}$. This spacing fits the $NTOT$ values into a total frequency range of $\text{EXTNT} \times H$, where $H$ is one-half the full width at half height of the slit function.

To start off the calculation, the first element of the $T$-table is evaluated using $NO$ to determine the number of points, as shown in Table A-3. Also listed are the number of new points (i.e., $\tau_{\text{mon}}$ values) used in subsequent iterations. The index $n$ along the left-hand side of the table is used by the program to determine the maximum number of iterations. When the $n$ value exceeds $NM$, the convolution stops iterating and takes the convergence failure error route.

For example, when $NO = 1$ and $NM = 5$, the first trapezoidal rule evaluation is made with five points. The corresponding $\tau_{\text{mon}}$ values are loaded into $T$. The next step involves a four-point midpoint rule evaluation. These two values are checked for convergence. If the convergence criterion is satisfied ($\text{AMTS} \leq \text{EPA}$), the convolved transmittance value is loaded into the array $TCI$. If there is no convergence, an eight-point midpoint rule evaluation is done and the $T$- and $M$-table values calculated and compared. The procedure continues until convergence or until the 32-point midpoint rule value is calculated. After this value, the convergence failure route is taken. In this way, up to 65 $\tau_{\text{mon}}$ values would be calculated and loaded into array $T$ in order of increasing frequency position. When moving to a new observed frequency position (next $VI$ value), the new $\tau_{\text{mon}}$ values that need to be calculated are written on top of the old $\tau_{\text{mon}}$ values which are no longer needed. In this way space is conserved and the values of $T$ can be efficiently retrieved.

As currently written, NSPEC generates its own observed frequency positions at which to calculate $\tau_{\text{con}}$ values. This can be easily changed to calculate $\tau_{\text{con}}$ values at specified nonuniformly spaced frequencies by passing the array of frequency positions to NSPEC and changing the scalar $VI$ to an array $V(I)$ of these frequency positions.
Table A3. The number of points in the first trapezoidal evaluation for different values of NO.

<table>
<thead>
<tr>
<th>NO</th>
<th>n = 0</th>
<th>n = 1</th>
<th>n = 2</th>
<th>n = 3</th>
<th>n = 4</th>
<th>n = 5</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>3</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>5</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>4</td>
<td>9</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>8</td>
<td>8</td>
<td>8</td>
<td>17</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>16</td>
<td>16</td>
<td>16</td>
<td>16</td>
<td>33</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>32</td>
<td>32</td>
<td>32</td>
<td>32</td>
<td>32</td>
<td>65</td>
</tr>
</tbody>
</table>

...
TIME=4, REGION=512K
/-JUGPARS- LINES=600,DISKID=3009
/NPL EXEC FJRXGC.PARM=(FORMAT,GOST4'T,
/- MAPIKREF=OPT(2),TIME=4,REGION=512K
/-FORT. SYSLIN OD DSN=TSG462.MSPEC.OBJ,DISP=(GL),PASS),
/- SPACE=(TK,(1,11))
/-FORT. SYSLIN ID D
DIMENSION UI1(360),PU1(360),TU1(360),U(50),PRES(50),TMP(50),
GMMIX1(5,50),H(200),P(200),T(200),R(5)
DIMENSION TCI(300)
REAL*8 VL, VU
COMMON M, PT, UI1, PU1, T1, PRES, TMP, RMIXR
REAU(5,0) LEVELS, ALAT, Z, HOBS, NGE, LUNIT
DO 100 I=1, LEVELS
REAU(10,0) H(I), T(I), P(I)
100 CONTINUE
CALL SNIDER(LEVELS, ALAT, G, Z, 0.0, HOBS, 82.0, 1)
READ(5,0) R(1), R(2) ! R(3), R(4), R(5)
CALL PATHSINGE,R,LEVTOP)
READ(5,0) VGL, VU, NVO, NMA, NO, EPA, EXTNTB, LIINTOP, TTOP, NTST
CALL NSPEC(VGL, VU, NVO, NMA, NO, EPA, EXTNTB, LIINTOP, LEVTOP, TTOP,
NTST, LUNIT, TCI)
DO 500 I=1, NVG
WRITE(1,110) TCI(I)
110 FORMAT(F8.5,1X,F11.5, IX,13)
CALL ESME(L, J, L, NTST, LIMIT, T)
END
DIMENSION VARCOM(200)
DIMENSION P(260)
DIMENSION H(200), T(200), GRAD(200), GAMMA(200)
DIMENSION Z(200)
DIMENSION THEAS(200), DELTH(200)
DIMENSION DHSTRA(200)
DIMENSION AIRS(200)
DIMENSION ESTR(200)
DIMENSION RHG(200), ZRHG(200)
DIMENSION XPTS(6), XGHT(6)
REAL*8 TITLE(13)
COMMON M, PT, VARCOM
EXECUTE SLANT/ VARCOM
EQUIVALENCE (VARCOM(1:6), (VARCOM(2),AIRWT), (VARCOM(3),)
1 RSTAR), (VARCOM(4), RADIUS), (VARCOM(5), CONST1), (VARCOM(6)
2 XPTS(1:7), (VARCOM(12), XGHT(1)), (VARCOM(18), FAKE)
EQUIVALENCE (VARCOM(2:6), REFM)
REAL*8 VARCOM(200)
FCNA1(Q00FL) = (1.0 + Q000F0L/2.0) * (1.0 + 2.0 * Q000F0L * (1.0 + Q000F0L/2.0) * 3.0)
FCNA1(Q00FL) = 1.0 * Q000F0L * (1.0 + Q000F0L/2.0) * 3.0
FCNU1(Q00FL) = 0.0 * Q000F0L * (1.0 + Q000F0L/2.0) * 3.0
FCNU1(Q00FL) = 0.0 * Q000F0L * (1.0 + Q000F0L/2.0) * 3.0
FCNU1(Q00FL) = 0.0 * Q000F0L * (1.0 + Q000F0L/2.0) * 3.0
FCNU1(Q00FL) = 0.0 * Q000F0L * (1.0 + Q000F0L/2.0) * 3.0
FCNU1(Q00FL) = 0.0 * Q000F0L * (1.0 + Q000F0L/2.0) * 3.0
FCNU1(Q00FL) = 0.0 * Q000F0L * (1.0 + Q000F0L/2.0) * 3.0
FCNU1(Q00FL) = 0.0 * Q000F0L * (1.0 + Q000F0L/2.0) * 3.0
FCNU1(Q00FL) = 0.0 * Q000F0L * (1.0 + Q000F0L/2.0) * 3.0
EQUATION(x)=PHI*Y/(RADIUS* X)
EQUATION(x)=PHI*Y/(RADIUS* X)
NTATA=3
NUMC=6
NITA=3=6
RDFL=2.06264866E+6
RDFL=1.74532936E-6
FAKE=-1000000.0
XPTS(1) = 466234757E+00
XPTS(2) = 339604693E+00
XPTS(3) = 119309593E+00
XPTS(4) = 119309593E+00
XPTS(5) = 33064693E+00
wHT(1) = 5662241E-01
wHT(2) = 18630786E+00
wHT(3) = 23395967E+00
wHT(4) = 23395967E+00
wHT(5) = 18630786E+00
wHT(6) = 5662241E-01
AVNMB = 6.02257E2b
LEVELS = MIC(LEVELS, 190)

IF (LEVELS GT 190) CALL ERRCR(1,0)
LEVELS = MIC(LEVELS, 190)

1000 CONTINUE
C1000 READ (NTATA2, 1021) (TITLE(I), I=1,13)
1021 FORMAT(13A6)
ALTRHR = 1.0

PHI = ALAT * RADCON
A = 6378160.0
S = 6556773.0
R = SQRT((A**2*(COS(PHI))**2 + B**2*(SIN(PHI))**2)) / (A - 2 * (COS(PHI)) - (SIN(PHI))**2)
X = COS(2.0 * PHI)
Y = COS(4.0 * PHI)
G = 980.6160 * (1.0 - (0.0026373 * X) + (0.0000059 * X**2))
G = G/169.0

PARTGZ = 3.7838462 E-06 + 2.27 E-02 X - 2.3 E-04 Y

RADIUS = 2.0 * G / PARTGZ
RAD = R
RSTAK = 631.439
AIRAt = 28.966
CONST1 = G * AIRAt/RSTAK
GEE = 9.80665
PHI = RADIUS / GEE
DU 1 I = 1, LEVELS
P(I) = P(I-1)**100.
H(I) = H(I)*1000.

1 CONTINUE

1051 CONTINUE
IF(P(I-1) EQ 0) P(I) = 101325.0
DO 1090 I = 2, LEVELS
CALL GETT(H(I-1), H(I), P(I-1), P(I), T(I-1), T(I))
1090 CONTINUE

1000 CONTINUE
DO 1125 I = 1, LEVELS
H(I) = FHC(H(I))
1125 CONTINUE

1150 CONTINUE
DO 1175 I = 2, LEVELS
GRAD(I-1) = (T(I-1) - T(I-1))/H(I-1)
GAMMA(I-1) = (CONST1/GRAD(I-1) + CONST1)
DELTH(I-1) = H(I) - H(I-1)
1175 CONTINUE
GAMMA(LEVELS) = 1.
GRAD(LEVELS) = G.
DELTH(LEVELS) = 0.0
SUMKMu = 0.0
DU 1190 I = 1, LEVELS
ZKH0(I) = AVNMB * P(I) / (RSTAK * T(I))
00000490
SU=KMHG = SUMRHC + ZRHO(I)*DELT(H(I))
00001060
1190 CONTINUE 00001070
RHO(I) = ZRHO(I)
00001080
OMSTRA = 1.0 -( RHO(I) / 2.9475521E25 )
00001090
DO 1230 I=2,LEVELS 00001100
CALL UM(M(I-1)+T(I-1)+T(I-1)+GAMMA(I-1)+OMEGA, DUMMY)
00001110
NLC = I-1
00001120
OMSTRA(NLC) = OMEGA
00001130
RHO(I) = RHO(I-1)+ (1.0-OMEGA)
00001140
CALL OPT1(M(I-1)+T(I-1)+T(I-1)+GAMMA(I-1)+RHO(I-1)+OMEGA+AIRS(I-1))
00001150
1)
00001160
1200 CONTINUE
00001170
AIRS(LEVELS)=0.0
00001180
DO 1225 I=2,LEVELS
00001190
IND=LEVELS+I-1
00001200
AIRS(IND)=AIRS(IND)+AIRS(IND+I)
00001210
1225 CONTINUE
00001220
STARD = AIRS(1)
00001230
C
00001240
REFAM = AIRS(1)
00001250
1243 FORMAT(IH1)
00001260
LINC = 1
00001270
ALTOZH = 1.0
00001280
CALL POUT(-1.0,0.0,0.0)
00001290
1250 CONTINUE
00001300
DD3 = DD3 * 1000.0
00001310
DD4 = DD4 * 1000.0
00001320
NLOP = 0
00001330
JMP = LSTOP + 1
00001340
NTF = 0
00001350
LINC = 1
00001360
GO TO (1257, 1258, 1261, 1253, 1254, 1255)
00001370
1256 GO TO 1400
00001380
1257 DD = DD + IN = 1.50
00001390
NTF = 0
00001400
NLOP = NLOP + 1
00001410
IF (NLOP. GT. NLOPT) GO TO 1400
00001420
1297 CONTINUE
00001430
ZO = DD1
00001440
ZS = ZG
00001450
OHGMT = DD3
00001460
HGMT = DD4
00001470
1258 WAVE = DD2
00001480
ZT = ZO
00001490
1270 IF (ALTOZH) 1280, 1290, 1280
00001500
1280 OHGMT=FHC(OHGMT)
00001510
HGMT = FHC(HGMT)
00001520
1290 CONTINUE
00001530
ZCS = ZO
00001540
ZT = ZO
00001550
1295 CONTINUE
00001560
NTF = NTF + 1
00001570
IF (NTF - 10) 1296, 1296, 1296
00001580
1296 CONTINUE
00001590
SECT2 = C
00001600
SECT3 = 0.0
00001610
SECT4 = C.0
00001620
RSAVE = 0.0
00001630
OSAVE = 0.0
00001640
PSAVE = 0.0
00001650
TSAVE = 0.0
00001660
HDIFF = 0.0
00001670
00001680
HTA=C.C
TP =273.15
To=TP
ZG=Z0*RA0CN
UTEPE=1.0/J/AVEL**2
EI = U*U
EI =CC0064328*C294981/(145.0-UTEMP)**2
60002554/(41.0-UTEMP)
DU =1360/INT=2/LEVELS
IF((1-HT)-OHGT) 130,1325,1325
1300 CONTINUE
CALL eRAO(2,G)
RETURN
1325 INT=INT-1
CALL uETT (HINT), OHGT, P(IHT), POB, T(IHT), T(IHT) 
RHOP = AVNMB / RSTAR*T(IHT)
RHOHIN = RHOP
TP = T(IHT)
DO 1335 IND=2/LEVELS
JNT=IND
IF((1-HT)-OHGT) 1335,1340,1340
1335 CONTINUE
CALL ERROR(30)
1337 FORMAT(2CH UPPER HEIGHT RESET)
1350 JNT=IND
1340 CONTINUE
ESTR (1) = FCNE (1, OFMSTG )
DO 1350 I=2, LEVELS
ESTR(I) = FCNE (ESTR(I-1), OMSTRA(I-1))
1350 CONTINUE
JN=1
HMINA=OHGT
IF ((205.LT.90.0) .IF ((HGHT-OHGT+05) 4500,4600,1373
CALL uN(HGHT,H(IHT),H(IHT),T(IHT),GAMMA(IHT),OMEGA,XXX)
EC=FCNE (ESTR(IHT),OMEGA)
ZCRIT = ASIN ((1.0 + ESTR (1) ) * ( 1.0 - OHGT / RADIUS ) / ( 1.000000021 )
1 + EO/1)
ZCRIT=3.141592653-ZCRIT
IF ((205.LT.ZCRIT+0000) .IF ((OHGT-HGHT+05) 4500,4600,1357
FVAL =SIN(ZG)/(1.0 + EO/(RADIUS-OHGT))
F1=(1.0 + ESTR(I)) / RADIUS - FVAL
DO 1351 I=2, LEVELS
K=I-1
F2=(1.0 + ESTR(I)) / (RADIUS-H(I)) - FVAL
IF((F2-F1) 1352,1352,1351
1351 F1=F2
GO TO 4500
1352 H1=H(K)
1353 CALL uN(H3,H3, H(K),H(K),T(K),GAMMA(K),W,XXX)
F3=(1.0 + FCNE (ESTR(K),W)) / (RADIUS-H3)-FVAL
H3=H3-F3*(H3-H2)/ (F3-F2) + (H3-H1)(F3-F1) - (H2-H1)(F2-F1))
IF((ABS(H3-H3) .LE.1.* ) GG TO 1354
H1=H2
H2=H3
F1=F2
F2=F3
GO TO 1353
1354 IF ((H4+GT-HGHT+05) 4500,4600,1357
HMINA=HM
ZGSAVE=ZG
HOSAVE=OHGHT
HSSAVE=HGT
ZG=1.370796326
OHGHT=HM
HGT=HOSAVE
T6=T(K)
JSKV=JHT
JHT=INT+1
INT=K
INS=2
GO TO 1374
1355 RSA VE=REFRS
OSAVE=SECT2
PSAVE = SECT3
TSAVE = SECT4
HGT=HSSAVE
JHT=JSAV
INS=3
GO TO 1374
1356 IF(HSSAVE. LT. HOSAVE) JNS=2
OHGHT=HOSAVE
GO TO 3950
1357 CALL OM(HGTH,H(JHT),H(JHT),T(JHT),GAMMA(JHT),W,XXX)
ZSAVE=ASIN((1.0+E0)/1.0+FCNE(ESTR(JHT),W)*(RADIUS-HGTH)/(RADIUS-HGT))
IHT=JHT
ZZ=20
ZG=ZSAVE
HOSAVE=OHGHT
HSSAVE=HGT
OHGTH=HSSAVE
HGT=HOSAVE
Z0=ZZ
INS=4
GO TO 1374
1358 JNS=1
OHGTH=HOSAVE
HGT=HSSAVE
GO TO 3950
1373 INS=1
1374 CONTINUE
CALL OM(OHGH T,H(IHT),H(IHT),T(IHT),GAMMA(IHT),OME,DUMMY)
CALL OM(H(IHT+1),OHGH T,H(IHT),T(IHT),GAMMA(IHT),OM0,TOO)
EC=FCNE(ESTR(IHT),OME)
VARCOM(I9)=RHO(IHT)*I*(1.0-OME)
IF(JHT.EQ.INT+1) GO TO 1380
US=FCNU(FCNA(E0),FCNB(E0),EC,OMG)
CALL ZCUP(10*RT(1)+1)*OHGH T,H(IHT+1),US,DELTZ,TETAS(IHT+1)
1)
CALL 2A09(THETAS(IHT+1),Z0,OHGH T,TOG,P(IHT+1),GAMMA(IHT),EO,SECT1,SECT2,SECT3,SECT4)
CALL POUT(SECT2,SECT3,SECT4)
ReFk =(DELT * SECT1)
REFRS=REFR*RADSEC
2010 DELRS=REFRS
2060 INDU=JHT-2
IHT1=IHT+1
IF(INDU.LT.IHT1) GO TO 1376
1360 CONTINUE
.DO 1375 I=IHT1,INGU
U=FCNU(FCNA(ESTR(I)),FCNB(ESTR(I)),ESTR(I),OMS TRA(I))
CALL ZCUMP(Z(I),Z(I+1),H(I),H(I+1),U,DELTZ,TETAS(I+1))
3991 FORMAT (IH,5X25HREFRACTION AIRM ASS TABLES,5X13A6,/) 0003790
340X38HALL HEIGHTS ARE IN GEOMETRIC METERS /,40X,*ALL TEMPERATURES0003710
3ES ARE IN DEGREES KELVIN/,40X,*ALL PRESSURES ARE IN N/SQ M / 0003720
4X4XON THE APPARENT AND ASTRONOMICAL ANGLES ARE/
340X34HIN DECIMAL DEGREES FROM THE ZENITH/
C WRITE ( 5 , 3993 ) MAX
3993 FORMAT ( 40X,'THE WAVELENGTH FOR THIS TABLE IS ',F5.2,' MICR OMETR 0003760
15.1//
C WRITE (6,3992)
3992 FORMAT (1X5SMLOWER,5X5SHPPER,5X4H41N,*, 7 X7CHAPMAN , 5X7OPTICAL)0663790
C WRITE (6,3995)
3995 FORMAT (1X5SHAPP, 2X4X5HEIGHT,4X6HEIGHT,4X6HEIGHT,5X6HAIR-MASS,4X0003810
18HAIR MASS,5X5MMHDPF,3X10REFRACTION, 4X6HAST. Z,6X 6HP(TEFF),4X6H0O0003820
LT(TEFF),6X6HP(TAN) ) 0003830
C WRITE (6,3996)
3996 FORMAT (5X3H1(1),7X3H(2),7X3H(3),7X3H(4),8X3H(5), 8X3H(6),10X3H(7), 0003850
1 6X3H(8),9X3H(9),9X4H(10),6X4H(11), 8X4H(12),/,1X ) 0003860
LINC=42 0003870
3999 LINC=LINC-1 0003880
ZFIN = ZEND * RADCGN 0003890
OHGHT = F2C(OHGHT ) 0003900
HGT = F2C(HGT ) 0003910
M1NA = F2C(M1NA ) 0003920
SCALHP = RSTART * TP /AIRWRT / G 0003930
XP = ( RADIUS + OHGHT ) / SCALHP 0003940
WHY = SRT(C.5 * XP ) * ABS(COS(ZFIN)) 0003950
FERF = EXP((WHY)**2.0) * ( 1.0 - ERF(WHY)) 0003960
4040 CONTINUE 0004210
4150 CONTINUE 0004270
LSTOP = 3 0004275
GO TO (1250,4100,1250,1256,1000),JMP 0004280
4160 CONTINUE IF (ABS(ZT-ZEND) .LT.0.0001) GOTO 4200 0004290
Z0S=ZT DERF 0004310
Z0=Z0S 0004320
GG TO 1245 0004330
4200 JMP=1 0004340
GO TO 3950 0004350
4500 CALL ERROR(4,0) 0004370
4510 FORMAT(1X4F9.5,6GX:O H *** NO SOLUTION *** ) 0004380
LINC=LINC-1 0004390
RETURN 0004400
4600 REFRS=C. 0004400
SECT2=C. 0004410
SECT3=C. 0004420
SECT4=C. 0004430
GO TO 3950 0004440
4700 IF (ABS(ZT-ZEND) .LT.0.0001) GO TO 4200 0004450
LINC=LINC-2 0004460
CALL ERROR(4,0) 0004470
4705 FORMAT(1H ,37H *** NO GCOL SOLUTION FOR LINE ABOVE *** ) 0004500
1063 FORMAT( 1H , 'UNREFRACTED RAY STRIKES DISC ' ) 0004520
RETURN 0004540
1460 CONTINUE 0004540
RETURN 0004560
END 0004560
SUBROUTINE UM(HHC,IV,H,GAMMA,MGEA,TO) 0004610
C CHAPMAN /SLANT/ G AIRWRT, RSTART, RADIUS, CONST1 0004620
GM=ABS(GAMMA) 0004630
IF(UM .LT.0.000001) GO TO 801 0004640
ONE6=1.0-GAMMA 0004650
ONE6=ONE6 0004660
IF(RADIUS+H) 500,550,630
500 CONTINUE
X=CONST*(RADIUS-HC)/TN
GO TO 700
600 CONTINUE
A=CONST*(H-3E)
T=TN+CONST*(H-3E)*(1+ONEG)/GAMMA
X=A/T
700 CONTINUE
Y=X/GAMMA
IF(Y*THETA(-30*30)) GO TO 600
IF(Y*THETA(-1*ONEG*Y)) 800,800*300
400 IF(Y*THETA(1*ONEG*Y)**(-1*ONEG)) RETURN
300 OMEGA=1+1*ONEG*Y**(-1*ONEG)
CONTINUE
600 CONTINUE
IF(Y*THETA(-30*30)) Y=0
1 FORMAT (1H,5E26*8)
IF(ABS(Y) GT 25*30) GO TO 10
CONTINUE
10 CONTINUE
RETURN
801 CALL ERROR(6*3)
802 FORMAT(IX,BH,GAMMA=0)
803 CALL ERROR(7*3)
804 FORMAT('30G800-*4E29*8')
RETURN
END
SUBROUTINE UPTI(H,H,H,T,GAMMA,HOC,OMEGA,AIMR)
CGM1**/SLANT/ GAIRM,H,STAR,RADIUS,CONST1
RAD=RADIUS-HO
XX=CONST/RAD/(T+GAMMA)
SM=H-HOC/RADIUS-HG
ONE=1.0-SM
OMG=GMMA-1.0
XX2=(1.0-OMG*SM)/XX/ONE
SM*U=0.0
SMV=0.0
XN=0*3
DENG=1.0
TERM=1.0
TEST=(0.0*G0.001/XX*GAMMA)
KCOUNT=0
1000 CONTINUE
KOUNT=KOUNT+1
XX=XX+1.0
DENG=DENG+ONE
FACT=AN/(XX*DENG)
TERM=TERM*FACT
TERMV=TERMV*FACT*XX
SUMU=SUMU+TERM
SUMV=SUMV+TERMV
IF (KOUNT-31) 1040,1090,1080
1040 IF(ABS(T(1*ABSTERM))) 1050,1050,1050
1050 IF(ABS(TERM)) 1060,1060,1075
1075 IF (KOUNT-35) 1060,1060,1075
1080 WRITE(610,1060)
1090 FORMAT(17H0,30G800 IN CPT1)
1100 AIR=(RADIUS**2/RAD)**HOC*(SUMU/(1.0-OMEGA)**SUMV/ONE)
RETURN
END
FUNCTION ASIN(X)(X)

CUNEC=C(2)
CUNEC=2.0
CUNEC=C(2)

END

DIMENSION XPTS(5),THTPTS(6),VALUES(6)
DIMENSION IS(3)
DIMENSION IS(3)

EQUIVALENCE (VARCOM(2),AIRWTI,IVARCOM)
EQUIVALENCE (VARCOM(12),RAIRWB,ivarcom)
EQUIVALENCE (VARCOM(18),FAKE)
EQUIVALENCE (VARCOM(19),RHO)
EQUIVALENCE (VARCOM(1),RADIUS)
EQUIVALENCE (VARCOM(2),RADIUS)
EQUIVALENCE (VARCOM(5),RADIUS)
EQUIVALENCE (VARCOM(12),RADIUS)
EQUIVALENCE (VARCOM(18),RADIUS)
EQUIVALENCE (VARCOM(19),RADIUS)

RETURN

END

SMALLR=KAOIuS-»-HO+hO**2/( RADIUS -HO )
V M
A -

A = FCfJ(A(EO )

HINT (I ) = FCfJ(THTPTS(I ),T)
HINT (I ) = FCfJ(THTPTS(I )

VALUES (I ) = FCfJ(VALuE(I ))
VALUES (I ) = FCfJ(VALuE(I ))

SUbkOUTINc wUADlThETA»ZC9H07

T»P9GAMMA,FCTSUM,VALM»PBAR11 BAR)
DIMCNSIt
NSIGN VALUCA(6)
DIMENSION VARCOM5Q)
DIMENSION isiNT(u)
DIMENSION XPTS(5),THTPTS(6) ?WGHT(6) ,VALUES(6)

SUbkOUTINc wUADlThETA»ZC9H07
VALM=VALC*VALP

PEAK = VALM*P
TDAM = VALM*T
RETURN

END

SUBROUTINE POUT(A1,A2,A3)

DIMENSION UED(3C),TED(3C),PED(3C),H(200),P(200),T(200)
COMMON H,P,T,UED,PED,TED,IED

IF (A1.EQ.-1.0) GO TO 100

RETURN

100 IED=1

RETURN

END

SUBROUTINE PATHSTINC 

DIMENSION UED(3C),TED(3C),PED(3C),H(200),P(200),T(200)
COMMON H,P,T,UED,PED,TED,IED

RETURN

100 IED=1

RETURN

END

SUBROUTINE PATHSTINC 

DIMENSION UED(3C),TED(3C),PED(3C),H(200),P(200),T(200)
COMMON H,P,T,UED,PED,TED,IED

RETURN

100 IED=1

RETURN

END
Du 200 J=1,NFCLU
K=NFOLD+J
UIN(K)=UIN(J)+UIN(K)
PUT(K)=PUT(J)+PUT(K)
T(J)=TU(J)+TU(K)

260 CONTINUE
270 J=NFOLD+1

K=0
IF (FTGT.LE.0.001) CALL ERRCRT(9,0)
SUMU=0.0
SUMTU=0.0
DU 400 J=J1,IEC
SUMU=SUMU+UIN(J)
SUMPU=SUMPU+PUT(J)
SUMTU=SUMTU+TU(J)
IF (SUMU+ST.TETCT/AGE) GO TO 390
GO TO 400

390 K=K+1
U(J)=SUMU
PRES(K)=SUMPU/SUMU
TMPI(K)=SUMTU/SUMU

420 CONTINUE
DU 500 J=1,K
DO 500 I=1,K
RMIX(I,J)=RMIX(I,J,PRES(J),RN)

500 CONTINUE
600 CONTINUE
RETURN
END

FUNCTION RMIX(I,P,RN)

END

DIMENSION RN(5)
RMIX=RN(I)
RETURN
END

SUBROUTINE HSPEC(VL,VU,NVCL,NM,NO,EP,A,EXTNT,H,LIBTOP,H,LINTOP,NLEVLS,
*TTOP,NT,IVINT,TCI)

REAL 3 IRUM(*)
C=4PLEX*16 AC/I1*2267931777164326002*0.0001)/A1/
+(2*14392368694706425002*0.0001)/A2/(1*81929533092181549002,
+0.000040)
+(1.736558465613541001*0.000050)
+(1.612562609773155001,0.000060)
+(5.91262609773155001,0.000070)
+(0.000080)
+(5.4572478795897737002*0.000090)
+(5.4878917719495792002,0.000100)
+(1.7354301821091472002,0.000110)
+(1.49929091224267501*0.000120)
+(2.1267931777164326002,0.000130)

DIMENSION H(1200),PX(1200),T(1200),UIN(1300),PUI(300),TUK(500)
REAL 3 VLUG,T,X,Y,ABSK,V0,V1,VK,VK,VL,VU,VBH,VONXT,VOU,VUP,DZABS
DIMENSION V(200),SG(200),ALL(200),EPP(200),TCI(300),
2 MOLN(C3C),NH(7),NSTw(T7),T(7,7),AMK(8),PRES(50),TMP(50),
3 U(50),AMIX(5,50),IACTV(200),AMAS(200),CEM(200)
REAL FRA (5) / 180.0, 44.0, 360.0, 0.0, 29.0 /
INTEGER * ART (5) / 2, 3, 2, 2, 2 /
COMPLEX HX, PA, TX, UINX, PUX, TUX, IECD, U, PRES, TMP, RMIXR
CALL CANDFL
ASSIGN 137 TO ISWT
IF (vU LE vL) GOTO 1350
NLINES = 0
NTAIL = 1
DO 20 JL = 1, 12

20 IF (NLINES.EQ.0) GOTO 1350
NLINES = NLINES + 1
VT = 101330.
F = 2.73
Curt = ALJG (2)
ALN = SORT (CONST)
PL = 3.141592654
CONST = ALN2 / SORT (PT)
IF (NM.EQ.7) CALL ERROR (10, G)
NM = MIN (NM, 7)
WID = EXTNT*H/2.
NTOT = 2*2*NM + 1
READ (LU1, T, 0, END = 1340) VCNX, SCNXT, ALNX, EPNX, MOLNX, CWNX
9010 FORM (19:3) = (10:3)
VCNX = VNXT + CWNX
DELVC = EXTNT*M/FLOAT (2**NM + 1)
110 I = 1
VI = vL
120 NBH = 1
VBM = VI - DELVC / FLOAT (NTOT + 1) / FLOAT (2)
NH (1) = 2**NM - NO
NST w (1) = 2**NM - NO
MTOP = NH - NO + 1
DO 125 M = 2, MTOP
NH (M) = 2**NM - NO - M
NST w (M) = 2**NM - NO - M
125 CONTINUE
EPA = EPA / FLONX (NST w (1)) / DELVC
130 NWL = 1
NST = NST w (1) / NWL
K = NH (1) / NST
NOUT = G
IF (NLINES .LE. 6) GOTO 132
131 IF (VU I ACMTV (I TAIL) ) + CENT (I ACMTV (I TAIL)) * GT * VI - WID) GOTO 132
ITAIL = MOD (ITAIL, LINTOP) + 1
NOUT = NOUT + 1
132 NLINES = NLINES + 1
133 IF (VUNX = CWNX.GT. VI + WID) GOTO 138
IF (VUNX = CWNX GT. VI + WID) GOTO 136
ILOAD = I ACMTV (100 (ITAIL + NLINES - 1, LINTOP) + 1)
VU (I LOAD) = VCNX
SU (I LOAD) = SCNXT/GNST
AMAS (I LOAD) = VCNXT + 0.581333E-07 / SQRT (FMAS (MOLNX))
ALL (I LOAD) = ALNX + ALN2 / PO * SQRT (T) / AMAS (I LOAD)
EPPI (I LOAD) = EPNX / 0.6946 / TC
MOLN (I LOAD) = MOLNX
CcnW (I LOAD) = CWNX
VOp = VUNX + CNX
J = NLINES - 1
NLINES = NLINES + 1
134 K1 = MOD (ITAIL, J + 1) LINTOP) + 1

INXT=IACTV(K1)

IF(VUP.K.LTAIL) GOTO 136
K=MOD(ITAIL+J,LINTUP)+1

IACTV(K1)=INXT

IF(J.EQ.3) GOTO 136
J=J-1

GU TO 134

136 CONTINUE

GU TO ISXT(I37,138)

137 READ(IU,II,9010,EQQ=133C) VMXT,SCXT,ALLNXT,EPNNXT,MOLNXT,CWNXT

VOXX=VCNX+CTNX

GU TO 133

138 CONTINUE

IF(ALINES.LE.0) GOTO 132

140 VK=VBR+DELC+PLCAT(IK)

IF(K.EQ.NTOT) GOTO 410

ALL=ALL(T)

AMASL=AMAS(L)

EPPL=EPPL(I)

NPARTL=NPART(MOLNML)

DO = SBC(IAT)+1,NEVLS

RT=TO/TEMP

ALD=AMASL*SWRT(TEMP)

BOLT=SIGN(RT**NPARTL)*EXP(EPLL*RT-1.0)

AKO=UL(IAT)*SOL*ALD/ALD*RMIXR(MOLNML,IAT)

Y=ALL*PRE5IAT/TEMP

X=VOL/ALD

Z=x=CHPLX(Y-x)

F=(1.0*(Z+H)*Z+H+3.0)*Z+H+2.0)*Z+H+1.0)*Z+H+0.0

ZVQV=1.0

DABS=AKO*ZVQV

D=AB=AKO*ZVQV

360 CONTINUE

IF(ABSK.G.E.TTUP) GOTO 210

200 CONTINUE

210 NK=AGQ(NBH+K-1,NTOT)+1

TINX=DEXY+ADSK

C

IF(NST.EQ.2) WRITE(14,9214) T(NK),VK

9014 FORMAT(1R8.5,1X,F15.5)

K=NST

460 GL TO 140

410 NHG=NST

CNVT=CN

SU=MT=C

MH(I)=NHG

620 NIK=MOD(VK+NHG,NHC-1,NTOT)+1

VK=VBR+DELC+FLOAT(NHC)

WT=CNST1/H*EXP(-SGL(VI-VK))*2.0*CONST2/H**2

CGNN=CNVT+WT*T(NK)

SU=MT=SNAT+WT

NHG=NHC-4ST

IF(NHC.LT.0) GOTO 510

560 GO TO 420


510  SUMT2=SUMVT
    TK3=CVNV
    IF(NST.1N.1) WRITE(13,9013) TKC
5913  FORMAT(5(14,1x)
    NNL=2
520  IF((NNL-1+N3+ST*M) GOTO 1310
    NST=NST+1
    K*VNT(NNL)*VST
530  VK*VNH+ELVC=FLOAT(K)
    IF(K.GT.NFGT) GOTO 510
    ABSK=K.
    DO 606 L1=1,NMLINES
    L=IACTV(*OD,ITAIL+L1-2,LINTCP)+1
    MGLML=MGLNLML
    SUL=SC(L)
    VGL=VK*VGL(L)+ALL2
    ALLL=ALL(L)
    AMASL=AMAS(L)
    EPPL=EPPL(L)
    NPARLT=NPAR(T-MGLNLML)
    DO 700 IAT=1,NLEVLS
    TEMP=TMP(IAT)
    RT=TO/TEMP
    ALD=AMASL*SCRT(TEMP)
    BOLT=SQRT(RT**NPARLT)*EXP(EPP**(RT-1.))
    AKG=UAT+SOFL*BOLT/ALDRMIXR(MGLNLML+IAT)
    Y=ALLL*PRES(IAT)/TEMP
    X=VGL/ALD
    ZH=CMPLX(Y,-X)
    F=('((((A0+ZH+A5)*ZH+A4)*ZH+A3)*ZH+A2)*ZH+A1)*ZH+A0)
    Z=('((((Z0+ZH+B5)*ZH+Z0)*ZH+Z0)*ZH+Z3)*ZH+Z0)*ZH+Z0)
    ZV=ZT-F
    DZAB=AKG*ZV
    ABSK=ABSK+DZAB
700  CONTINUE
    IF(ABSK>ST+TTOP) GOTO 610
600  CONTINUE
610  NK=MG0(KBH+K-1*NTGT)+1
    T(NK)=DEXP(-ABSK)
    IF(NST.EQ.2) WRITE(14,9314) T(NK),VK
700  CONTINUE
800  GO TO 530
810  NN=C-K-NST
    CGNV=0.
    SUK=N0
    NNMLT=NN
820  NIK=MUH(NBH+NNH-1,NTOT)+1
    VIK=VBD+DELVE FLOAT(NHC)
    M=CONST1/H**EXPL(-SMGL(VI-VIK)**2*CONST2/H**2)
    CGNV=CGNV+HT**T(VI)
    SUMT=SU14N+K
    NNHC=NNHC+VST
    IF(NHC.LT.0) GOTO 910
900  GO TO 620
910  SU14N2=SUK*ST2+SUMT
    CGNV=CGNV/FLOAT(2**2*(NNL-2))
    IF(NWL.LE.2) GOTO 1010
    NSTPR=NNL-2
    DO 1000 NCR=1,NSTPR
    FNCR=FLOAT(4**2*NCR)
    AMK=(FNCR*CONVT-AMK(L,CR))/1(FNCR-1.0)
    AMK(NCR)=CONVT
CUNV=AKKN
1000 CONTINUE
1010 AKK(NNL-1)=CQ.VT
AMTS=ADSF(TK0-CUNV)
IF(AKTS.LE.QPA) GOTO 1110
DAVF=LAGAT(2*4**INML-1)/FLCAT(4**NNL-1-1)
TK0=CUNV+DAVF*(TK0-CUNV)
IF(NST.EQ.1) WRITE(13,9013) AMK,TK0
NNL=NNL+1
1160 GO TO 320
1110 TCI(I)=FLCAT(INST(I)/2)*DELVC*(CUNV+TK0)
IF(INST.EQ.11) WRITE(13,9013) AMK
1140 IF(I.EQ.NVO) RETURN
I=1+1
VI=VL*FLOAT(I-1)*(VU-VL)/FLCAT(NVC-1)
VDB=TV*VDBH/DELVC*FLOAT(INTCT(I)/2)
IF(VDB*GE.*FLUGAT(NTOT-I)) GOTO 12C
NDBH=I*TVDBH
NDB=MID(NDB+NBH-1,NCT)+1
VDB=VDB+DELVC*FLOAT(NDBH)
JSTOP=NN-NK+1
GO TO 1200 J=1,JSTOP
NH(I)=NH(J)-NDBH
1200 CONTINUE
NCH=1
NST=NSTw(I)
1490 NHM=NH(NCH)
1500 IF(NHM*GE.*NST) GOTO 1510
NHM=NHM+NST
GO TO 1500
1510 NH(NCH)=NHM
1520 NCH=NCH+1
IF(NCH.GT.(AKM-NG+1)) GOTO 1500
NST=NSTW(NCH)
GO TO 1490
1660 CONTINUE
GO TO 130
1310 TCI(I)=TKG*DELVC*FLOAT(NSTW(I))
CALL ERROR(11,C)
GO TO 1120
1320 TCI(I)=1*C
CALL ERROR(I2,C)
GO TO 1120
1330 ASSIGN 138 TO JSX
VNUM=CAI+XX+VU*10.*EXTNT
GO TO 134
1340 CALL ERROR(I3,C)
ITAIL=MGD(ITAIL+LINTOP-NLINES-1,LINTOP)+1
NLINES=LINTOP
Y912 Ferruch(13 ERROR IN LINE Sorter)
GO TO 134
1350 CALL ERROR(I4,C)
RETURN
END
SUBROUTINE ERROR(I,J)
DIMENSION IER(30)
COMMON /ERK/N,NML,IER
IF (J.NE.1) GOTO 132
IF (I.EQ.11) GOTO 500
N=N+1
IER(N)=I
RETURN
500   M11=M11+1
      RETURN
1000  WRITE(6,*) M11+IER
      RETURN
END

//GL.SYSLIN  DD  USN=TSG462*NSPEC*OBJ*DISP=SHR
//GU.FT13F001  DD  USN=TSG462*SNIDER*DATA*(SAVE)*DISP=SHR
//GU.FT13F001  DD  USN=TSG462*LIMPAR*DATA*DISP=SHR
//GL.FT12F001  DD  SYSCUT=A
//GU.FT13F001  DD  SYSCUT=A
//GU.SYSIN   DD *
  190 45.0 95.0 45.0 15 11
  3.19E-06 322.0 0.0 0.0 0.0
  1900.0 1900.0 5 2 7 1 0.035 5.5 0.05 20.0 10.0 0
//
APPENDIX B

THE LINE PARAMETER SETUP PROGRAM

This program reads the AFGL line listing tape and creates a file of selected line parameters. The two-step JCL routine runs the FORTRAN program to read and select the line parameters and then calls for an all core sort using the IBM system sort routine to put the lines in increasing order of the lowest frequency value at which they have significant absorption. A sample of the line parameter output after sorting is also included. As written, the program selects NaO lines from 2550 - 2560 cm$^{-1}$ for a ground-based observer looking straight up at the sun. The line parameter listing example is for a different case.
00010 // REGION=192K,TIME=2
00020 /*SETUP UNIT=TAPE9,ID=(AFCRL,J229,READ)
00030 /*NTAPE EXEC FORTRAN,TIME=2,REGION=192K
00035 /*CMP.SYSPRINT DD SYSOUT=X
00040 /*CMP.SYSIN DD DSN=TS0462.BOB.FORT,DISP=SHR
00045 /*GO.SYSLOUT DD SYSOUT=X
00050 /*GO.OUTF001 DD LABEL=(1,BLP,IN),
00060 // UNIT=TAPE9, VOL=SER=AFCRL, DISP=(OLD,KEEP), DCB=(LRECL=3200,RECFM
00070 // BLKSIZE=3200)
00080 //GO.OUTF001 DD LABEL=(2,BLP,IN),
00090 // UNIT=TAPE9, VOL=SER=AFCRL, DISP=(OLD,KEEP), DCB=(LRECL=3200,RECFM
00100 // BLKSIZE=3200)
00110 //GO.OUTF001 DD LABEL=(3,BLP,IN),
00120 // UNIT=TAPE9, VOL=SER=AFCRL, DISP=(OLD,KEEP), DCB=(LRECL=3200,RECFM
00130 // BLKSIZE=3200)
00140 //GO.OUTF001 DD LABEL=(4,BLP,IN),
00150 // UNIT=TAPE9, VOL=SER=AFCRL, DISP=(OLD,KEEP), DCB=(LRECL=3200,RECFM
00160 // BLKSIZE=3200)
00170 //GO.OUTF001 DD LABEL=(5,BLP,IN),
00180 // UNIT=TAPE9, VOL=SER=AFCRL, DISP=(OLD,KEEP), DCB=(LRECL=3200,RECFM
00190 // BLKSIZE=3200)
00200 //GO.OUTF001 DD DSN=&LINE, DISP=(MOD,PASS), UNIT=SYSDA,
00210 // SPACE=(TRK,(1,1)), DCB=(RECFM=FB,LRECL=42,BLKSIZE=2100)
00220 // S EXEC SORT
00230 // S.SORTIN DD DSN=&LINE, DISP=(OLD,DELETE)
00240 // S.SORTOUT DD DSN=TS0462.L2.DATA, DISP=SHR
00250 // S.SYSIN DD *
00260 SORT FIELDS=(1,9,CH,A), SIZE=E200
END OF DATA
DIMENSION G(40), SS(40), AP(40), A(9, 40), ISOT(40), MOL(40),
# ID(40), EE(40), UM(6), EPSLON(2)
INTEGER IPOKE
REAL*8 G
DATA UINIT, UFINAL, BOUND, H, DEPTH
# .2550.0, 2560.0, 2.0, .30, 0.010/
KOUNT = 0
UBOT = UINIT - (BOUND + H)
UTOP = UFINAL + (BOUND + H)
UM(4) = 5.30E18
P = 1.0
EPSLON(1) = DEPTH/UM(1) * 3.1415927 * P
EPSLON(2) = DEPTH/UM(2) * 3.1415927 * P
MF = 9
IF (UBOT .GT. 500.0) MF = 10
IF (UBOT .GT. 1000.0) MF = 11
IF (UBOT .GT. 2000.0) MF = 12
IF (UBOT .GT. 5000.0) MF = 13
3 REWIND MF
1 CONTINUE
READ (MF, 2, END=6, ERR=4) (G(I), SS(I), AP(I), EE(I), A(J, I),
4 J = 1, 9), ID(I), ISOT(I), MOL(I), I = 1, 40)
2 FORMAT (40(F10.3, E10.3, F5.3, F10.3, 8A4, A3, I3, I4, I5))
IF (G(40) .LT. UBOT) GO TO 1
IF (G(1) .GT. UTOP) GO TO 9
DO 2002 I = 1, 40
IF (MOL(I) .NE. 4) GOTO 2002
IF (SS(I) / AP(I) .LT. EPSLON(MOL(I))) GOTO 2002
KOUNT = KOUNT + 1
CENTW = SORT(SS(I) * UM(MOL(I)) * AP(I) * P / 3.1415927 / 0.001
#(AP(I) * P) ** 2)
IG = G(I) * 1.0D3
IC = CENTW * 1000.0
00341        G(I)=DFLOAT(IG-IC)/1.0D3
00351        CENTW=FLOAT(IC)/1000.0
00352        WRITE(14,100) G(I),SS(I),AP(I),EE(I),MOL(I),CENTW
00353 100 FORMAT(F9.3,E10.3,F6.3,F9.3,I2,F6.3)
00354        IF (KOUNT .GE. 200) GO TO 9
00355 2002 CONTINUE
00360          GO TO 1
00370          6 MF = MF + 1
00380          GO TO 3
00390          4 WRITE (6, 605) MF
00400 605 FORMAT( '0 ERROR ON UNIT *', I3)
00410 9 CONTINUE
00420          STOP
00430          END
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