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# ERROR ANALYSIS OF INVERSION TECHNIQUES


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FINAL REPORT

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GODDARD SPACE FLIGHT CENTER

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SUMMARY

The background of the nonlinear inversion method is briefly described. A specific form of the nonlinear technique has been developed to infer unique atmospheric temperature profiles from satellite radiometer data. This particular version of nonlinear inversion utilizes the ground temperature, as sensed in a spectral window, to fix the inferred profile, which consist of a set of ramp functions. Application of the nonlinear algorithm to a spectral scan necessitates the approximation of actual band transmittances with an exponential model. A mathematical technique for fitting transmittance data is described, together with details of a computer program to accomplish this task. An error analysis of the nonlinear inversion algorithm is being performed by a computer program called INVERSIM. This program performs the inversion of noisy synthetic radiance data calculated at those frequencies which are optimal for Prony's method to apply. Details of INVERSIM and its component subroutines are presented with appropriate flow charts. The INVERSIM program has been applied to the 691 to 712.5 $cm^{-1}$ region of the 15 micron band of carbon dioxide using typical model atmospheres. The results of attempting to infer two and three ramp profiles are analysed with respect to noise level. It is concluded that the window radiance method is not a stable inversion algorithm for the above frequency region. Other conclusions and recommendations for future study are also presented.

## INTRODUCTION

During the past two years an error analysis of the nonlinear inversion technique has been pursued under Contract NAS5-3352. In order to describe the background of this problem, we first summarize the development of the nonlinear method and then outline our approach to an error analysis of the technique.

The context in which the nonlinear method first arose was the study of limb-darkening curves. The radiative transfer equation relates the upwelling radiant intensity at a given nadir angle to the Planck source function B. The relation between the intensity I and source function B is simply that of a Laplace transform. It was found that if one approximated the source function by a set of slabs, then the positions of these slabs could be determined by a nonlinear algorithm, the so-called Prony method. In reference 1, the variable slab inversion method is developed in a manner applicable to limb-darkening scans.

We realized that the slab method could be applied to any piecewise polynomial function: e.g., ramps, parabolic sections, etc. This class of functions has been termed "spline" functions in the mathematical literature (Ref. 2). When the variable slab method was applied to various analytic Laplace transforms, we soon found that the polynomial roots arising in Prony's method did not always correspond to physical slab boundaries. However, in cases where we used rounded or truncated values of the transform, the weights associated with such "bad" roots were usually negligible in comparison to the weights of good roots. This finding suggested the stability of the Prony algorithm against noise in the data.

In an attempt to confirm the error properties of the Prony method, we developed a computer program to apply the algorithm to various analytical Laplace transforms. The models chosen for analysis involved functions which should lead to bad roots. The results of this study are reported in Ref. 3. We found that noise could be considered equivalent to rapid oscillations in the inverse function and that the Prony method would lead to bad roots when the number of slabs became just sufficient to resolve the structure of these oscillations. The smoothing properties of nonlinear inversion were then traced to the inability of slabs to resolve fine structure in the inverse function.

The first application of the nonlinear method to actual radiance data involved the inference of a vertical temperature profile consisting of two ramps. The data was obtained by the U.S. Weather Bureau from a balloon flight from Palestine, Texas in September 1964. The process of inference is reported in Ref. 4; we mention here only a few important points.

The radiance data to be inverted were obtained by a grating spectrometer looking directly downward. Measurements were taken at six selected frequencies in the carbon dioxide 15 micron band. Since the resolution of each channel was about 5 $cm^{-1}$, one could not assume the simple exponential law of absorption which would hold for monochromatic viewing. An appropriate band transmission model had to be assumed in order to retain the Laplace transform character of the upwelling intensity. The model described in Ref. 4 is similar in spirit to the Mayer-Goody statistical model, but it was based on calculated transmissivities supplied by the Weather Bureau.

Application of the Prony method to limb scans in a plane-parallel atmosphere requires that measurements be taken at integral values of the secant of the nadir or zenith angle, the so-called air mass. This requirement, translated into spectral language, established certain viewing channels at which data should be obtained. The available data, however, was not measured at these optimal frequencies; hence, interpolation of the radiance data was necessary.

Also the choice of ramp functions to represent the temperature profile left an ambiguity in the parameters of the ramp which fitted the top of the atmosphere. The ambiguity was resolved by trying several different ramp parameters based on climatological information. The results of the nonlinear inversion, as shown in Ref. 4, were sufficiently encouraging to prompt an effort at eliminating the defects which arose because the data was not optimally suited to the nonlinear inversion method.

The first problem was to adapt the nonlinear method to spectral viewing. Realistic, nonexponential band transmittances would have to be used instead of the exponential transmittances of a limb scan. The TRANSFIT program was developed to fit real band transmittances with exponential models; the method used is outlined in later sections.

The second problem was to obtain data at the optimal viewing frequencies. If one had a continuous spectral scan across the band, there would be no difficulty. Continuous data is not available at present; hence, it was decided to work completely with synthetic data. Radiance data would be calculated at frequencies which correspond with integral values of the equivalent air mass.

The third problem was to develop a version of the nonlinear inversion technique which permitted a unique specification of the inferred temperature profile. Study of ramp profiles showed that a crossing property could be proved (cf. Ref. 3): each ramp should cross the true profile in at least two points. It also became evident that certain choices of the initial ramp could improve the overall fit of the spline function. A method was then developed for determining a unique profile by letting the inferred ground temperature equal the actual ground temperature. If a measurement of ground temperature was available by viewing in a spectral window, then only radiance data would be necessary for a unique inference. The window radiance method was chosen as the appropriate form of nonlinear inversion for an extensive error analysis.

Because the inversion algorithm is nonlinear, a linear error analysis is not possible. Therefore, we decided to carry through the entire inversion process for different noise levels. For this purpose the INVERSIM program was prepared. By comparing the inferred profile with the original profile used to synthesize the radiance data, one could relate error in the inverted profile to the error in the data.

In the following sections we present an account of the inversion method and details of the INVERSIM program. The results of several runs of the program are summarized, and finally conclusions are made on the success of the inversion method.

## NONLINEAR INVERSION UTILIZING WINDOW RADIANCE

The upwelling radiation intercepted by a narrow band radiometer pointing vertically downward is given by the transfer equation as

$$I(\nu) = - \int_0^\infty B[\nu, T(u)] \frac{\partial \tau(u,\nu)}{\partial u} du \tag{1}$$

where $\nu$ is the wave number at the band center, $\tau$ the transmittance, and B the Planck intensity. The absorbing mass cross section u is the height variable, reckoned positive downward with the origin at the satellite level.

To permit the integral in Equation (1) to be written as a Laplace transform, one introduces a general model transmittance of the form

$$\tau(u,\nu) = \exp[-s(\nu)\ t(u)] \quad . \tag{2}$$

The parameter t is a function of absorber mass only and plays the role of an effective optical depth. The parameter s depends only on wave number; it can be defined in such a way that it is analogous to the secant of a nadir angle, or the so-called "air mass thickness."

Using Equation (2), one derives the expression

$$I(s) = \int_0^\infty B(t) \exp(-st) s\, dt \quad , \tag{3}$$

where the Planck intensity has been expressed as a function of t only. The dependence of B on wave number has been removed by referring all intensities to a standard wave number (see below).

In the following we consider only the case of inferred ramp profiles. Since the actual atmosphere is not semi-infinite as implied in Equation (3), the effect of ground emission must be considered. It is sufficient to assume that the temperature profile becomes isothermal at great depths:

$$\lim_{t \to \infty} B(t) = B(\infty) \quad , \quad \lim_{t \to \infty} dB/dt = 0 \quad . \tag{4}$$

We then integrate Equation (3) by parts twice, obtaining

$$s[I(s) - B(0)] - B'(0) = \int_0^\infty B''(t) \exp(-st)\, dt \tag{5}$$

where primes denote differentiation with respect to t.

In the ramp approximation one assumes that the function $B(t)$ consists of a series of linear segments (ramps). In mathematical terminology $B(t)$ is taken as a spline function of order 2.(ref. 2) A simple characterization of such a spline function is that its second derivative is a sum of delta functions:

$$B''(t) = \sum_{i=1}^{n} \Delta B_i' \, \delta(t-t_i) \tag{6}$$

The quantities $\Delta B_i'$ represent the change in slope at the joint $t_i$. Substitution of Equation (6) into Equation (4) yields the basic result

$$s[I(s) - B(0)] - B'(0) = \sum_{i=1}^{n} \Delta B_i' \, (x_i)^s \tag{7}$$

where

$$x_i = \exp(-t_i) \quad .$$

When the secant parameter s takes on integral values

$$s = \ell = 0,1,2,\ldots \tag{8}$$

Equation (7) become moment equations, which are solved by using Prony's algorithm. A mathematical treatment of the moment problem and its implications for the nonlinear inversion method is given in ref. 3.

To solve the moment equations one must know the initial values $B(0)$ and $B'(0)$. However, it is possible to utilize relations (4) to fix the spline function $B(t)$ completely. By taking the limit $s \to 0$ in Equation (3), one shows the identity

$$I(0) = B(\infty) \quad . \tag{9}$$

In other words, measurement of the radiance in a spectral region with negligible absorption directly implies the temperature of the ground or cloud top. The method to be described presently may be used when a window radiance is available.

Condition (4) leads to the expression

$$B(t) = B(\infty) + \int_t^{\infty} \int_{t'}^{\infty} B''(t'') \, dt'' \, dt' \quad . \tag{10}$$

If one uses Equations (6) and (9) in expression (10), the following result emerges:

$$B(t) = I(0) + \sum_{i=1}^{n} \Delta B_i' \, (t_i - t) \, H(t_i - t) \quad . \tag{11}$$

where the Heaviside unit step function is defined by

$$H(x) = \begin{Bmatrix} 0 : x < 0 \\ 1 : x > 0 \end{Bmatrix} \quad .$$

One simple consequence of Equation (11) is the relation

$$B(0) = I(0) + \sum_{i=1}^{n} \Delta B_i' \, t_i \quad . \tag{12}$$

If I(0) is known, then Equation (12) can be used in conjunction with the moment equation (7) to specify $B'(0)$. A complete determination of the profile B(t) can be made only if B(0), $B_i'(0)$, $\Delta B_i$, and $x_i$ (i=1,...,n) are determined. One must, therefore, have 2n + 2 equations in order to fix the profile.

Equation (12) can be used with 2n + 1 moment equations ($\ell$=0,1,...2n), thus insuring uniqueness of the inversion. The initial slope $B'(0)$ can be eliminated by subtracting the moment equation for $\ell + 1$ from the equation for $\ell$; the resulting moment equations are

$$\ell \, I(\ell) - (\ell + 1) \, I(\ell + 1) + B(0) = \sum_{i=1}^{n} w_i (x_i)^{\ell}, \quad (\ell=0,\ldots,2n-1) \tag{13}$$

where the weights are given by

$$w_i = \Delta B_i' \, (1 - x_i) \quad . \tag{14}$$

Equations (12) and (13) are of transcendental type for general n; their solution requires an iterative method. Since Equation (13) can be solved by Prony's method to give the weights $w_i$ and roots $x_i$ as nonlinear functions of B(0), use of these values in Equation (12) leads to a nonlinear equation for B(0):

$$B(0) = F[B(0)] \quad . \tag{15}$$

Equation (15) can be solved by a standard iterative technique, such as Wegstein's method (ref. 5).

## THE TRANSFIT PROBLEM

In reference 4 a transmittance of the form

$$\tau(u,\nu) = \exp[-u/u_e)^m] \tag{16}$$

was found to represent data in the 15 micron $CO_2$ band over a range of absorber mass u. In order to generalize Equation (16) to the form given in Equation (2), one first introduces the variable

$$y(u,\nu) \equiv \ell n\{\ell n[1/\tau(u,\nu)]\} \tag{17}$$

Then Equation (2) becomes

$$y(u,\nu) = \ell n[s(\nu)] + \ell n[t(u)] \quad .$$

Thus, if the variable y is plotted against any function of u, then curves for different wave number $\nu$ have the same shape, but are displaced relative to one another along the y axis.

Applying the same argument to Equation (16), we find

$$y(u,\nu) = \alpha(\nu) + m\ell n(u) \quad . \tag{18}$$

An obvious generalization of Equation (18) would be to express y as a polynomial in the independent variable

$$x \equiv \ell n(u) \quad . \tag{19}$$

Thus, we consider fitting functions of the form

$$y(u,\nu) = \alpha(\nu) + \sum_{\ell=1}^{m} a_\ell \, x^\ell \quad . \tag{20}$$

In order to determine the parameters $\alpha(\nu)$ and $a_\ell$ which best fit the data, one must use a method appropriate to this problem. It was decided to use weighted least squares. Defining residuals

$$r(u_i,\nu) \equiv y(u_i,\nu) - \alpha(\nu) - \sum_{\ell=1}^{M} a_\ell (x_i)^\ell$$

we require that the following quantity be minimized:

$$R = \sum_{i,\nu} W(u_i,\nu)[r(u_i,\nu)]^2 \quad . \tag{21}$$

The regression equations appropriate to Equation (21) are derived in Appendix I;they are a simple generalization of the usual least square equations.

The weights appearing in Equation (21) must now be specified. Since the model transmittance will be used to compute radiances from the transfer equation (1), the maximum weight should be assigned to those values of u which contribute most to the integral. If we assume that the independent variable in Equation (1) is taken to be x as in Equation (19), then a suitable weighting function would be

$$W(x,\nu) \equiv -\partial\tau(u,\nu)/\partial x \quad . \tag{22}$$

Inserting the form (16) into Equation (22), we obtain

$$W(x,\nu) = m\,\tau(u,\nu)\,(u/u_e)^m \propto \tau\,\ell n(1/\tau) \quad . \tag{23}$$

Equation (23) suggests that we choose as weights for Equation (21) the quantities

$$W(u_i,\nu) = C(\nu)\,\tau(u_i,\nu)\,\ell n\,[1/\tau(u_i,\nu)] \tag{24}$$

where the constant $C(\nu)$ is such as to allow the normalization

$$\sum_i W(u_i,\nu) = 1 \quad .$$

A program TRANSFIT has been prepared to compute transmittances and to solve the regression equations derived from Equation (21). TRANSFIT uses the SYNDAT subroutine to be discussed in the next sections. A flow chart of the TRANSFIT program is shown in Fig. 1.

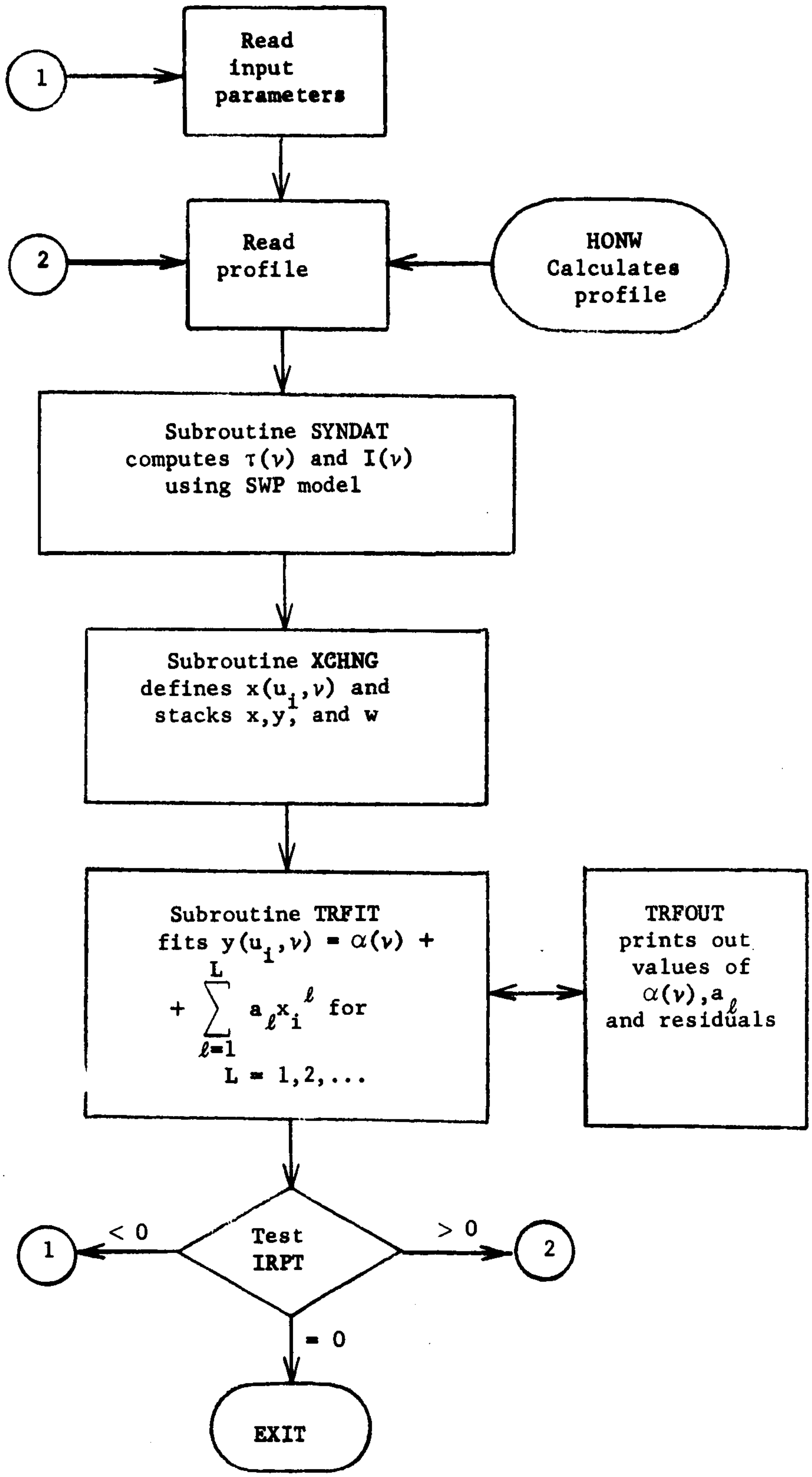


Figure 1. Flow chart of TRANSFIT program.

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# THE INVERSIM PROGRAM

The error analysis performed under the present contract will determine the effect of instrumental accuracy on inferred temperature profiles. Because of the nonlinear character of the inversion technique under study, linear error analysis cannot be used. Therefore, a synthetic approach to the error problem has been pursued. Radiances are computed from various model atmospheres, and the resulting synthetic data, with or without random error, are inverted to recover the temperature profile. A comparison of the original and inverted profile provides the measure of error.

The synthetic approach to error analysis has been coded as a computer program called INVERSIM. The first application of INVERSIM has been inversion in the 15 micron absorption band of $CO_2$, but the capability of inversion in other spectral regions is built into the program. The INVERSIM program has been written in FORTRAN II for the IBM 7094 computer at Goddard Space Flight Center.

The present form of INVERSIM will infer two or three ramp profiles from synthetic radiance with or without noise. Nonlinear inversion, using the window radiance as described above, can be applied to any model atmosphere. The capability of interpreting an extensive file of temperature profiles has also been incorporated into the present version of INVERSIM.

A simplified flow chart of INVERSIM is given in Figure 2 . A more complete description of the FORTRAN subroutines shown in Figure will be found in the following sections. Here we describe briefly the functions of each routine.

The first block indicates the input of various parameters necessary for transmittance generation and control purposes. The second block refers to FORTRAN subroutine called OPTMZ. The purpose of subroutine OPTMZ is to calculate the optimal wave numbers for application of the nonlinear inversion method, and then to interpolate the transmittance data of Stull, Wyatt, and Plass (SWP) for computation of transmittances at the optimal sampling frequencies.

Next the temperature profile is read in and radiances at the optimal sampling frequencies are calculated by subroutine SYNDAT. The subroutine called HONW is used to interpret the compact data format in the available file of profiles and to interpolate at pressure levels for which data is not given.

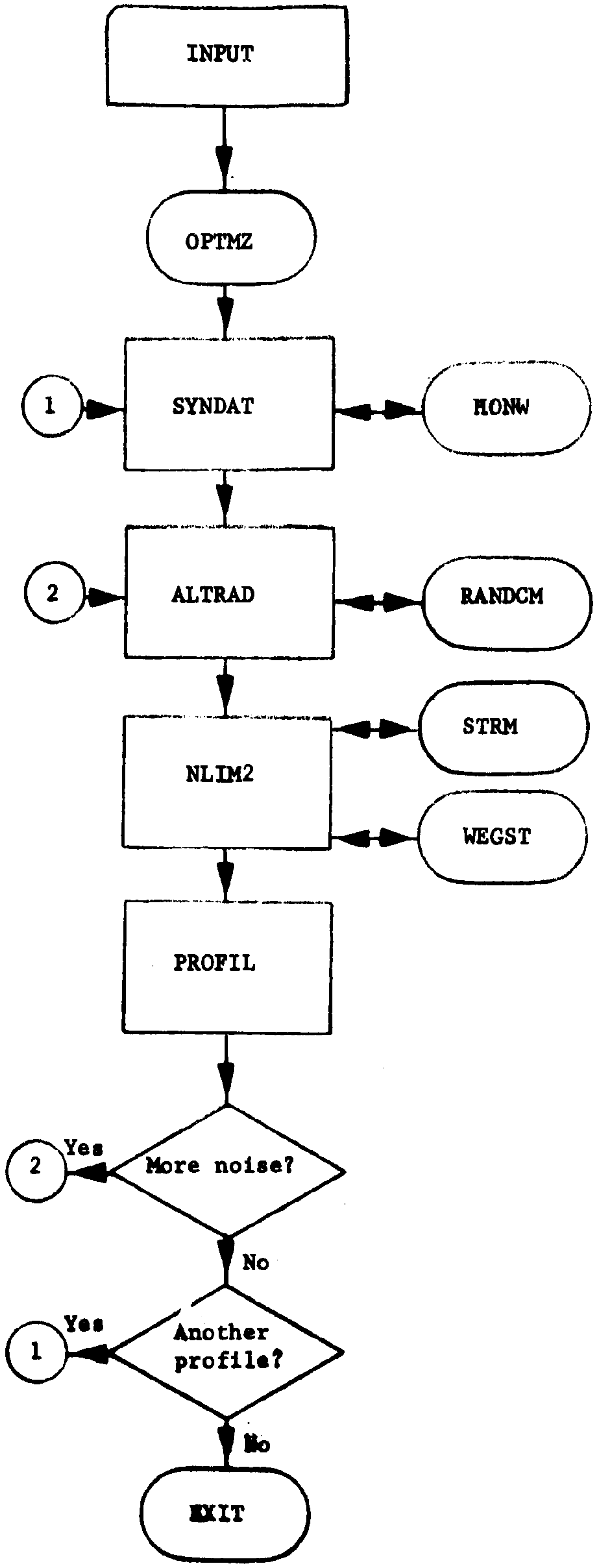


Figure 2. Flow chart for INVERSIM.

The synthetic radiance data are then converted to effective blackbody temperatures by subroutine ALTRAD. Random noise, generated by RANDCM, is used to simulate a brightness temperature fluctuation, and finally ALTRAD converts the noisy blackbody temperatures back into radiances at a standard wavenumber.

The converted radiance data is then inverted by subroutine NLIM2. The present version of NLIM2 attempts in subroutine WEGST to infer the ramp profile uniquely by applying Wegstein's method to find B(0). If a unique inversion is not possible, an average value of B(0) is used. Subroutine STRM is used to apply Sturm's test for the number of good roots and, thus, the number of possible ramps.

Finally, subroutine PROFIL converts the ramp profile to meteorological units and compares the inferred temperature structure with the model profile.

The program then either adds a higher level of noise to the radiance data or processes another model profile. Although it is not shown in Figure 2 , one has option of repeating the entire program.

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## SYNTHETIC RADIANCE GENERATION IN THE INVERSIM PROGRAM

### A. Transmittance Model

In order to generate realistic radiances from model atmospheres without an unduly complicated computer program, we have attempted to develop a semiempirical transmittance model for the INVERSIM program. Although several theoretical models can be used for $CO_2$ transmittance calculations, it was decided to employ data from the tables of Stull, Wyatt, and Plass (SWP, Ref. 6). These tables list $\tau$ as a function of wave number $\nu$, absorber mass u, pressure p, and temperature T. If one is computing transmittance along a vertical path toward the satellite radiometer, then the single variable

$$u^* \equiv u \frac{p}{p_o} \left(\frac{T_o}{T}\right)^{\frac{1}{2}} \tag{25}$$

is often used as the path parameter. There remains a temperature dependence in the transmittance which must be accounted for separately. This additional temperature variation has been handled in a manner such that the methods embodied in the TRANSFIT program can be used extensively. The linear pressure scaling in Equation (25) has been retained because it seems satisfactory for the 15 micron $CO_2$ absorption band.

We have attempted to fit the Stull, Wyatt, Plass (SWP) transmittance tables with polynomials in the form

$$y = \sum_{\ell=0}^{L} c_\ell x^\ell \quad , \tag{26}$$

where

$$x = \ell n(up)$$

$$y = \ell n \; \ell n[1/\tau(u,\nu)] \tag{27}$$

and p is the pressure in atmospheres. The polynomial coefficients $c_\ell$ depend on wave number $\nu$. The temperature variation of transmittance $\tau$ has been accounted for in the manner discussed below.

For a single frequency it was noted that the three curves

$$y = f(x,T) \quad , \quad (T = 200^o, 250^o, 300^oK) \tag{28}$$

were practically identical in shape, and could be brought into coincidence by suitable translation along the x axis. In mathematical terms, Equation (28) could be written

$$y = f(x + \Delta x_T, T_o) \quad , \tag{29}$$

where $\Delta x_{T_o} = 0$. For $(T - T_o)$ small, we see from Equation (27) that

$$x + \Delta x_T \cong x + \gamma(T - T_o) = \ell n[up(T/T_o)^{\gamma}] \quad . \tag{30}$$

The translated form (29) implies that one can introduce an effective absorber mass

$$u^* = up(T/T_o)^{\gamma} \quad .$$

Temperature effects can, thus, be incorporated by scaling the path parameter (up).

The displacements $\Delta x_T$ have been determined by using the TRANSFIT approach to solve the equations

$$x_T = \bar{c}_o(T) + \sum_{k=1}^{K} \bar{c}_k y^k$$

for T = 200°, 250°, 300°K. Only $\bar{c}_o$ was temperature dependent. The displacements were found from

$$\Delta x_T = \bar{c}_o(250) - \bar{c}_o(T) \quad .$$

The results of fitting the SWP tables showed that the linear approximation in Equation (30) was inadequate and that we should choose the effective x-parameter to be given by

$$\bar{x} \equiv \ell n(up/p_o) + \gamma \ell n(T/T_o) - \epsilon(T-T_o)^2/T_o^{\,2} \quad , \tag{31}$$

where $T_o$ = 250°K. Equation (31) suggests that we define an effective absorber mass $u^*$ so that

$$\bar{x} = \ell n(u^*) \quad . \tag{32}$$

For a homogeneous path

$$u^* = u \frac{p}{p_o} \left(\frac{T}{T_o}\right)^{\gamma} \exp[-\epsilon(T-T_o)^2/T_o^{\,2}] \quad . \tag{33}$$

Both parameters $\gamma$ and $\epsilon$ are functions of wave number. The limits of $\gamma$ are -.175 at 675 $cm^{-1}$ to 4.13 at 712.5 $cm^{-1}$. Such a wide range for $\gamma$ implies that the transmittance is a strong function of temperature in the wings of the band, but has a weak temperature dependence near the band center.

The coefficients $c_{\ell}$ were found by fitting the data reduced to the standard temperature $T_o$ = 250° as indicated in Equation (29). It was found that a polynomial fit of order L = 3 was sufficient to represent the SWP data. The final parameters for the range $\nu$ = 667.5 - 712.5 are listed in Table 1.

## TABLE 1

| WAVE NUMBER (1/CM) | GAMMA | EPSILON | C0 | C1 | C2 | C3 |
|---|---|---|---|---|---|---|
| | | | TRANSMITTANCE PARAMETERS | | | |
| 667.5 | .3585 | .0499 | 1.5157716 | .4476082 | -.0014096 | .0007941 |
| 670.0 | .4616 | -.1204 | .8821655 | .3414661 | .0203809 | .0060891 |
| 672.5 | .2214 | -.4200 | .5248257 | .4594480 | .0293006 | .0049725 |
| 675.0 | -.1747 | -.6804 | .2398565 | .5947729 | .0196186 | .0017591 |
| 677.5 | -.1534 | -.6980 | .2975750 | .5830430 | .0166053 | .0014264 |
| 680.0 | .0131 | -.3023 | .2872236 | .5740368 | .0142166 | .0011619 |
| 682.5 | .2703 | .0288 | .2366465 | .5677631 | .0131058 | .0011204 |
| 685.0 | .6361 | .2777 | .1016491 | .5708233 | .0149217 | .0014006 |
| 687.5 | 1.0735 | .3519 | -.0072655 | .5644598 | .0131665 | .0012549 |
| 690.0 | 1.4578 | .3126 | -.1279677 | .5583442 | .0122800 | .0012186 |
| 692.5 | 1.8921 | .4433 | -.2970365 | .5513266 | .0106778 | .0010569 |
| 695.0 | 2.2127 | .6453 | -.4704916 | .5483322 | .0103056 | .0009905 |
| 697.5 | 2.7022 | .8113 | -.6772594 | .5457561 | .0091351 | .0007908 |
| 700.0 | 3.1864 | .8492 | -.8341421 | .5427234 | .0088101 | .0007542 |
| 702.5 | 3.6664 | 1.3178 | -1.0051480 | .5399849 | .0077101 | .0005298 |
| 705.0 | 3.9035 | 1.3226 | -1.1804948 | .5366890 | .0067321 | .0003629 |
| 707.5 | 4.0289 | 1.0458 | -1.4100608 | .5356166 | .0068380 | .0003080 |
| 710.0 | 4.0145 | .3464 | -1.6180453 | .5363707 | .0076581 | .0002973 |
| 712.5 | 4.1275 | -.2476 | -1.8182142 | .5373851 | .0077548 | .0002860 |

For nonhomogeneous optical paths in the atmosphere one must account properly for the variation of temperature along the path. The foregoing development immediately leads to a generalization for nonhomogeneous paths. We take the effective absorber mass to be

$$u^* = \int_{p_1}^{p_2} (T/T_o)^\gamma \exp[-\epsilon(T-T_o)^2/T_o^2]\,(p/p_o)\,du \qquad ,(34)$$

where $p_o$ = 1013.25 millibars.

B. Subroutine OPTMZ

In the INVERSIM program the transmittance is represented in the form

$$\tau = \exp[-\exp(y)] \quad . \qquad (35)$$

As described above, the nonlinear algorithm requires that y as a function of wave number $\nu$ and absorber mass u have the separable form

$$y(u,\nu) = \alpha(\nu) + \sum_{k=1}^{m} a_k x^k \qquad (36)$$

where

$$x = \ell n(u\bar{p}/p_o) \quad . \qquad (37)$$

The pressure $p_o$ is taken as atmospheric pressure, 1013.25 millibars; the average pressure in a nonuniform path may be taken as the arithmetic mean

$$\bar{p} = \int_{u_1}^{u_2} p\,du/(u_2-u_1) = \tfrac{1}{2}(p_2+p_1)(u_2-u_1) \quad . \qquad (38)$$

Because the transmittance in the wings of the 15 micron band is more strongly dependent on temperature than at the band center, it is necessary to compute the parameters $\alpha(\nu)$ and $a_k$ from transmittances for a standard temperature profile. For example, the U.S. Standard Atmosphere, 1962 can be chosen for this purpose. We then apply the TRANSFIT program described above to transmittance data generated by the SYNDAT subroutine (see below). The resulting parameters $\alpha(\nu)$ and $a_k$ are input to subroutine OPTMZ.

The most transparent channel in the SWP tables has been chosen to be $\nu$ = 712.5 $cm^{-1}$. Since this channel corresponds to s = 1 in the Prony algorithm, the effective secant parameter for other SWP frequencies is given by

$$s(\nu) = \exp[\alpha(\nu) - \alpha(712.5)] \quad . \qquad (39)$$

The first task of OPTMZ is to determine the optimal wave numbers $\nu_\ell$ for use in SYNDAT. in the present program Equation (35) is used to calculate transmittances and y is found from

$$y(u,\nu) = \sum_{k=0}^{3} c_k(\nu)\bar{x}^{\,k} \quad , \tag{41}$$

where $\bar{x}$ is defined in Equation (42). The parameters $c_k(\nu)$ have been obtained by fitting the SWP data with the form (41): they seem to be rather smooth functions of $\nu$. Hence, the optimal parameters

$$c_{k,\ell} \equiv c_k(\nu_\ell) \tag{42}$$

can be obtained by interpolation. In this approach we interpolate the entire transmittance curve in frequency rather than specific points on it. It is felt that such a functional interpolation is more justified for our application.

It has been found that all SWP parameters $(\gamma,\epsilon,c_k)$ show a somewhat irregular dependence on frequency, which precludes polynomial interpolation with respect to $\nu$. However, since $\alpha(\nu)$ will reflect some of the irregularity, one can use $\alpha(\nu)$ as the independent variable in place of $\nu$. The results of the TRANSFIT program bear out the correctness of this assumption.

Since $\gamma(\nu)$, $\epsilon(\nu)$, and $c_k(\nu)$ can be regarded as smooth functions of $\alpha(\nu)$, polynomial interpolation is suitable. The Aitkin-Neville scheme, in which interpolates are found recursively, is used because of the irregular spacing of $\alpha(\nu_\ell)$ and because the appropriate order may be chosen for each parameter.

C. Subroutine SYNDAT

The purpose of the SYNDAT subroutine is to generate transmittances and radiances at the optimal sampling frequencies $\nu_\ell$ ($\ell$=1,...,6) required by the Prony algorithm. The generating parameters for computing SWP model transmittances are interpolated by OPTMZ, as described above.

The model atmosphere input to SYNDAT consists of a set of pressure levels $p_i$ and associated temperatures $T_i$. The effective absorbed mass $u_i^*$ corresponding to level i is found from Equation (34) by quadrature.

$$u_i^* = \sum_{j=1}^{i-1} \exp\left[-\epsilon(\bar{T}_j-T_o)^2\big/T_o^{\,2}\right]\frac{c_2}{4}\left(T_j^{\,\gamma}+T_{j+1}^{\gamma}\right)\left(p_{j+1}^{\,2}-p_j^{\,2}\right)\Big/p_o^{\,2}, \tag{43}$$

where

$$\bar{T}_j = \frac{1}{2}(T_j + T_{j+1})$$

and $c_2$ = 249.0 if the pressures are given in millibars. Since $\epsilon$ and $\gamma$ in Equation (43) are functions of frequency, the effective absorber mass depends on $\nu_\ell$.

SYNDAT calculates the radiance from Equation (1) by a numerical quadrature utilizing Simpson's rule:

$$I(\nu_\ell) = \sum_{j=1}^{N-1} \frac{1}{6}\left\{B\left(\nu_\ell, T_j\right) + B\left(\nu_\ell, T_{j+1}\right) + 4B\left(\nu_\ell, \bar{T}_j\right)\right\} \left[\tau\left(u_j^*, \nu_\ell\right) - \tau\left(u_{j+1}^*, \nu_\ell\right)\right] \quad . \tag{44}$$

The wavenumber dependence of $u_j^*$ has not been indicated in Equation (44).

Weighting functions are defined by

$$W_{i,\ell} \equiv \left[\tau\left(u_i^*, \nu_\ell\right) - \tau\left(u_{i+1}^*, \nu_\ell\right)\right] \Big/ \log_{10}\left(p_{i+1}\; p_i\right) \quad . \tag{45}$$

The weighting functions can be used to visualize the relative contribution of different pressure levels to the upwelling radiances. They are also used in TRANSFIT for the weights in Equation (21).

## INVERSIM PROGRAM: NONLINEAR INVERSION

### A. Subroutine ALTRAD

One purpose of this subroutine is to convert radiances $I(\nu_\ell)$ at the optimal wave numbers $\nu_\ell (\ell = 1,\ldots,6)$ to effective blackbody temperatures $T_\ell$ by the relation

$$I(\nu_\ell) = B(\nu_\ell, T_\ell) \quad , \tag{46}$$

where B is the Planck intensity function. Then noise is added to these temperatures according to the specification

$$\tilde{T}_\ell = T_\ell + \chi_\ell \Delta T \quad . \tag{47}$$

The variables $\chi_\ell$ are a set of statistically independent random variables satisfying a normal probability distribution; they are simply generated in the computer by a random number subroutine RANDCM.

The parameter $\Delta T$ may be called an equivalent rms temperature fluctuation. The INVERSIM program can input up to 10 values of $\Delta T$.

Having defined temperatures with noise by Equation (47), subroutine ALTRAD then converts them into radiances at a standard wave number $\nu_s$:

$$\tilde{I}(\ell) = B(\nu_s, \tilde{T}_\ell) \quad . \tag{48}$$

The radiances $I(\ell)$ are then input to NLIM2 for application of Prony's algorithm.

### B. Subroutine NLIM2

The theory behind the form of the nonlinear inversion method embodies in NLIM2 has already been discussed above. Our purpose here is to describe some of the computational details which have been developed in the course of applying this method to synthetic radiance data. The case of three ramps is considered here explicitly; only minor variations are involved for two ramps.

The first task of NLIM2 is to solve the following moment equations by Prony's algorithm:

$$\alpha_\ell \equiv \ell\tilde{I}(\ell) - (\ell+1)\tilde{I}(\ell+1) + B(0) = \sum_{i=1}^{3} w_i (x_i)^\ell, \quad (\ell = 0,1,\ldots,5) \quad . \tag{49}$$

The weights are related to the ramp slope discontinuities by

$$w_i = \Delta B_i' \,(1 - x_i) \quad .$$

The orthogonal polynomial $P_3$ whose roots are $x_i$ is given explicitly by the determinantal form

$$P_3(x) = \begin{vmatrix} \alpha_o & \alpha_1 & \alpha_2 & \alpha_3 \\ \alpha_1 & \alpha_2 & \alpha_3 & \alpha_4 \\ \alpha_2 & \alpha_3 & \alpha_4 & \alpha_5 \\ 1 & x & x^2 & x^3 \end{vmatrix} = \sum_{k=0}^{3} c_k x^k \quad . \tag{50}$$

Since the moments in Equation (49) depend linearly on B(0), one can show that the coefficients $c_k$ are linear functions also:

$$c_k = \gamma_k + \epsilon_k B(0) \quad . \tag{51}$$

In the present form of NLIM2 the parameters $\gamma_k$ and $\epsilon_k$ are determined by evaluating Equation (5) for B(0) = 0 and B(0) = $B_1$. Thereafter $P_3$ can be calculated for an arbitrary value of B(0) from Equation (51).

A three-ramp profile can be inferred only if all roots of $P_3$ lie in the interval (0,1), that is, are "good". Experience has shown that not all values of B(0) lead to three "good" roots. Let $R_3$ denote the connected region of B(0) for which $P_3$ has three good roots, and $R_2$ denote a similar region where $P_3$ has only two good roots. A search routine has been incorporated into NLIM2 in order to find the endpoints of $R_3$, or, failing that, to find the endpoints of $R_2$. Figure 3 shows a flow chart of the search method in its present version.

The search is made on a preset mesh and attempts to find the lower and upper endpoints B(0) = $b_1$ and B(0) = $b_2$ of $R_3$. At every value of B(0), Sturm's test for the number of roots in (0,1) is applied by subroutine STRM. If both endpoints of $R_3$ are found, subroutine WEGST is called to test for the possible application of Wegstein's method to fix a unique value of B(0). If only one endpoint of $R_3$ is found, then the search interval is contracted around that endpoint and the search is repeated on a finer mesh.

During the first search, the endpoints of $R_2$ are determined and stored. If no point of $R_3$ has been found, then the search interval is contracted about the point $B_c$ at which one root vanishes. We have found that one endpoint of $R_3$ is often the value of B(0) for which $x_1$ = 0. This critical value $B_c$ can be found from Equation (18) as

$$B_c \equiv - \gamma_o/\epsilon_o \quad . \tag{52}$$

If $R_3$ has not been defined after a second or third search, then the endpoints $b_1$ and $b_2$ of $R_2$ are used to define an average B(0):

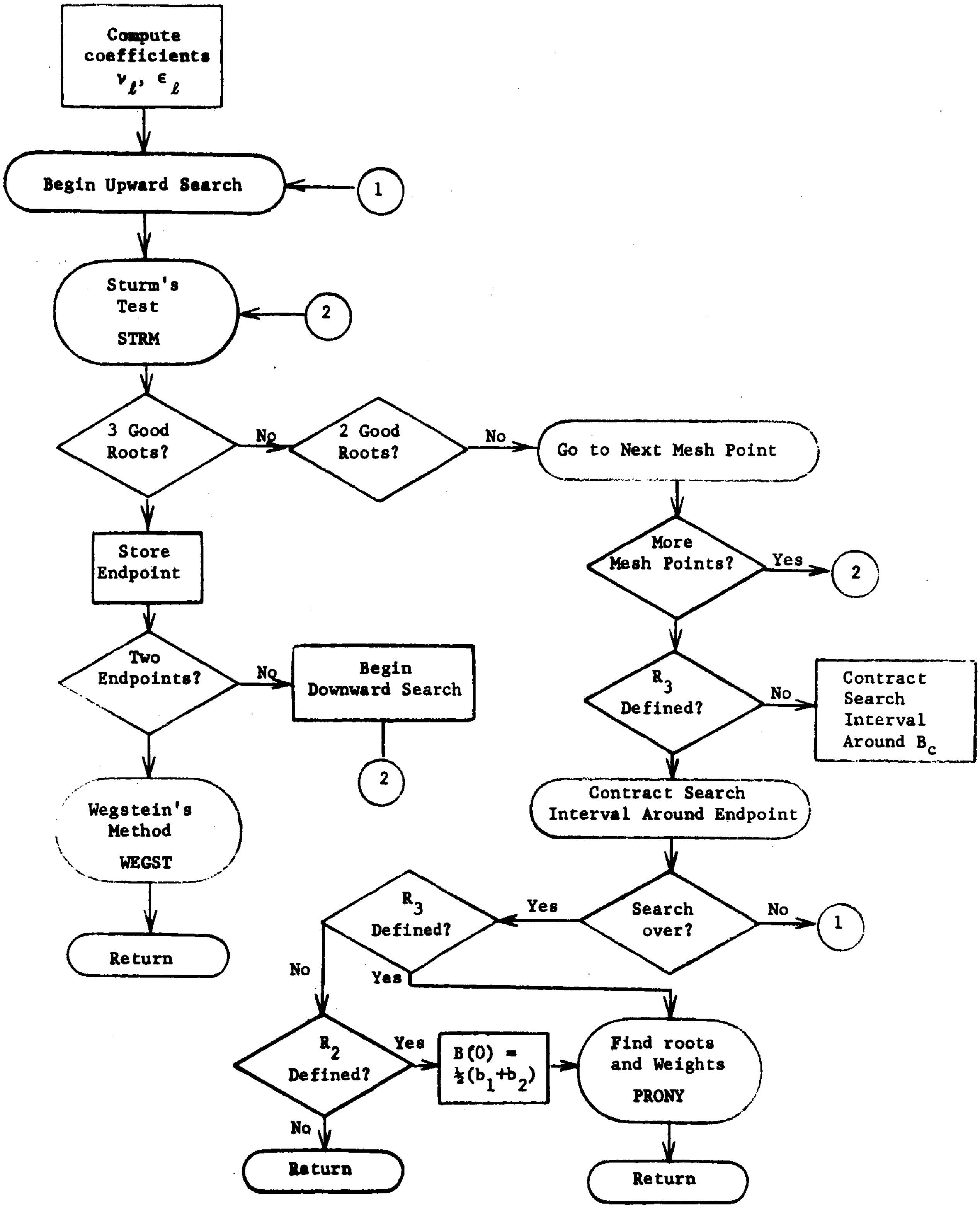


Figure 3. NLIM2 Version 6 Flow chart.

$$\overline{b} = \frac{1}{2}(b_1 + b_2) \tag{53}$$

In this case the roots and weights are computed by subroutine PRONY, and we return to the main program.

Figure 4 shows the Flow Chart for subroutine WEGST which attempts to fix B(0) unique by the method of the window radiance. The unique value of B(0) is defined to be such that the inferred $B(\infty)$ is just the window radiance I(0). However, we turn the condition around by computing for a given B(0) what the inferred B(0) would be when the profile is anchored at the ground by using the window radiance. The inferred value is computed from Equation (54):

$$\overline{B(0)} \equiv F[B(0)] = I(0) + \sum_{i=1}^{3} \Delta B_i' \, \ell n(1/x_i) \quad . \tag{54}$$

In NLIM2 $\overline{B(0)}$ is calculated from Equation (54) at the endpoints $b_1$ and $b_2$ of region $R_3$ by subroutine PRONY. It has been determined by experiment that solution point $B(0)^*$ satisfying $F[B(0)^*] = B(0)^*$ can be found if $b_1 < B(0)^* < b_2$. Then Wegstein's method, which is a form of the method of false position, can be applied to find $B(0)^*$ iteratively. Thus, iteration can begin if $(b_1 - b_1)\ (b_2 - b_2) < 0$. The left branch in Figure 4 shows this case.

If F(y) does not cross y in the interval derived from the search procedure, then the following procedure is suggested. We have found that crossings often occur when one root, say $x_1$, becomes very small. Then $\overline{B(0)}$ in Equation (54) tends to $-\infty$. This will be the case if $B_c$ defined in Equation (52) is an endpoint of $R_3$. If $B_c$ appears to be an endpoint of $R_3$, then a value of B(0) between $B_c$ and the nearest endpoint $b_i$ is selected. A test is made to see if Wegstein's method is applicable. If not, a point closer to $B_c$ is chosen and the test reapplied.

If Wegstein's method cannot be applied or if complex roots are encountered (a common occurrence), then an average B(0) is used for the final profile.

The form of Wegstein's method shown in the flow chart is not used; instead the expression

$$b_{n+1} = b_n - \frac{(b_n - b_{n-1})\ (\overline{b}_n - b_n)}{\overline{b}_n - b_n - \overline{b}_{n-1} + b_{n-1}}$$

gives the (n-1)th iterate. Each time subroutine PRONY is called, except in the Wegstein iteration, the roots, weights and other parameters of interest are output so that the reasons for failure may be more readily ascertained.

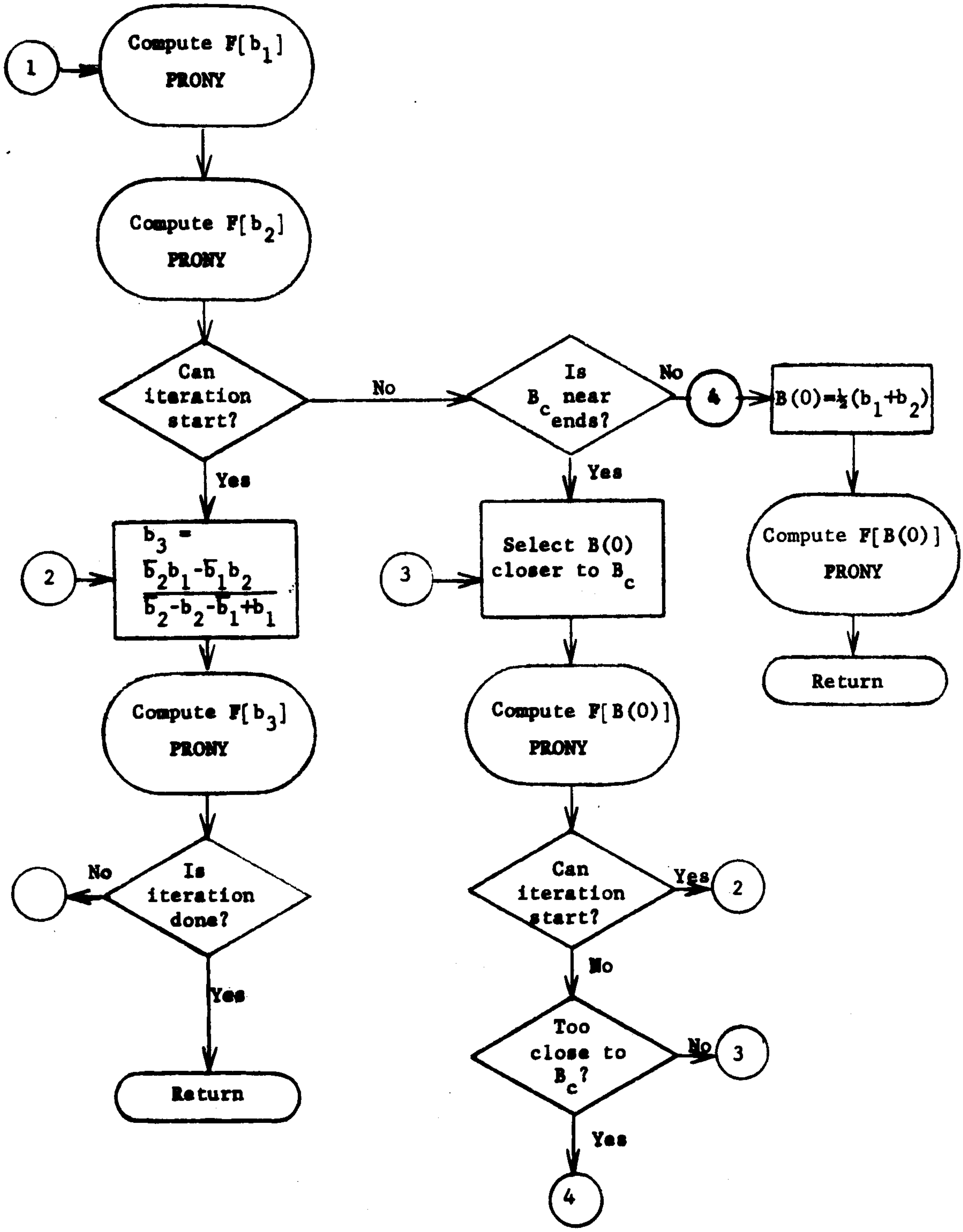


Figure 4. Flow chart for Wegstein's method.

# RESULTS OF INVERSIM PROGRAM

## A. Features of Present INVERSIM Version

The present FORTRAN version of INVERSIM has been coded to handle inversion of radiance data from two different sets of optimal frequencies. The second set of data is inverted after all levels of noise are applied to the first radiance data set. The option of inverting the second data set provides an opportunity to compare inversion using radiances calculated with actual transmittances computed from the SWP parameters and inversion using exponential transmittances [Equation (2)] computed from the parameters derived with the TRANSFIT program.

By comparing the effects of noise on the real and exponential transmittance data, one can evaluate the effects of the temperature non-linearity in the actual transmittance [effects of $\gamma(\nu)$ and $\epsilon(\nu)$]. Thus one can estimate the approximation made in replacing the actual weighting in Equation (1) by the Laplace transform in Equation (3). The validity of this replacement is essential for application of nonlinear inversion.

Many parts of the INVERSIM program have been specifically designed to find three-ramp profiles. The possibility of deriving four or five ramps seems out of the question because of the sensivity of the additional ramps to noise in the data. It has been previously shown (Ref. 3) that with five joints only three decimal accuracy in the root is obtained with exact eight-place moments. This result would seem to rule out inversion using more than three ramps.

## B. Model Atmospheres

Initial production runs have been made on three types of model atmosphere:

(1) The U.S. Standard Atmosphere 1962 assuming a satellite height of 60 km;

(2) A temperature sounding in the vicinity of Palestine, Texas on 8 May 1966, taken to represent the balloon flight of the IRIS instrument assuming a float altitude of about 30 km.

(3) A set of climatological temperature profiles representing four seasons at stations along the meridian at 100°W; satellite altitude taken as 60 km.

The third category of profiles includes mean soundings at 20°, 30°, 45°, 60°, and 75° north latitude for January, April, July and October. In addition to these 20 mean profiles are included an actual sounding taken on 12 August 1964 at a location 63.75°N, 165°W.

The TRANSFIT program was applied to both the U.S. Standard Atmosphere and the Palestine sounding in order to obtain approximate exponential transmittances. Twelve transmittances in the wavenumber interval 685.0 to 712.5 were computed with subroutine SYNDAT and fitted with polynomials [see Equation (20)] of order up to five. It was found that the order four fit was sufficient. The parameters from the Standard Atmosphere were also used to invert the climatological profiles.

The optimal SWP parameters as output from the OPTMZ subroutine are given in Tables 2 and 3. It should be noted that the sampling frequencies in the Palestine case are slightly displaced toward smaller wavenumbers (toward the band center).

## TABLE 2

## APPLICATION OF TRANSFIT TO U.S. STANDARD ATMOSPHERE 1962

| WAVE NUMBER (1/CM) | OPTIMAL TRANSMITTANCE PARAMETERS | | | | | |
|---|---|---|---|---|---|---|
| | GAMMA | EPSILON | C0 | C1 | C2 | C3 |
| 712.50 | 4.1275 | -.2476 | -1.8182142 | .5373851 | .0077548 | .0002860 |
| 704.21 | 3.8417 | 1.3211 | -1.1235187 | .5377290 | .0070407 | .0004156 |
| 699.27 | 3.0495 | .8381 | -.7884749 | .5436122 | .0089054 | .0007649 |
| 695.95 | 2.3866 | .7082 | -.5499090 | .5473563 | .0098621 | .0009149 |
| 693.34 | 2.0118 | .5111 | -.3551700 | .5503218 | .0105530 | .0010347 |
| 691.03 | 1.6516 | .3664 | -.1973356 | .5554534 | .0116200 | .0011521 |

## TABLE 3

## APPLICATION OF TRANSFIT TO PALESTINE, TEXAS PROFILE

| WAVE NUMBER (1/CM) | OPTIMAL TRANSMITTANCE PARAMETERS | | | | | |
|---|---|---|---|---|---|---|
| | GAMMA | EPSILON | C0 | C1 | C2 | C3 |
| 712.50 | 4.1275 | -.2476 | -1.8182142 | .5273851 | .0077548 | .0002860 |
| 704.22 | 3.8425 | 1.3211 | -1.1241382 | .5377162 | .0070369 | .0004150 |
| 699.31 | 3.0575 | .8387 | -.7910955 | .5435605 | .0088999 | .0007643 |
| 696.02 | 2.3997 | .7128 | -.5555318 | .5472853 | .0098299 | .0009094 |
| 693.47 | 2.0290 | .5216 | -.3641894 | .5501653 | .0105335 | .0010312 |
| 691.20 | 1.6822 | .3755 | -.2089685 | .5549668 | .0115090 | .0011408 |

## C. Results of Production Runs

Production runs of INVERSIM were made on all profiles to infer three ramps; all but the Standard Atmosphere were also inverted to infer two-ramp profiles. Because of an operator error, three climatological profiles were not run to obtain three ramps; hence, the total number of three-ramp inferences is less than that of two-ramp inferences.

In order to indicate typical results we describe here in detail the results of the Palestine profile inversion. The computed radiance profile from 680 to 712.5 is compared in Figure 5 with IRIS data obtained on the Palestine balloon flight. Optimal sampling frequencies are also indicated to show the significant radiances for nonlinear inversion. The discrepancy between calculated and measured data cannot be explained at the present time.

In the INVERSIM program noise levels $\Delta T$ = 0.0, 0.02, 0.04, 0.06, 0.08, 0.1, 0.2, 0.5$^{o}$K were used with both real and exponential transmittances. When three-ramp profiles were attempted, one obtained three ramps in only four cases. With real transmittance the case with $\Delta T$ = 0.06$^{o}$K give three ramps for $46.17 < B(0) < 46.97$. For the exponential model transmittance we inferred three ramps for noise levels $\Delta T$ = 0.0, 0.02, 0.06$^{o}$K. However, only with exact radiances did we find that the window fix method, using Wegstein iteration, could be applied.

Therefore, out of 16 inversions, only a single case led to a unique temperature profile. This inferred profile is shown in Figure 6. One can see that the inferred temperatures differ at the most by 5$^{o}$K from the sounding. It should also be noted that the tropospheric section of the profile (pressure less than 100 mb) requires two ramps.

Eleven inferred profiles contained two ramps and one case (exponential transmittance, $\Delta T$ = 0.5$^{o}$K) allowed only one ramp to be inferred.

For the Palestine case two-ramp inferences were attempted for real transmittances only. All noise levels allowed two ramps to be inferred, but only a single case ($\Delta T$ = 0.08$^{o}$K) led to a unique inference. This profile is shown in Figure 6. One observes that the two-ramp profile is unable to delineate any thermal structure in the stratosphere. The reason for the failure to determine the stratospheric temperature structure lies in the nature of the weighting functions for the optimal wavenumbers. The weighting functions for the Palestine profile are plotted in Figure 7.

The figure shows that the optimal weighting functions give greatest weight to the tropospheric section below 100 mb. Since two-ramp inversion uses radiances calculated in the interval 696.0 to 712.5 wavenumbers, the stratospheric contribution to each radiance is a small fraction of the tropospheric contribution. Hence, the effects of noise and the temperature dependence of the transmittance are sufficient to prevent utilization of information in the radiances about the stratospheric section of the of the temperature profile.

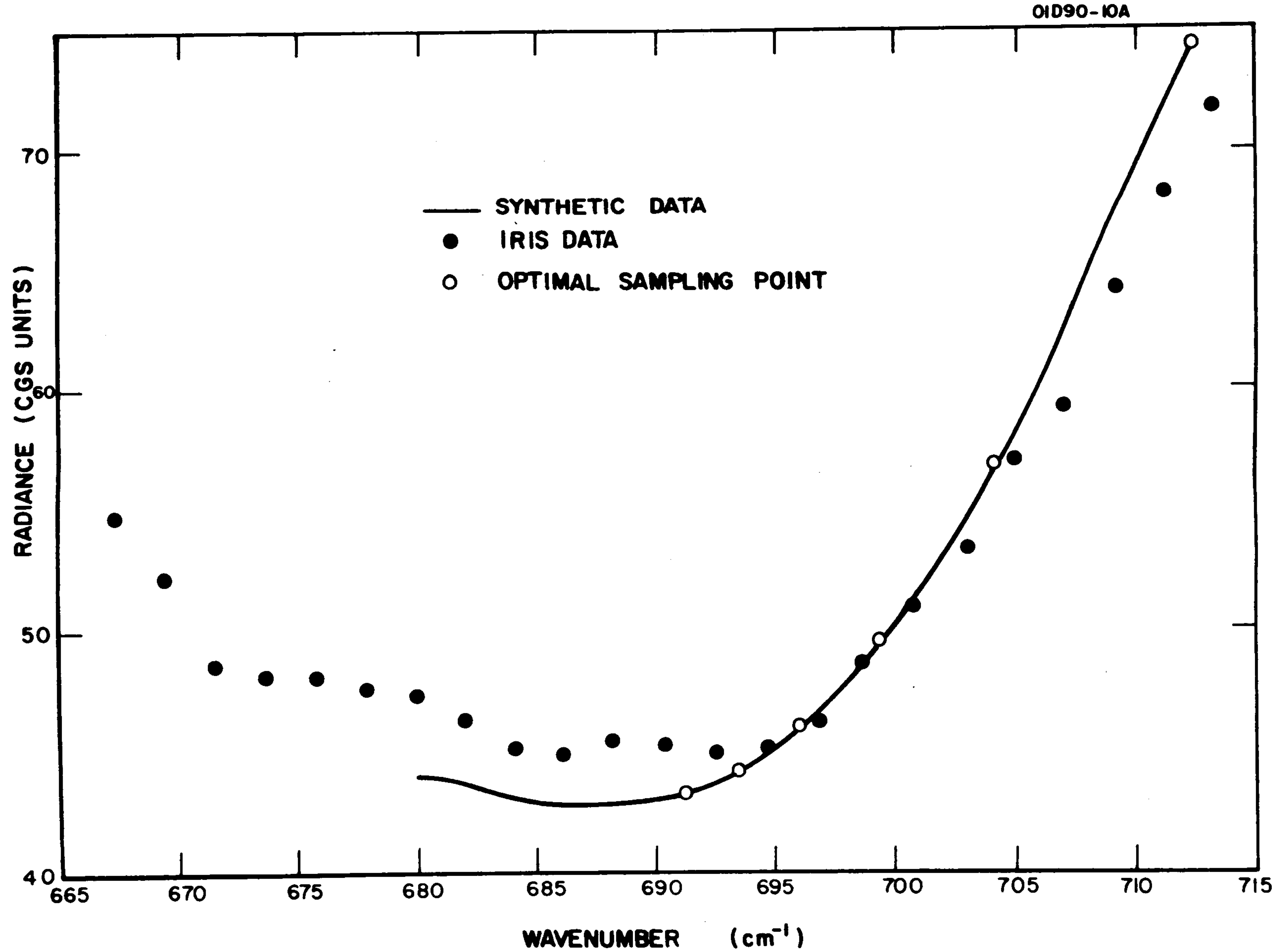


Figure 5. Comparison of IRIS data from Palestine balloon flight 8 May 1966 with synthetic radiances.

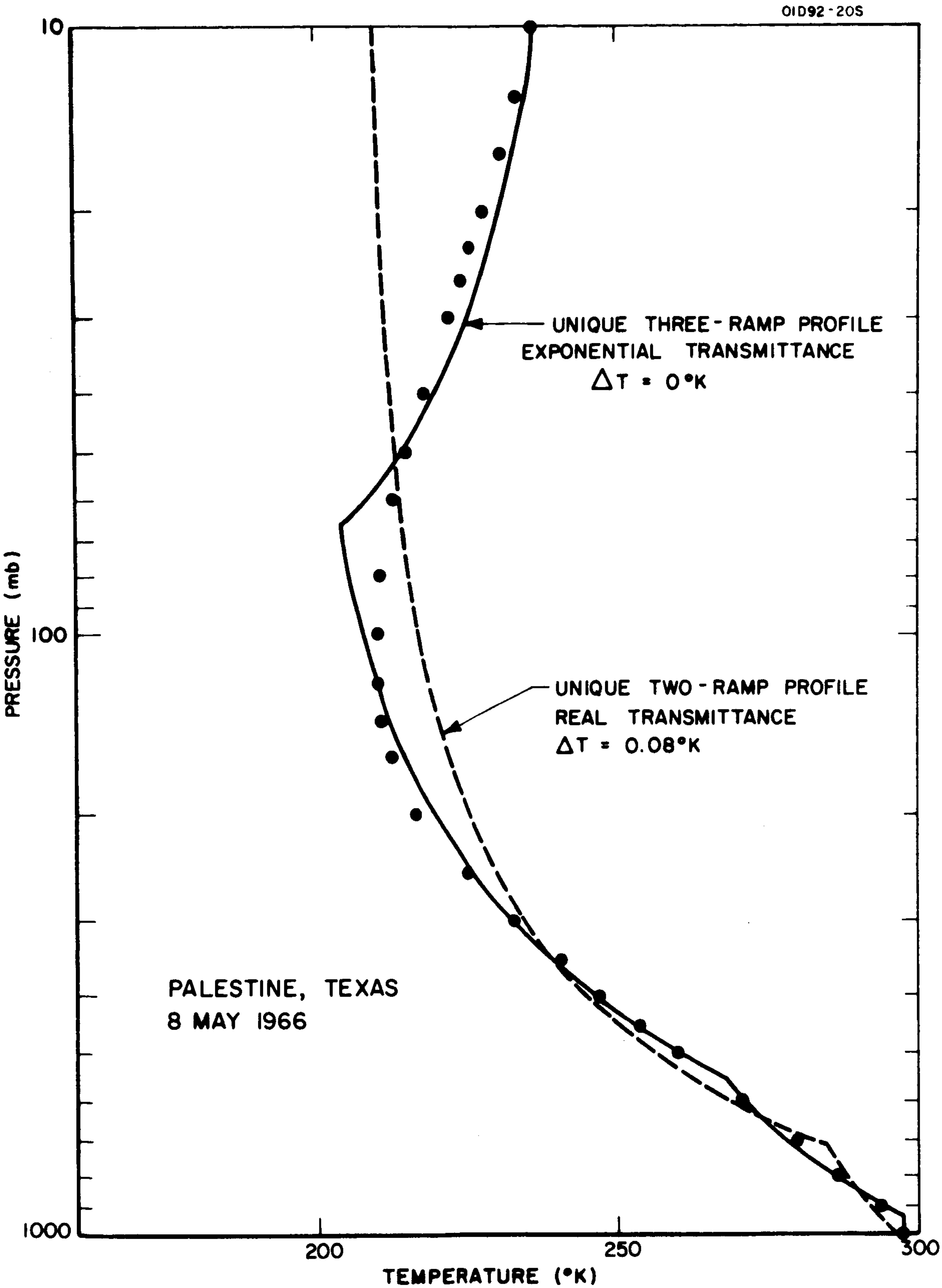


Figure 6. Unique two- and three- ramp inversions of Palestine, Texas profile.

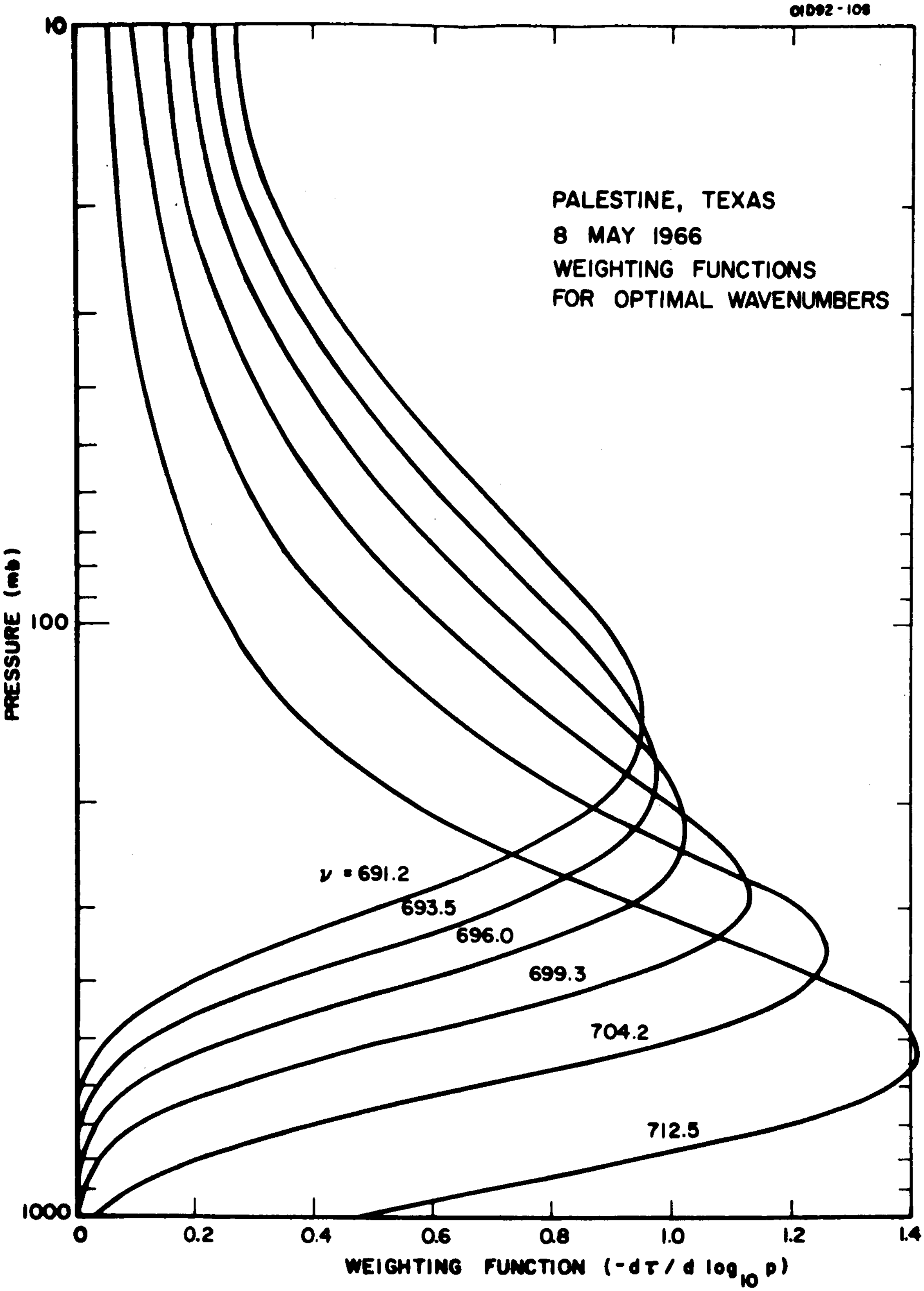


Figure 7. Weighting functions for optimal wavenumbers with Palestine, Texas profile.

In short, information about the stratosphere is contained in the last few decimal places of the radiances at s = 1,2,3,4; noise can easily render this information irretrievable.

The findings described above are further borne out by the results with climatological profiles. Table 4 gives a breakdown of the inversion results when both three-ramp and two-ramp profiles were sought.

As Table 4 shows, only 39 cases led to three-ramp profiles. About 75% of the three-ramp profiles were obtained for low noise levels ($\Delta T \leq 0.02^{o}K$). This finding reveals the instability of inversion with the given data sampling. It is also important to note that 13 of the 39 three-ramp profiles were obtained with real transmittances.

The vast majority of inferred profiles involved only two ramps. The chance of inferring a single ramp was more likely if one attempted to invert with 5 data points than with 7 data points. This result shows that the additional two radiances contained some information which was not completely destroyed by noise.

If we examine the distribution of unique profiles, then certain facts about inversion using the window radiance can be drawn. According to Table 4 , 15 unique three-ramp profiles were inferred and 16 two-ramp profiles were also unique. However, the distribution of unique inferences with respect to noise level depends noticeably on the number of ramps. The unique three-ramp profiles are most likely found from data with no noise; whereas unique two-ramp profiles are found at all noise levels. Thus, unique inversion shows extreme instability in the case of three ramps. This finding bears out the result of the Palestine inversion - that information about the stratospheric temperature is not retrievable in the presence of noise because the additional data are close to the minimum in the radiance curve.

The 15 unique three-ramp profiles may be further classified by transmittance model. All unique inversions with no noise were associated with the exponential model. One of the cases for $\Delta T = 0.02^{o}K$ involved an exponential transmittance. The remaining two profiles were obtained with real transmittances. We conclude from these statistics that the temperature nonlinearity in the "real" SWP transmittance introduces a systematic error in the radiance data which prevents one from inferring unique three-ramp profiles.

In fact, the temperature effect prevents the inferrence of three-ramp profiles, since all but two cases with real transmittance required $\Delta T \neq 0$ for three-ramp inversion.

TABLE 4

INVERSION OF CLIMATOLOGICAL PROFILES

| Noise Level ($\Delta T^o K$) | 3 ramps found | 2 ramps found | 1 ramp found | Unique |
|---|---|---|---|---|
| 3 ramps sought | | | | |
| 0.0 | 16 | 17 | 3 | 12 |
| 0.02 | 13 | 23 | 0 | 2 |
| 0.05 | 6 | 30 | 0 | 1 |
| 0.1 | 4 | 31 | 1 | 0 |
| 0.2 | 0 | 35 | 1 | 0 |
| 0.5 | 0 | 32 | 4 | 0 |
| Totals | 39 | 168 | 9 | 15 |
| 2 ramps sought | | | | |
| 0.0 | | 42 | 0 | 2 |
| 0.02 | | 42 | 0 | 3 |
| 0.05 | | 42 | 0 | 3 |
| 0.1 | | 41 | 1 | 2 |
| 0.2 | | 38 | 4 | 5 |
| 0.5 | | 19 | 23 | 1 |
| Totals | | 224 | 28 | 16 |

A more direct indication that temperature effects in the transmittance model lead to instability of inversion can be found by examining the range of B(0) for which three ramps can be inferred. If this range is found to be less than about 5 cgs units (erg/sq. cm. sec wavenumber), then one can assert that the profile is a very sensitive function of the assumed B(0). In 13 of the three-ramp inferences one observed such a narrow range of B(0). Three cases corresponded to the exponential transmittance model, while ten were associated with real transmittances. Apparently the chance of instability, as manifested in a narrow B(0) range, is higher with real transmittances, which are influenced by temperature nonlinearities.

We next discuss successful unique inversions in order to evaluate the accuracy of the inferred temperature profiles. First three-ramp profiles will be considered. In all of these cases a single ramp represented the stratospheric section of the profile, and two ramps were used to fit the tropospheric section (See Figure 6). The reason for two tropospheric ramps is related to the pressure dependence of the optical depth t(u). The function B(t), which is being approximated by a spline function of order two, has considerable curvature in the troposphere. This fact explains the necessity of two ramps in order to fit the tropospheric section with least error.

In Figure 8 we show a comparison of functions B(t) for two transmittance models. The case labeled "Model 1" corresponds to a neglect of the pressure dependence in the optical depth. On the other hand, the profile labeled "Model 2" is typical of a realistic model transmittance such as used in the INVERSIM program. It is apparent from Figure 8 that three ramps are necessary as a minimum to approximate B(t) without serious error.

Two unique profiles should be singled out as of particular interest: January 45°N and April 75°N both had profiles with a pronounced temperature inversion near the ground. In both cases the uniquely inferred profile also showed a temperature inversion. In Figure 9, the actual and inferred profiles are compared for the January 45°N case. Shown on the same figure is a three-ramp inference from data calculated with the real transmittance model; this latter profile, which is not unique, indicates the existence of a low-level inversion layer. It is evident from the figure that only three-ramp profiles could reveal such detailed temperature structure.

Figures 10 and 11 give examples of unique two-ramp inferences. Figure 10 shows a case in which the tropospheric structure seems quite adequately represented by a single ramp and in which the stratosphere is also quite well approximated by one ramp. Figure 11, on the other hand, reveals a variability in the deduced temperature structure which is not desirable in a stable inversion procedure. Note that some noise was required in order to obtain a unique inference. It seems clear in this example that the exponential model led to a more satisfactory inversion than the real transmittance model.

It should be further pointed out that the last profile considered, April 45°N, was mentioned above as having an inversion layer near the ground. Figure 11 shows that two-ramp profiles are unable to infer the inversion layer, instead predicting an isothermal layer at the same temperature as the ground.

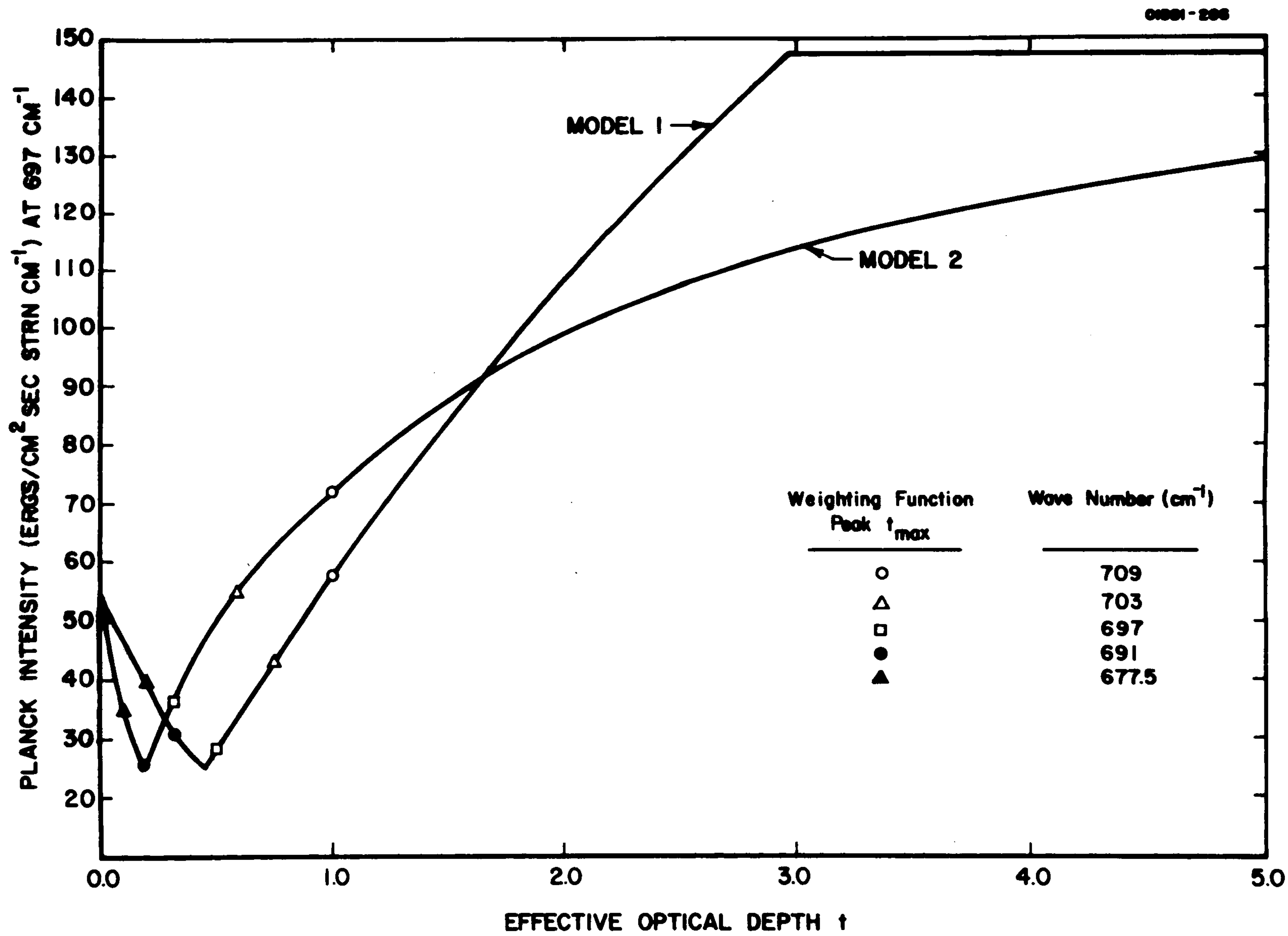


Figure 8. The function B(t) for two transmittance models: Model 1 - no pressure dependence; Model 2 - realistic pressure dependence.

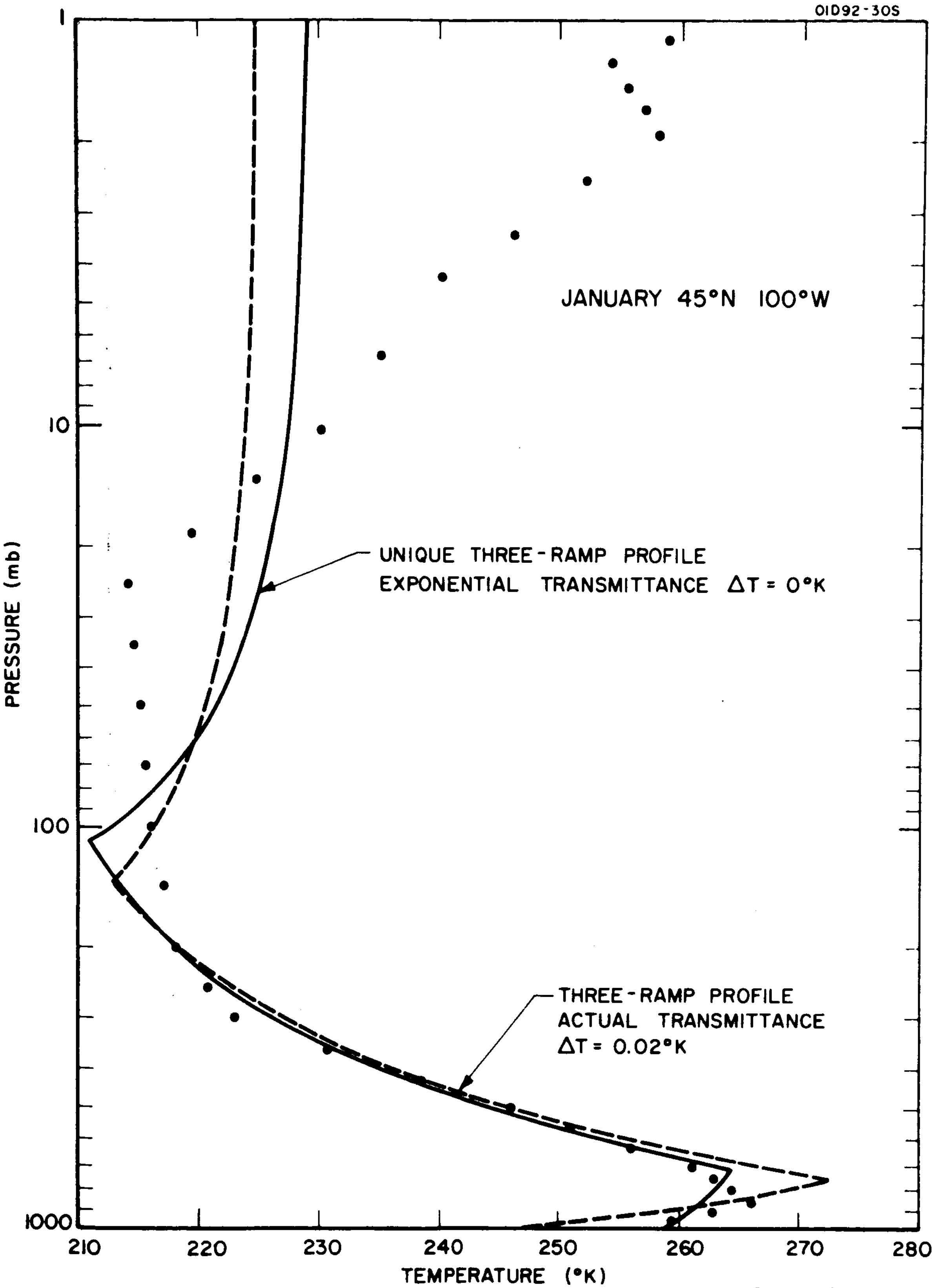


Figure 9. Three-ramp inversions for January 45°N 100°W climatological profile.

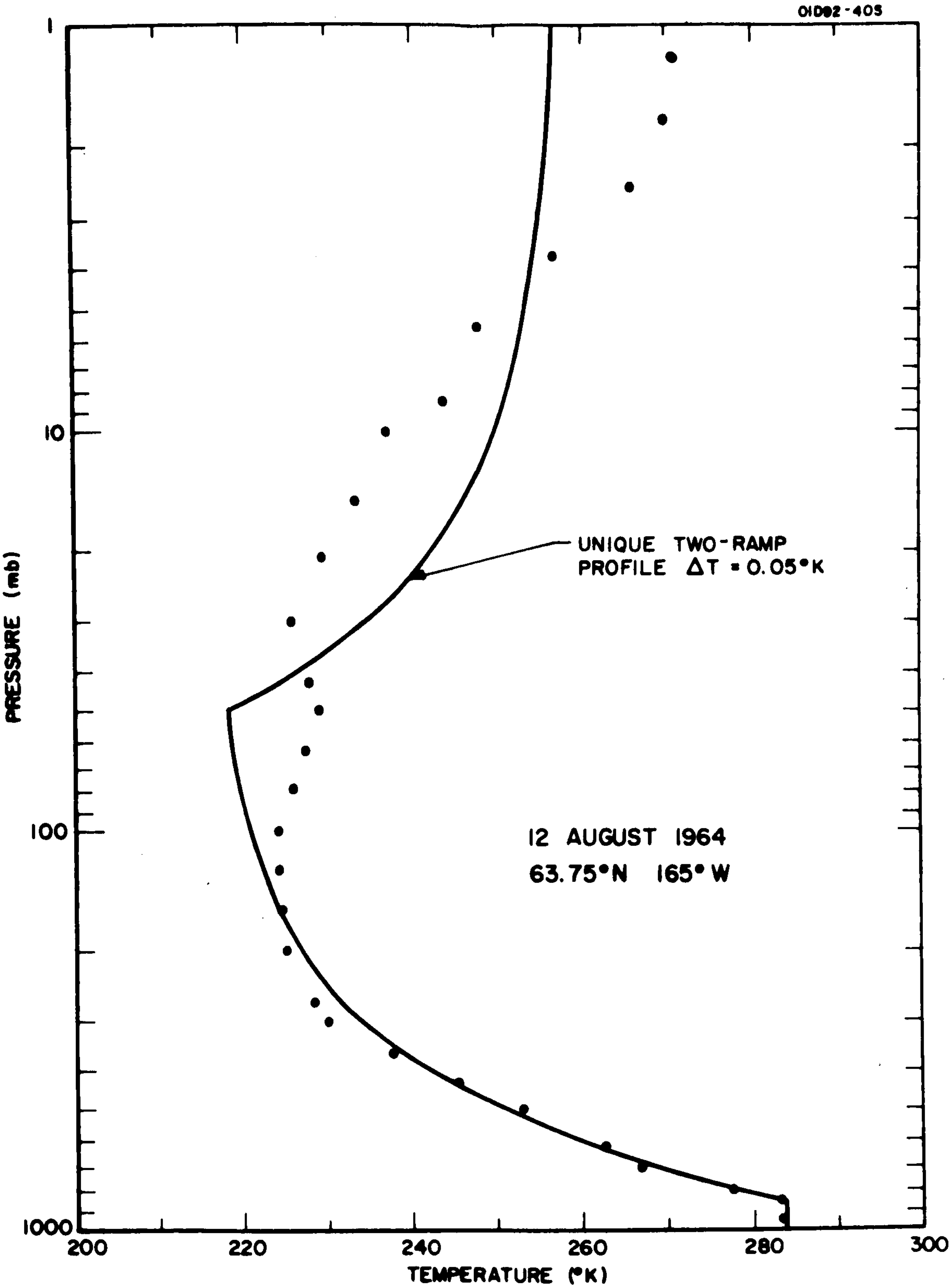


Figure 10. Unique two-ramp inversion of sounding taken on 12 August 1964 at 63.75°N 165°W.

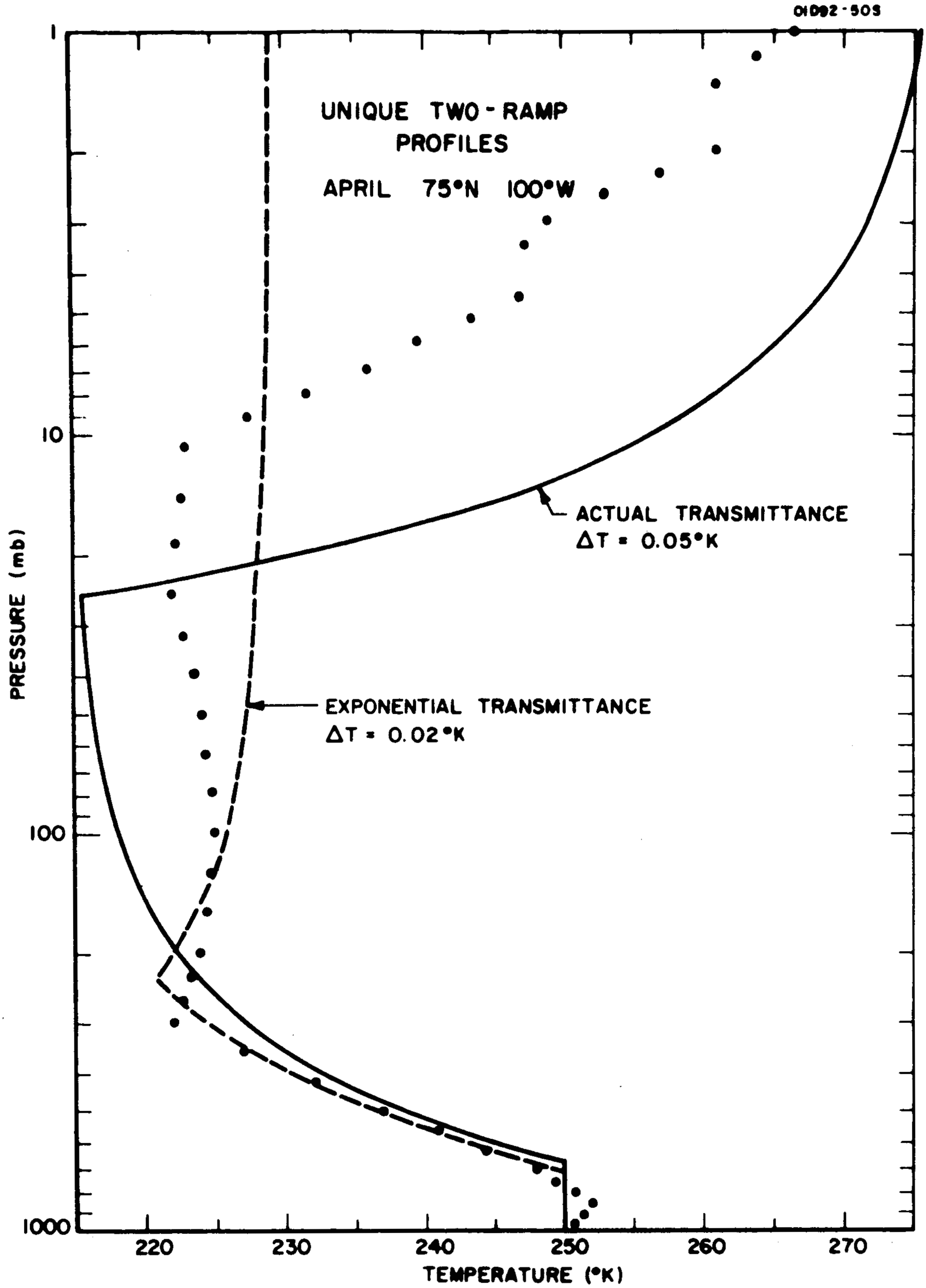


Figure 11. Unique two-ramp profiles for April 75°N 100°W climatological profile.

# CONCLUSIONS

## A. Evaluation of INVERSIM Results

The INVERSIM program was developed in response to the need for a quantitative evaluation of the nonlinear inversion method as a technique for handling radiometer data which contains significant noise. Since the results of inversion may depend on the particular problem to which it is applied, a general error analysis is not possible. Therefore, it was decided to test the nonlinear inversion algorithm on synthetic radiance data in the 15 micron carbon dioxide band. The specific spectral interval chosen was the range from 690 to 712.5 wavenumbers.

The decision was also made to select one particular inversion technique which seemed most able to extract the relevant information from radiance data in the above spectral interval. As described in the previous sections, the method chosen infers a unique profile by using the radiance in a spectral window plus radiances at effective air masses $s = 1,2,\ldots,2n$, where $n$ is the maximum number of ramps in the inferred profile.

The conclusions stated in this section should be taken as applicable only to the above-mentioned frequency range with the specific inversion method outlined in previous sections. Since production runs of INVERSIM were achieved so late in the contract period, only more qualitative conclusions will be stated. Quantitative measures of the inferred profile error are useful, in any case, only when an optimal inversion technique has been found. As we shall try to indicate, the present method is not optimal.

There are two qualitative tests which one can apply to any inversion algorithm in order to assess its response to error in the input data:

Test I - How well can one approximate actual temperature profiles with the selected finite set of basis functions;

Test II - Is the algorithm stable against random errors in the radiance data.

The purpose of Test I is to ascertain what error in inherent in the choice of basis functions. In other words, because only a finite set of functions can be selected as a basis, some temperature profiles may be difficult to fit accurately with the given function set. It is important to know what temperature error will be caused by the finiteness of the basis set before considering effects of noise in the data.

Test II refers to error in the inferred profile caused by random error in the radiance data. If the temperature error is subject to wild oscillations or if physically impossible profiles are inferred, then we call the inversion method "unstable." A stable method of inversion usually requires the presence of constraints which prevent the profile error from exceeding reasonable values.

The two tests above are not mutually exclusive, since some methods of rendering an algorithm stable may depend on the choice of basis set. The nonlinear method is a good example of the interaction of the two tests since the matehmatical stability of spline functions affects their ability to represent a wide range of temperature profiles. That is, the effect of noise causes a loss of one or more joints. With nonlinear inversion, fewer ramps must approximate the same temperature profile when one has noisier data.

In analyzing the nonlinear inversion method then one should first ascertain the ability of ramps to fit typical temperature profiles. Applying Test I to the nonlinear inversion method, we ask if two and three ramp profiles provide adequate approximations to actual temperature structure. In the last section we tried to indicate that to fit the troposphere adequately requires two ramps because of the curvature caused by pressure effects in the transmittance. Thus, to obtain an inferred profile with good accuracy in both stratospheric and tropospheric sections, one needs at least three ramps. The requirement of a minimum of three ramps applies to the spectral interval 690 to 712.5 wavenumbers.

Of course, one can point to particular profiles (for example, that in Figure 10) which are satisfactorily represented by only two ramps. These cases, however, seem to be nontypical. If small temperature error in the inferred profile is desired at all meteorologically significant pressure levels, then two-ramp inference is not sufficient.

The necessity for obtaining three-ramp profiles in order to fit actual atmospheric temperature structure causes us to re-examine the finding of our mathematical study (Ref. 3) that the nonlinear algorithm is stable in the presence of noisy data. That is, we must consider stability in the context of the present application of nonlinear inversion as the ability to infer at least three ramps from noisy data.

Because nonlinear inversion reacts to noise by reducing the number of inferred ramps, Test II can be applied by studying the effect of noise on the inference of three ramps. The results of the INVERSIM program outlined in the last section demonstrate the difficulty of inferring three ramps from noisy data. Specifically, of the radiance curves inverted for three ramps, only 18 percent of the cases resulted in the determination of three good roots. Furthermore, in a number of these cases the acceptable range of B(0) was so narrow that the NLIM2 subroutine found the three-rott region only with difficulty.

Hence, the present realistic attempt to apply nonlinear inversion to the 15 micron carbon dioxide band has led to the conclusion that the nonlinear algorithm is unstable with respect to noise levels, typical of present instrumental capabilities.

At this point we should like to indicate reasons for not attempting to infer four or five ramps. One reason is that taking differences of radiance measurements is required by the specific inversion technique used in INVERSIM. Since data corresponding to x = 7,8,9,10 will be very close together, the amount of additional information carried by these points does not seem sufficient to permit a better definition of the inferred profile. Another reason is that the selection of optimal sampling frequencies requires fitting the real transmittances with exponential ones. Because temperature effects are not uniform across the band, the exponential model transmittances, as found by the TRANSFIT program, are more accurate when the spectral interval is as narrow as possible. For example, near the band center the weighting functions are more spread out than in the wings of the band. This fact makes modelling of the entire 667.5 to 712.5 interval impossible.

Test II can also be applied to the inference of unique profiles by the window radiance method. In this context, we inquire as to the sensitivity of B(0) to noise in the data. Since three-ramp profiles are difficult to obtain and since radiances associated with more transparent frequency ranges in the absorption band should contain more information about the temperature profile near the ground, one should consider two-ramp inversion as a more appropriate application of the window radiance method than three-ramp inversion.

Although two-ramp profiles were relatively easy to obtain even with high noise levels, the chance of finding a unique profile was only about 7 percent. Since the choice of 712.5 $cm^{-1}$ as the most transparent channel was made to otpimize the window radiance method, the results of INVERSIM show that the method does not generally permit the inference of unique profiles, even where its should be most applicable. The resulting instability of the window radiance method leads us to the conclusion that the method cannot be applied anywhere in the 15 micron band.

A further confirmation of the above conclusion is based on the analysis of temperature in the transmittance. INVERSIM results show that systematic error caused by the temperature dependence of $\tau$ prevents three-ramp inversions. Since these nonlinear temperature effects are most extreme in the wings of the band, one concludes that three-ramp inference is made more difficult in the wings by temperature effects. Hence a channel at 712.5 $cm^{-1}$ may even be too far from the band center to be considered as $s = 1$ for application of nonlinear inversions.

To summarize the main conclusions derived from the INVERSIM program results:

(1) In order to achieve a satisfactory approximation to the typical atmospheric temperature profile, one must employ a spline function consisting of at least three ramps. Although an occasional profile can be fitted with only two ramps, meteorological accuracy seems to require a minimum of two ramps in the tropospheric section of the profile.

(2) The optimal sampling frequencies required by the Prony algorithm do not seem well chosen if one uses 712.5 $cm^{-1}$ as the most transparent channel. For one finds that this choice leads to ill-conditioning of the inversion method. Three-ramp profiles are obtained in only 20 percent of the cases, and most of these cases contain only very low levels of noise. Typical noise levels expected with state-of-the-art spectrometers are about $\Delta T \sim 1^{o}K$; inversion with such high noise levels results in at most one or two ramps.

(3) The window radiance method of uniquely fixing the temperature profile is also found to be badly conditioned. Since the temperature dependence of the transmittance seems to affect the method adversely and since utilization of a more transparent channel than 712.5 $cm^{-1}$ would involve stronger temperature dependence, we have concluded that the window radiance method of uniquely fixing the inferred profile is not applicable to the 15 micron band.

B. Recommendations for Future Study

The negative results of the INVERSIM runs summarized above lead one to ask how the nonlinear inversion technique might be modified in order to give more satisfactory temperature profiles. In particular, is there an alternative method to the window fix for determining a unique B(0).

Since the lower troposphere seems most difficult to fit with ramps, it appears logical to select a channel for $s = 1$ with a weighting function whose peak is located nearer to the tropopause. Use of 710, 707.5, or 705 wavenumbers for the most transparent channel is abviously suggested. There is an upper limit to the choice of a most transparent channel, however.

As one nears the Q branch at the band center (667 $cm^{-1}$), the shape of the weighting function changes. Rather than the height of the peak continuing to rise, the weighting function tends to broaden. It then becomes more difficult to fit an exponential model to the transmittance over the necessary frequency range. For example, the present version of TRANSFIT cannot be used with 705 $cm^{-1}$ as the most transparent channel.

It may be possible to retain the present approach to nonlinear inversion with only a minor change to fix the value of B(0). That is, instead of utilizing the window radiance, we use the radiance associated with a large effective air mass. Then B(0) would be found from Equation (7) instead of Equation (12). The solution of

$$B(0) = F\,[B(0)]$$

can be found with Wegstein's method, as in the present version of INVERSIM.

The success of the above method will depend on the stability of three-ramp inversion. Furthermore, because of the problem of fitting exponential transmittances in the Q branch, it may not be possible to obtain a value of $s(\nu)$ large enough to stabilize the determination of B(0).

We recommend, therefore, that INVERSIM be applied in its present form with 707.5 and 710 wavenumbers as most transparent channels in order to demonstrate the feasibility of nonlinear inversion nearer to the band center. If three-ramp inversion is found to be more stable or if two-ramp profiles appear more accurate representations of the temperature structure, then modification of the nonlinear inversion method as suggested above should be undertaken.

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## GLOSSARY OF FORTRAN ACRONYMS

| | |
|---|---|
| ALTRAD | A subroutine converting radiances to a standard wavenumber and adding random error |
| HONW | A subroutine to compute the temperature profile from data in a compact format |
| INVERSIM | The main program which simulates nonlinear inversion applied to synthetic radiance data |
| NLIM2 | A subroutine to perform nonlinear inversion using the window radiance |
| OPTMZ | A subroutine to compute SWP parameters at optimal frequencies |
| PROFIL | A subroutine to compare the inferred and model profiles |
| PRONY | A subroutine to calculate roots and weights in Prony's method |
| RANDCM | A subroutine to produce random numbers |
| STRM | A subroutine to apply Sturm's test for the roots of a polynomial |
| SYNDAT | A subroutine to compute transmittances, weighting functions, and radiances |
| TRANSFIT | The main program which fits exponential models to real transmittances |
| TRFIT | A subroutine to fit data to a polynomial by least squares |
| TRFOUT | A subroutine to print the output of TRFIT |
| WEGST | A subroutine applying Wegstein's method to fix the profile with the window radiance |
| XCHNG | A subroutine to prepare transmittance data for polynomial fitting. |

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# APPENDIX I

## LEAST SQUARES FITTING OF TRANSMITTANCE DATA

The problem treated in this Appendix is the least squares determination of parameters $\alpha(\nu)$ and $a_\ell$ to fit data $y(p,\nu)$ to a polynomial in the independent variable $x(p)$. The mathematical formulation involves minimizing the weighted residual sum

$$R(\alpha,a) = \sum_{p,\nu} w(p,\nu)\left\{y(p,\nu) - \alpha(\nu) - \sum_{\ell=1}^{M} a_\ell[x(p)]^\ell\right\}^2 \qquad (I.1)$$

The regression equations are obtained by differentiation of R with respect to $\alpha(\nu)$ and $a_\ell$. If the normalization condition

$$\sum_{p} w(p,\nu) = 1 \qquad (I.2)$$

is satisfied, the regression equations take the form

$$\sum w(p,\nu)\left\{y(p,\nu) - \alpha(\nu) - \sum_{\ell=1}^{M} a_\ell[x(p)]^\ell\right\} \qquad (I.3)$$

$$\sum_{p,\nu} w(p,\nu)[x(p)]^\ell\left\{y(p,\nu) - \alpha(\nu) - \sum_{m=1}^{M} a_m[x(p)]^m\right\},\ 1 \leqq \ell \leqq M \quad . \qquad (I.4)$$

To simplify Equations (I.3) and (I.4) let us introduce the notation

$$X_\ell(\nu) \equiv \sum_p w(p,\nu)[x(p)]^\ell \qquad (1 \leqq \ell \leqq 2M) \qquad (I.5)$$

$$Y_\ell(\nu) \equiv \sum_p w(p,\nu)\ y(p,\nu)[x(p)]^\ell \qquad (0 \leqq \ell \leqq M) \quad . \qquad (I.6)$$

Then with Equation (I.2) the regression Equation (I.3) can be solved explicitly for $\alpha(\nu)$:

$$\alpha(\nu) = Y_o(\nu) - \sum_{\ell=1}^{M} a_\ell\, X_\ell(\nu) \qquad (I.7)$$

If we then insert the values (I.7) for $\alpha(\nu)$ in (I.4), we obtain a linear equation for $a_\ell$:

$$\sum_\nu [Y_\ell(\nu) - X_\ell(\nu)Y_o(\nu)] = \sum_{m=1}^{M} a_m \sum_\nu [X_{\ell+m}(\nu) - X_\ell(\nu)X_m(\nu)] \qquad (I.8)$$

$$(1 \leqq \ell \leqq M) \quad .$$

The solution of Equation (I.8) for the parameters $a_\ell$ involves a matrix inversion. The values $a_\ell$ are then inserted into Equation (I.7) to determine $\alpha(\nu)$. A FORTRAN subroutine called TRFIT has been written to carry out this procedure. It is basically a modification of the standard polynomial least square routine.