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**ON THE ESTIMATION OF
RELATIVE HUMIDITY PROFILES FROM
MEDIUM RESOLUTION INFRARED SPECTRA
OBTAINED FROM A SATELLITE**

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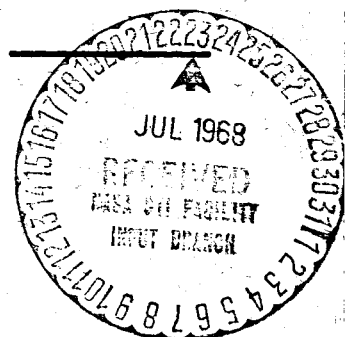
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ABSTRACT

Measurements of radiation emitted by the atmosphere of the earth in an infrared absorption band of water vapor, obtained with satellite borne instrumentation, contain information on atmospheric relative humidity. Two methods are developed for estimating tropospheric relative humidity profiles from infrared spectral measurements for which the spectral resolution elements are narrow compared to the total width of the absorption band, but wide compared to a single absorption line. The methods, which are essentially complementary, consist of a direct estimation technique which requires a minimum of a priori knowledge of the behavior of the relative humidity profile and a statistical estimation technique which can make full use of a knowledge of the statistics of tropospheric humidities in situations where such knowledge exists. An analysis of the propagation of errors in the measured spectral intensities indicates that meaningful estimates should be obtained from the 6.3 micron water vapor band in the presence of realistic instrumental noise for most types of atmospheres. One exception is the polar winter atmosphere where catastrophic error propagation occurs because of the behavior of the temperature profile. An examination of the effects

on the inferred relative humidity profile of errors in the temperature profile employed in the estimation reveals that the relative humidities inferred in the lowest layers of the troposphere are extremely sensitive to errors in the surface temperature, and this may prove to be the limiting factor in obtaining complete relative humidity profiles. Examples of applications of the techniques to synthetic data from model atmospheres and to real data obtained with a balloon borne infrared interferometer spectrometer are given.

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I. Introduction

Remote radiometric measurements of the thermally emitted infrared radiation from the atmosphere and the surface of the earth, performed with satellite-borne instruments, contain information on a number of parameters of interest in atmospheric physics and meteorology. Among these parameters are the temperature profile and the vertical distribution of non-uniformly mixed optically active gases. A considerable literature exists on the problem of estimating temperature profiles from radiometric measurements (see Wark and Fleming, 1966, and references therein), and the problem of obtaining the vertical distribution of non-uniformly mixed gases was treated formally by King (1963). In the present study, we shall be concerned with the specific problem of obtaining estimates of the vertical humidity distribution in the troposphere.

Several in the TIROS series of meteorological satellites carried instrumentation for making measurements in the 6 to 6.5 micron water vapor absorption region and the 8 to 12 micron "window" in addition to other passbands. These measurements have been used in estimating average tropospheric relative humidities, employing a method developed by Möller (Möller, 1961, 1962; Möller and Raschke, 1964; Raschke and Bandeen, 1967). Recently Smith (1967) has

developed a technique for making estimates of the water vapor mixing ratio as well as temperatures in the troposphere for a proposed 5-channel radiometer experiment.

Several forthcoming meteorological satellites will carry infrared interferometer spectrometer (IRIS) experiments (cf. Hanel and Chaney, 1965). The first of these will cover the spectrum from 5 to 20 microns with a resolution of 5 cm^{-1} . A spectrum obtained with an instrument of this type during a high altitude balloon flight near Palestine, Texas, on 8 May 1966 is shown in Figure 1. Included in this spectral region is the 6.3 micron water vapor absorption band. The possibility of having such measurements on a global basis provides motivation for the development of the theory of the estimation of tropospheric relative humidity profiles from spectra for which the individual spectral resolution elements are small compared to the total width of the absorption band but large compared to an individual absorption line. It is the purpose of the present study to investigate certain aspects of that theory.

In the development of any complete inversion technique a large number of factors must be taken into consideration. Here we shall confine ourselves to the development of basic approaches to the problem. The general principles of constituent inversion will be considered, and a direct estimation method will then be developed and used to study the sensitivity of the relative humidity estimates to errors in both the intensity measurements and in the temperature profile used

in the inversion. A statistical estimation method will then be examined. Examples of applications to synthetic data calculated from model atmospheres and real data from an IRIS balloon flight will be given. The effects produced by the possible presence of particulate matter will not be included in the scope of this study.

II. Basic Principles

For a nonscattering atmosphere in local thermodynamic equilibrium the spectral intensity at the top of the atmosphere can be written from the solution to the radiative transfer equation in the form

$$I(\nu) = B(\nu, T_s) \tau(\nu, X_s) - \int_{X_\infty}^{X_s} B[\nu, T(X)] \frac{\partial \tau(\nu, X)}{\partial X} dX \quad (1)$$

where $B(\nu, T)$ is the Planck function at wavenumber ν and temperature T , X is an arbitrary independent variable taken as increasing downward toward the surface, and $\tau(\nu, X)$ is the transmissivity at wavenumber ν of the column of gas between level X and the top of the atmosphere. The subscript s refers to surface values. It is assumed in (1) that the surface has unit emissivity, so the contribution from the surface is given by the first term. The second term in (1) represents the atmospheric contribution and for a given wavenumber can be regarded as an average of the source function over the weighting function $-\partial \tau(\nu, X)/\partial X$ which is everywhere positive since τ decreases with increasing X .

The principle of obtaining information on the atmospheric water vapor content from measurements of $I(\nu)$ can be seen in the following way. Since $\tau(\nu, X)$ at any level X depends on the amount of water vapor above that level, a change in the water vapor content of the atmosphere will cause a change in the weighting function relative to the temperature profile so a different segment of the source function will be sampled, and $I(\nu)$ will be changed. This effect is illustrated in Figure 2 where weighting functions in the 6.3 micron water vapor absorption band are shown for two model atmospheres with the same temperature profile but different relative humidities. To obtain information at several different atmospheric levels, measurements must be made at several points in the absorption band ranging from the more opaque band center to the less opaque band wings. Weighting functions at two different points in the 6.3 micron water vapor band are included in Figure 2. The calculations employed in Figure 2 were made using the water vapor transmissivities given by Möller and Raschke (1964) and correspond to resolution elements about 40 cm^{-1} wide. The sampling of the source function by the weighting function is not very sensitive to structure in the humidity profile which is of a scale small compared to the characteristic width of the weighting functions themselves. Any attempt at retrieving this fine structure can result in an instability against errors in the measured intensities just as occurs in the temperature inversion problem. Thus, the information obtainable on the humidity profile will be limited by the noise in the measurements of $I(\nu)$.

III. Direct Estimation

Throughout the remainder of this paper we shall utilize the transmissivities of Möller and Raschke (1964) in all of our examples. The use of these functions limits us to consideration of spectral resolution elements no narrower than about 40 cm^{-1} . However, the techniques considered should be equally applicable to data of higher spectral resolution when used with appropriate transmissivities.

There are a number of approaches which can be taken to the water vapor inversion problem; we shall consider two of these here. The first of these might be called a direct estimation of the relative humidity profile.

Let us assume that we have available to us measurements of outgoing spectral intensities, and call this measured spectrum $\hat{I}(\nu)$. Let us further assume we have available to us the temperature profile $T(X)$. Now if we arbitrarily assume some representation for the relative humidity profile containing a number of free parameters a_1, a_2, \dots, a_n and substitute this into (1) we obtain a parametric representation of the spectrum in terms of the a 's. For example, the a 's may be constants in some analytic form or coefficients in an expansion in terms of some function set. For convenience of notation let us denote the measured and theoretical intensities at the i th wave number by \hat{I}_i and I_i respectively and define the n -dimensional vector \mathbf{a} whose components are a_1, a_2, \dots, a_n . We can try to evaluate \mathbf{a} and hence get an estimate of the relative humidity profile by setting the measured intensities equal to the theoretical representation at m points ($m \geq n$) in the absorption band; i.e.,

$$I_i(\mathbf{a}) = \tilde{I}_i; i = 1, 2, \dots, m \quad (2)$$

Since in the practical situation we can extract only a few independent pieces of information with many of the measured intensities being redundant to within the experimental error, we will generally have many more measurements than parameters to be determined in experiments such as the IRIS. Hence (2) will be an overdetermined generally nonlinear system of algebraic equations.

A number of techniques exist for evaluating such a system of equations. The method which we have chosen is a generalization of the Newton-Raphson method. A Taylor expansion is made about some first guess, say \mathbf{a}^0 , and truncated after the linear term. This gives

$$\Delta I_i = \sum_{j=1}^n \left(\frac{\partial I_i}{\partial a_j} \right)_{\mathbf{a}=\mathbf{a}^0} \Delta a_j; i = 1, 2, \dots, m \quad (3)$$

where

$$\Delta I_i \equiv \tilde{I}_i - I_i(\mathbf{a}^0)$$

and

$$\Delta a_j \equiv a_j - a_j^0$$

An ordinary least-squares solution can now be obtained for $\Delta \mathbf{a}$ from the overdetermined linear system (3) which can be expressed in the well known matrix form

$$\Delta \mathbf{a} = (\mathbf{A}^* \mathbf{A})^{-1} \mathbf{A}^* \Delta \mathbf{I} \quad (4)$$

where

$$A_{ij} \equiv (\partial I_i / \partial a_j)_{\mathbf{a} = \mathbf{a}^0}$$

and A^* is the matrix transpose of A . The corrections $\Delta \mathbf{a}$ can be used to obtain what is hopefully an improved approximation to \mathbf{a} which can be used as a new first guess and the process iterated until some convergence criterion is satisfied, assuming convergence is obtained.

The above procedure is equivalent to making a least-squares fit of $I(\nu; \mathbf{a})$ to the measured spectrum $\tilde{I}(\nu)$. This does not imply that the resulting estimate for the relative humidity profile is necessarily a best fit to the true profile in a least-squares sense. One would prefer to have a technique which provides a least-squares fit to the true relative humidity profile, but of course this cannot be done directly since the true profile is unknown. However, it can be done in a statistical sense, and this approach will be considered in the following section.

The estimates obtained with this technique will generally depend on the representation assumed. There will be two types of errors involved, one of which is that due to the inability of the representation chosen to fit the profile exactly even for perfect measurements. The other type of error is due to errors in the inferred values of the parameters of the representation, resulting from errors in the measured values of the spectral intensities. In order to make the representation error as small as possible, a priori knowledge of the

humidity profiles can be used to make a reasonable choice of representation. One particular class of representations is that in which the relative humidity profile $r(X)$ depends on the parameters in a linear fashion, i.e.,

$$r(X) = \sum_{i=1}^n a_i \phi_i(X) \quad (5)$$

where the ϕ 's are arbitrary functions of X which might be members of some orthogonal function set or might be chosen such that $r(X)$ is expressed in terms of step functions or ramps. We shall consider examples using the form (5), but such a restriction is not a necessary one.

The transmissivities which we are employing for our examples can be written (Möller and Raschke, 1964)

$$\tau(\nu, X) = \exp \left\{ - \frac{1.97 \ell_\nu u^*(X)}{[1 + 6.57 \ell_\nu u^*(X)]^{1/2}} \right\} \quad (6)$$

where ℓ_ν is the generalized absorption coefficient at wave number ν , and u^* is the reduced absorber mass

$$du^* = (p/p_0)^{0.72} \sqrt{\frac{T_0}{T}} du \quad (7)$$

with T_0 and p_0 referring to standard temperature and pressure. The temperature factor $\sqrt{T_0/T}$ has been neglected in the present study. It has been found convenient to choose the independent variable X as the atmospheric pressure p for

the present application. Use of the form of the transmissivity given by (6) allows us to express in a rather simple form the quantities $\partial I_i / \partial a_j$ required for each step of the Newton-Raphson calculation. It is convenient to start with the integration by parts form of (1)

$$I_i = B_i(0) + \int_0^{P_s} \frac{\partial B_i(p)}{\partial p} \tau_i(p) dp \quad (8)$$

where the subscript i denotes values for the i th spectral resolution element in the absorption band. Making use of the well known approximate relationship between specific humidity and relative humidity

$$w \text{ (g/kg)} \simeq 622 \frac{e_s}{p} r \quad (9)$$

and relation (7), along with the expression for the absorber mass

$$du = \frac{1}{g} w dp \quad (10)$$

we obtain from (8)

$$\frac{\partial I_i}{\partial a_j} = \int_0^{P_s} \frac{\partial B_i(p)}{\partial p} \frac{\partial \tau_i(p)}{\partial u^*} \psi_j(p) dp \quad (11)$$

where

$$\psi_j(p) = \frac{622}{g} \int_0^p \left(\frac{p'}{p_0} \right)^{0.72} \frac{e_s(T)}{p'} \phi_j(p') dp' \quad (12)$$

The gravitational acceleration is represented by g , and e_s is the saturation vapor pressure which is a function of temperature only. The factor $\partial \tau_i / \partial u^*$ occurring in the integrand in (11) is to be evaluated at each iterative step using the value of the relative humidity profile estimated in the previous step.

In order for such a computational scheme to be of value, the region of convergence must be sufficiently large to allow one to make a reasonable first guess. It appears that the question of convergence can best be examined empirically. To obtain some feeling for the behavior of this method of estimation, synthetic data were calculated and inversions performed for a number of model atmospheres.

Application to a rather wet mid-latitude model is shown in Figure 3. A 3-parameter representation consisting of two ramps linear in pressure with the break point at the 500 mb level was employed. Synthetic data for nine 40 cm^{-1} wide spectral resolution elements between 1200 cm^{-1} and 1520 cm^{-1} were used with a "first guess" of a completely saturated atmosphere with 100% relative humidity at all levels. Convergence to the solution shown was obtained in about six iterations. For most model atmospheres tried, the a 's were found to change less than 1% after five or six iterations. In practice, one could probably make better first guesses than the crude one used here.

An inversion of synthetic data from a tropical model is shown in Figure 4. Once again a 3-parameter 2-ramp representation with the break point at 500 mb

was employed. Because of the higher atmospheric opacity due to the larger amount of water vapor present, it was necessary to go further into the band wing in order to insure some sensitivity to the lower-most layers of the troposphere. Ten spectral resolution elements between 1160 cm^{-1} and 1520 cm^{-1} were employed.

One very important aspect of any inversion technique is the stability of the estimation against random errors in the measured intensities. The root-mean-square fluctuation in the estimated values of the parameters σ_a due to the presence of a given rms error in the intensities σ_I can be approximated for small errors by

$$\sigma_{a_i} = \left[\sum_{j=1}^m \left(\frac{\partial a_i}{\partial I_j} \right)^2 \sigma_{I_j}^2 \right]^{1/2} \quad (13)$$

The factors $\partial a_i / \partial I_j$ required in (13) are just the elements of the matrix $(A^* A)^{-1} A^*$ of (4) which are required in the inversion. If the σ_{I_j} are the same for all spectral resolution elements we can define an error amplification factor

$$K_i = \left[\sum_{j=1}^m \left(\frac{\partial a_i}{\partial I_j} \right)^2 \right]^{1/2} \quad (14)$$

such that

$$\sigma_{a_i} = K_i \sigma_I \quad (15)$$

In the two ramp representation used in the examples above, the three parameters solved for were the relative humidities at the 100 mb, 500 mb, and 1000 mb levels.

The error amplification factors corresponding to these three parameters for the mid-latitude and tropical models used above are given in Table I.

Table I
Error Amplification Factors K_i ($\text{erg cm}^{-2} \text{sec}^{-1} \text{ster}^{-1} \text{cm})^{-1}$

Parameter	Model Atmosphere		
	Mid-Latitude	Tropical	Polar
2-Ramp $\left\{ \begin{array}{l} r_{100 \text{ mb}} \\ r_{500 \text{ mb}} \\ r_{1000 \text{ mb}} \end{array} \right.$	0.376	0.334	—
	0.231	0.237	—
	0.603	0.730	—
2-Layer $\left\{ \begin{array}{l} r_{100-575 \text{ mb}} \\ r_{575-1000 \text{ mb}} \end{array} \right.$	—	—	0.102
	—	—	1.246

The error which is due to the representation alone will be dependent on how well the assumed form can be made to fit a given profile, so will vary from case to case. Some idea of typical errors of representation can be gotten from Figures 3 and 4. The IRIS experiment provides an example of the random error in the measurement of the spectral intensities which might be expected in the practical situation. The rms error expected in that experiment is about $0.5 \text{ erg cm}^{-2} \text{sec}^{-1} \text{ster}^{-1} \text{cm}$. In order to meet the constraints of the transmissivities employed in the examples above, the IRIS data would have to be averaged over about eight 5 cm^{-1} wide resolution elements, so the resulting effective rms error would be about $0.2 \text{ erg cm}^{-2} \text{sec}^{-1} \text{ster}^{-1} \text{cm}$. The effects of such an error on the three parameters of the inversion are shown by the error bars in

Figure 4. In this particular case the error due to noise in the measurements is about the same size as the representation error.

Figure 5 shows an inversion of synthetic data for a polar winter model atmosphere which is probably a worst case for inferring relative humidities. The representation used in this case was a step function consisting of two layers of constant relative humidity divided at the 575 mb level. Once again the error bars indicate the effects of a $0.2 \text{ erg cm}^{-2} \text{ sec}^{-1} \text{ ster}^{-1} \text{ cm}$ random error in the measured intensities. It can be seen that the inferred relative humidity for the bottom layer is quite unstable against errors in the measurements. This is primarily due to the behavior of the temperature profile which is also shown in the figure. The average temperature in the bottom layer is very near the surface temperature so that layer looks very much like an extension of the blackbody surface and the outgoing intensities are highly insensitive to the actual value of the relative humidity in the layer.

A quantity of considerable interest which can be calculated from the relative humidity profile along with the temperature profile is the total water vapor in an atmospheric column. The inferred total water vapor using exact intensities is compared with the actual value in each of the examples shown in Figures 3, 4, and 5. The lack of complete agreement is due to the representation errors in the relative humidity profiles. The percentage rms error in the inferred total amount of water vapor due to rms intensity errors of $0.2 \text{ erg sec}^{-1} \text{ cm}^{-2} \text{ ster}^{-1}$

cm is 12% for the mid-latitude model, 9% for the tropical model, and 41% for the polar winter model.

In the examples considered, we have used representations for the relative humidity profile containing considerably fewer parameters than the number of spectral intensity measurements employed in the inversions. Attempts at using more complex representations containing additional parameters, lead to such strong propagation of instrumental errors that the results would be of little value. The instrumental noise of $0.2 \text{ erg sec}^{-1} \text{ cm}^{-2} \text{ ster}^{-1} \text{ cm}$ for intensities averaged over 40 cm^{-1} constitutes an error of almost 10% in the most opaque parts of the 6.3 micron band. This is due primarily to the low values of the Planck intensities in this spectral region (see Figure 1). It is only through the use of a number of spectral intensities in a redundant sense such as in a least-squares calculation that we are able to obtain inversions in the presence of such errors.

Up to this point we have assumed an exact knowledge of the temperature profile. In the practical situation, we will presumably have to rely upon temperature profiles estimated from spectral measurements in the 15 micron carbon dioxide absorption band, for example. Since these temperature estimates will contain errors, it is important to investigate the effects of errors in the temperature profile on the relative humidity estimates.

It was pointed out by Möller (1962) that the intensity at the top of the atmosphere for a spectral interval in a water vapor absorption band is not dependent on the temperature profile provided the following conditions are satisfied: (a) the relative humidity is constant at all levels to which the outgoing intensity is sensitive, (b) the optical thickness of the atmosphere is large enough to prevent there being a significant contribution from the surface, (c) the temperature lapse rate is constant, (d) the atmospheric transmissivity from a given level to the top of the atmosphere depends only on the total amount of water vapor between that level and the top of the atmosphere. When these conditions are met, the same temperature will always occur at the same optical depth regardless of the absolute value of the temperature at any given height. Conditions (a), (c), and (d) will never be rigorously satisfied in the practical situation, and (b) is not satisfied when we use data from the wings of the absorption band in an effort to get information on the lower-most layers of the troposphere. Therefore, an empirical investigation was made of the effects of perturbations in the temperature profile on the estimated relative humidities.

Temperature perturbations of -1° K were introduced successively into the region between 50 mb and 300 mb, the region between 350 mb and 550 mb, the region between 600 mb and 950 mb, and the surface temperature for a mid-latitude model atmosphere, and a relative humidity inversion was performed for each case as well as the case of the exact temperature profile. The perturbations resulting for the three relative humidities forming the parameters for the two

ramp representation are given in Table II. The effect on estimations of the total water vapor amount is also indicated. It can be seen that the relative humidity estimates are not particularly sensitive to small errors in the atmospheric temperature, but are quite sensitive to errors in the surface temperature. The reason for this extreme sensitivity is that in using the spectral region between 1200 cm^{-1} and 1520 cm^{-1} rather transparent portions of the band wings have been included in order to obtain information on the lower-most layers of the troposphere. Here the boundary term in (1) is large compared to the atmospheric contribution so the surface temperature is the parameter to which the intensities are most sensitive. This sensitivity can be reduced by not using the intensities as far out into the band wings; however, this will reduce the information gained on the humidity in the lower part of the troposphere. It should be noted that while reasonable estimates of relative humidity might be made when there are errors in the estimated atmospheric temperatures, the resulting estimates of the absolute humidity may contain large errors due to the strong sensitivity of the saturation vapor pressure to the temperature.

If the temperature profile used in estimating the relative humidity profile must come from an inversion in the 15 micron carbon dioxide absorption band, there is an additional complication due to the finite water vapor absorption in this region as well as the "window" region near 11 microns from which the surface temperature must be obtained. Thus, the water vapor and temperature

Table II
Effects on 2-Ramp Inversion Parameters of Temperature
Perturbations of -1°K at Selected Levels

Region of Temperature Perturbation	u (g cm^{-2})	δu (g cm^{-2})	$r_{100 \text{ mb}}$	$\delta r_{100 \text{ mb}}$	$r_{500 \text{ mb}}$	$\delta r_{500 \text{ mb}}$	$r_{1000 \text{ mb}}$	$\delta r_{1000 \text{ mb}}$
Unperturbed	2.28	—	0.222	—	0.345	—	0.546	—
50-300 mb	2.25	-0.03	0.273	0.051	0.352	0.007	0.531	-0.015
350-550 mb	2.33	0.05	0.212	-0.010	0.341	-0.004	0.573	0.027
600-950 mb	2.08	-0.20	0.236	0.014	0.333	-0.012	0.525	-0.021
Surface	1.72	-0.56	0.147	-0.075	0.405	0.060	0.321	-0.225

inversions are essentially coupled. One approach to this problem is an overall iterative scheme which takes advantage of the relatively weak dependence of the window and 15 micron band intensities on the humidity profile. A first guess at the relative humidity profile is made and the surface temperature and atmospheric temperature profile are estimated from the window and 15 micron regions. These temperatures are then used along with measured intensities in the water vapor band to obtain an improved relative humidity profile. The process is then iterated until convergence is obtained. An example of such a calculation on synthetic data from the mid-latitude model used above is shown in Figure 6. Five iterations were required to obtain the solution shown. The representation assumed for the temperature profile consisted of two ramps linear in the logarithm of the pressure with the break points chosen at the 200 mb and the 800 mb levels and the temperature above 200 mb assumed constant.

As a final example of a direct estimation of relative humidity, an inversion of actual IRIS data was performed. The data were obtained during a high altitude balloon flight 8 May 1966 near Palestine, Texas (Chaney, et al., 1967). The results are shown in Figure 7.

IV. Statistical Estimation

Up to this point we have used the a priori information available on humidities in the troposphere only as a guide in picking reasonable representations for approximating the relative humidity profile. For those geographic regions for

which a large amount of information is available, it would seem desirable to make better use of this information. One possible approach would be to employ as the function set in expansion (5) empirical orthogonal functions (Obukhov, 1960; Holmström, 1963) constructed from radiosonde data collected in the past at the station in question. This method has been applied to the temperature inversion problem (Alishouse et al, 1967; Wark and Flemming, 1966). Another approach is to attempt to devise a regression relation between the measured intensities and the relative humidity at each level. This method will be investigated here.

As mentioned earlier, the least squares fitting of the measured spectrum does not in general imply a least squares fit of the representation for the relative humidity profile to the true relative humidity profile. We can, however attempt to minimize the mean square deviation of the estimated profile from the true profile in a statistical sense. A formulation of this type has been given for general linear systems by Foster (1961) and for the temperature inversion problem by Rodgers (1966) and by Strand and Westwater (1968). The procedure below follows the general derivation given by these authors.

Let us consider an ensemble consisting of q measurements of the m -component intensity vector $\tilde{\mathbf{I}}$ and the corresponding n -component relative humidity vector $\tilde{\mathbf{r}}$. Define the m by q matrix $\tilde{\mathbf{A}}$ such that each column corresponds

to a member of the ensemble of intensity measurements from which the ensemble mean has been subtracted. Similarly, let $\tilde{\rho}$ be an n by q matrix whose columns correspond to the measured relative humidity profiles minus the ensemble mean. Now define a linear estimate $\hat{\rho}$ to the true relative humidity profiles of the form

$$\hat{\rho} = H\tilde{\rho} \quad (16)$$

where H is an n by m matrix of coefficients to be determined. Even though the relationship between relative humidities and spectral intensities is generally nonlinear, the assumed linear form should give reasonable results at least in the vicinity of the ensemble mean. If it is found necessary, higher order terms can be added to (16).

The elements of H can be determined by requiring that the mean square deviation of the estimated profiles $\hat{\rho}$ from the true profiles ρ be a minimum which is equivalent to requiring that the diagonal elements of the matrix

$$Q = \frac{1}{q} (\rho - \hat{\rho}) (\rho - \hat{\rho})^* \quad (17)$$

be minimized. This results in

$$H = CR^{-1} \quad (18)$$

where C is the n by m cross-covariance matrix

$$C = \frac{1}{q} \rho \tilde{\rho}^* \quad (19)$$

and R is the n by n covariance matrix of the measured intensities

$$R = \frac{1}{q} \tilde{\mathcal{I}} \tilde{\mathcal{I}}^* \quad (20)$$

To be able to calculate C , we need to know the true relative humidity profiles ρ when in fact all we have available are the measured values $\tilde{\rho}$ which will generally contain errors

$$\tilde{\rho} = \rho + \eta \quad (21)$$

where η is the matrix of errors associated with the measurements. If the errors are random with zero ensemble mean, then ρ can simply be replaced with $\tilde{\rho}$ in (19).

Since it does not appear to be practical to assemble the necessary ensemble of both intensity measurements and corresponding relative humidity measurements, we must rely on the measured relative humidity profiles alone and use radiative transfer theory and an a priori knowledge of the instrumental noise in the spectral measurements to obtain C and R . Let us assume the measured intensities $\tilde{\mathcal{I}}$ can be represented by

$$\tilde{\mathcal{I}} = \mathcal{I} + \epsilon \quad (22)$$

where \mathcal{I} is the matrix of true intensities, and ϵ represents the matrix of instrumental noise, assumed to have zero mean and to be uncorrelated with the measured relative humidities. The calculation can be simplified by expanding the theoretical relationship between the intensities and the relative humidity profile about the ensemble mean and truncating after the linear term, i.e.,

$$\mathcal{I} \simeq \mathbf{P}\rho \quad (23)$$

where \mathbf{P} is the m by n Jacobian matrix whose elements are of the form $\partial I_i / \partial r_j$ and are evaluated using the ensemble mean relative humidity profile. This approximation is consistent with (16) and allows us to write \mathbf{C} and \mathbf{R} explicitly in terms of the covariance matrix of the true relative humidity profiles. In calculating the true values of \mathcal{I} required in (22), we need the true values of ρ , but again we have available only the ensemble of measurements $\tilde{\rho}$. By utilizing (21) and the previous assumptions on η , along with the additional assumption that η and ϵ are uncorrelated, we obtain

$$\mathbf{H} \simeq \mathbf{S}\mathbf{P}^* (\mathbf{P}\mathbf{S}\mathbf{P}^* + \mathbf{N})^{-1} \quad (24)$$

where \mathbf{N} is the covariance matrix of the instrumental noise

$$\mathbf{N} = \frac{1}{q} \epsilon \epsilon^* \quad (25)$$

and \mathbf{S} is the covariance matrix of the true relative humidity profiles

$$\mathbf{S} = \frac{1}{q} (\tilde{\rho} \tilde{\rho}^* - \eta \eta^*) \quad (26)$$

Thus, if the covariance matrix $1/q \eta \eta^*$ is known, the effect of the random errors in the measured relative humidity profiles $\tilde{\rho}$ can be taken into consideration in the computation of \mathbf{S} .

We can now use \mathbf{H} in the estimation of a relative humidity profile from actual intensity measurements $\tilde{\mathbf{I}}$, providing the ensemble used in calculating \mathbf{S} is representative of the conditions to which the intensity measurements pertain.

The estimated relative humidity profile is then given by

$$\hat{\mathbf{r}} \simeq \langle \mathbf{r} \rangle + \mathbf{SP}^* (\mathbf{PSP}^* + \mathbf{N})^{-1} [\hat{\mathbf{I}} - \mathbf{I}(\langle \mathbf{r} \rangle)] \quad (27)$$

where $\langle \mathbf{r} \rangle$ denotes the ensemble mean relative humidity profile, which is used along with the temperature profile in the computation of \mathbf{P} and $\mathbf{I}(\langle \mathbf{r} \rangle)$. The residual variances Q_{ii} are given by the diagonal elements of the residual covariance matrix (17) evaluated using (16) and (24),

$$\mathbf{Q} \simeq \mathbf{S} - \mathbf{SP}^* (\mathbf{PSP}^* + \mathbf{N})^{-1} \mathbf{PS} \quad (28)$$

As the previous authors have pointed out, the inversion is stable against instrumental noise in the sense that $Q_{ii} \rightarrow S_{ii}$ as $N \rightarrow \infty$.

In order to obtain some feeling for the behavior of such an estimation scheme, we have employed an ensemble of twenty-five humidity profiles based on radiosonde data taken at Guam Island during the months of July and August over a three year period. The covariance matrix for the relative humidities was calculated, and the ensemble mean profile along with the standard deviation for each level ($= \sqrt{S_{ii}}$) is shown in Figure 8. In many situations, the noise covariance matrix will reduce to a single noise variance σ_N^2 times the unit matrix. The residual standard deviation $\sqrt{Q_{ii}}$ at each level is shown in Figure 8 for the case where $\sigma_n = 0.2 \text{ erg cm}^{-2} \text{ sec}^{-1} \text{ ster}^{-1} \text{ cm}$, demonstrating the amount by which the variance is reduced in this particular case by the spectral data over that for the a priori statistics alone.

Figure 9 shows the results of an estimation using synthetic data from a model atmosphere which employed as a relative humidity profile a member of the original ensemble which lies fairly close to the ensemble mean profile. The fit in terms of both the relative humidity profile and the total water vapor amount is quite satisfactory. A similar inversion on synthetic data is shown in Figure 10. In this case the model atmosphere is based on a member of the ensemble which differs considerably from the ensemble mean. The fit is not quite as good as in the previous case, especially above the 500 mb level; this is partly due to the assumption of the linear relationship (16) which becomes increasingly poor the further the sounding is from the ensemble mean.

To obtain some feeling for the dependence of the results of an estimation on the type of ensemble employed relative to the type of profile sought, the covariance matrix and ensemble mean for the tropical ensemble were used to perform an inversion on the synthetic data from the mid-latitude model considered previously. The results are shown in Figure 11. The fit is not as good as in the previous examples, presumably because the sounding is atypical with reference to the ensemble used.

V. Summary and Discussion

Two possible approaches to the problem of estimating tropospheric relative humidity profiles from medium resolution infrared spectra obtainable from an earth satellite have been developed. The direct estimation technique should be applicable in those situations for which little a priori knowledge of the behavior

of the humidity profile is available. For applications to regions for which a considerable amount of information exists on the statistical behavior of the relative humidity profile, it is highly desirable to take this information into consideration in performing inversions. The statistical estimation technique which has been described here provides one means of accomplishing this. Hence, the two methods are essentially complementary.

Calculations using both model atmospheres and actual data from a balloon borne infrared interferometer spectrometer experiment indicate reasonably stable inversions can be obtained using the direct estimation technique with a three parameter representation, in the presence of realistic instrumental noise. One exception is the polar winter type atmosphere for which the measured intensities are insensitive to the humidities because of the behavior of the temperature profile.

An empirical study of the influence of errors in the temperature profile on the relative humidity estimates indicates that the relative humidity inferred is not extremely sensitive to errors in the atmospheric temperatures. However, absolute quantities such as mixing ratios obtained from these relative humidities and temperatures will be quite sensitive to temperature errors because of the strong dependence of the saturation vapor pressure on temperature. When the more transparent wings of the absorption band are employed in an effort to obtain information on lower tropospheric layers, it is found that the inferred

relative humidities are very sensitive to errors in the surface temperature. This may prove to be the limiting factor in the accuracy of estimates of complete relative humidity profiles. The surface temperature must be determined in satellite experiments from measurements in an atmospheric "window" such as that near 11 microns. The temperatures obtained in this way will be influenced by instrumental errors and by uncertainties in the atmospheric transmissivities in the window region. The window transmissivities will be dependent not only on water vapor, but also on the particulate matter present which will generally be an unknown parameter.

The linear statistical estimation technique when applied to synthetic data from model atmospheres shows sufficient promise to warrant further development in the future. The success of the method depends strongly on having a good estimate for the relative humidity covariances for the location in question and also the covariances for the noise associated with the instrument employed. Further study is required to determine those geographical regions for which the method might be reliably used. Other areas of future investigation include the possibility of obtaining an improvement by including nonlinear terms in (16) and the possibility of combining measurements in the 6.3 micron band, the window region, and the less opaque parts of the 15 micron band to perform a combined statistical estimation of tropospheric temperature and water vapor.

This study has concentrated primarily on the 6.3 micron water vapor band because the first of the satellite experiments to which the work is applicable will include that band. However, the basic techniques developed here should be equally applicable to the rotation water vapor band beyond 20 microns and that spectral region should not be neglected in future work. The transmissivities of Möller and Raschke have been used here, but other transmissivities such as those given by Williamson and Houghton (1965) could be fit into the computational techniques equally well.

There are a number of factors which must be taken into consideration in the development of methods for obtaining relative humidity profiles from satellite measurements on a truly global basis which have not been included within the scope of this study. Perhaps foremost among these is the problem of treating the case in which the field-of-view of the instrument is partly cloud filled. Smith (1967) has proposed a technique for treating this problem based on the availability of additional information in the form of spatial scans within the principal area for which the inversion is to be performed. For experiments for which this additional information is not available, other techniques must be developed. Also, quantitative estimates of the effects of atmospheric turbidity which may be enhanced in spectral regions of strong water vapor absorption (Deirmendjian, 1960) are needed. However, the computational methods considered here should provide a basis for utilizing the forthcoming satellite experiments to develop techniques which can eventually be incorporated into operational systems.

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References

- Alishouse, J. C., L. J. Crone, H. E. Fleming, F. L. Van Cleef, and D. Q. Wark, A Discussion of Empirical Orthogonal Functions and Their Application to Vertical Temperature Profiles, Tellus, 19, 477-481 (1967).
- Chaney, L. W., S. R. Drayson, and C. Young, Fourier Transform Spectrometer Radiation Measurements and Temperature Inversion, Applied Optics, 6, 347-349 (1967).
- Diermendjian, D., Atmospheric Extinction of Infra-red Radiation, Quart. J. R. Met. Soc., 86, 371-381 (1960).
- Foster, Manus, An Application of the Wiener-Kolmogorov Smoothing Theory to Matrix Inversion, J. Soc. Indust. Appl. Math., 9, 387-392 (1961).
- Hanel, R. A., and L. Chaney, The Merits and Shortcoming of a Michelson Type Interferometer to Obtain the Vertical Temperature and Humidity Profile, in Proceedings of the XVII International Astronautical Congress, Madrid, 9-15 October 1966, Vol. II (1966).

Holmström, I., On a Method for Parametric Representation of the State of the Atmosphere, Tellus, 15, 127-149 (1963).

King, J. I. F., Meteorological Inferences from Satellite Radiometry. I, J. of Atmos. Sci., 20, 245-250 (1963).

Möller, F., Atmospheric Water Vapor Measurements at 6-7 Microns from a Satellite, Planet. Space Sci., 5, 202-206 (1961).

Möller, F., Einige Vorläufige Auswertungen der Strahlungsmessungen von Tiros II, Arch. Meteorol. Geophys. Bioklimatol. Ser. B., 12(1), 78-94 (1962).

Möller, F., and E. Raschke, Evaluation of Tiros III Radiation Data, Contractor Report CR-112, National Aeronautics and Space Administration, Washington (1964).

Obukhov, A. M., The Statistically Orthogonal Expansion of Empirical Functions, Izvestiya, Seriya Geofizicheskaya, Akademiya Nauk, SSSR, No. 3, 432-439 (1960). (English translation by the American Geophysical Union, 288-291, Nov. 1960.)

Raschke, E., and W. R. Bandeen, A Quasi-Global Analysis of Tropospheric Water Vapor Content from Tiros IV Radiation Data, J. of Appl. Meteor., 6, 468-481 (1967).

Rodgers, C. D., Satellite Infrared Radiometer; A Discussion of Inversion Methods, University of Oxford Clarendon Laboratory Memorandum No. 66.13, 25 pp. (1966).

Smith, William L., An Iterative Method for Deducing Tropospheric Temperature and Moisture Profiles from Satellite Radiation Measurements, Monthly Weather Review, 95, 363-369 (1967).

Strand, O. N., and E. R. Westwater, Minimum-RMS Estimation of the Numerical Solution of a Fredholm Integral Equation of the First Kind, to be published in SIAM Journal on Numerical Analysis (1968).

Wark, D. Q., and H. E. Fleming, Indirect Measurements of Atmospheric Temperature Profiles from Satellites: I. Introduction, Monthly Weather Review, 94, 351-362 (1966).

Williamson, E. J., and J. T. Houghton, Radiometric Measurements of Emission from Stratospheric Water Vapor, Quart. J. R. Met. Soc., 91, 330-338 (1965).

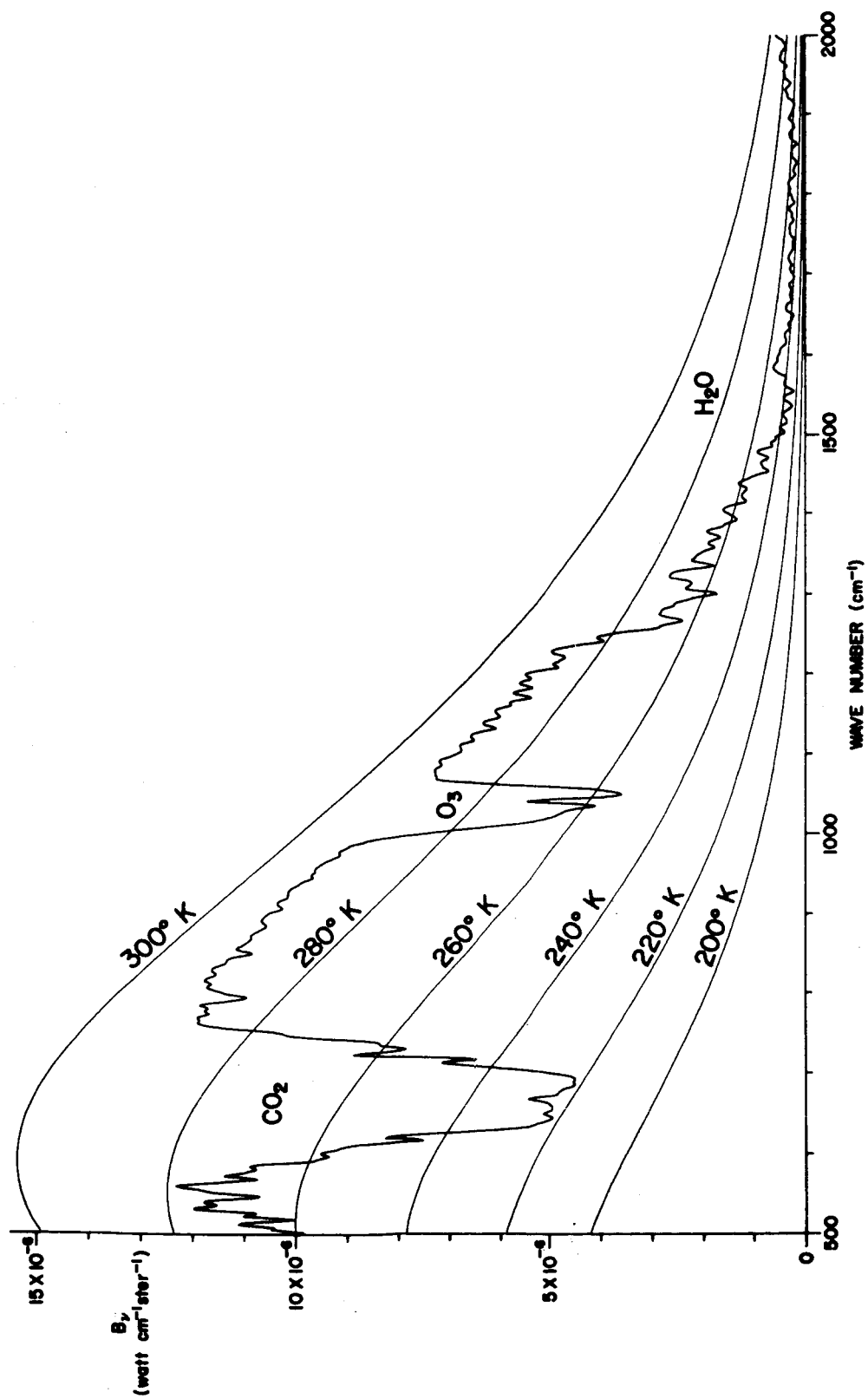


Figure 1—Spectrum obtained with an infrared interferometer spectrometer (IRIS) flown in a high altitude balloon 8 May 1966 near Palestine, Texas.

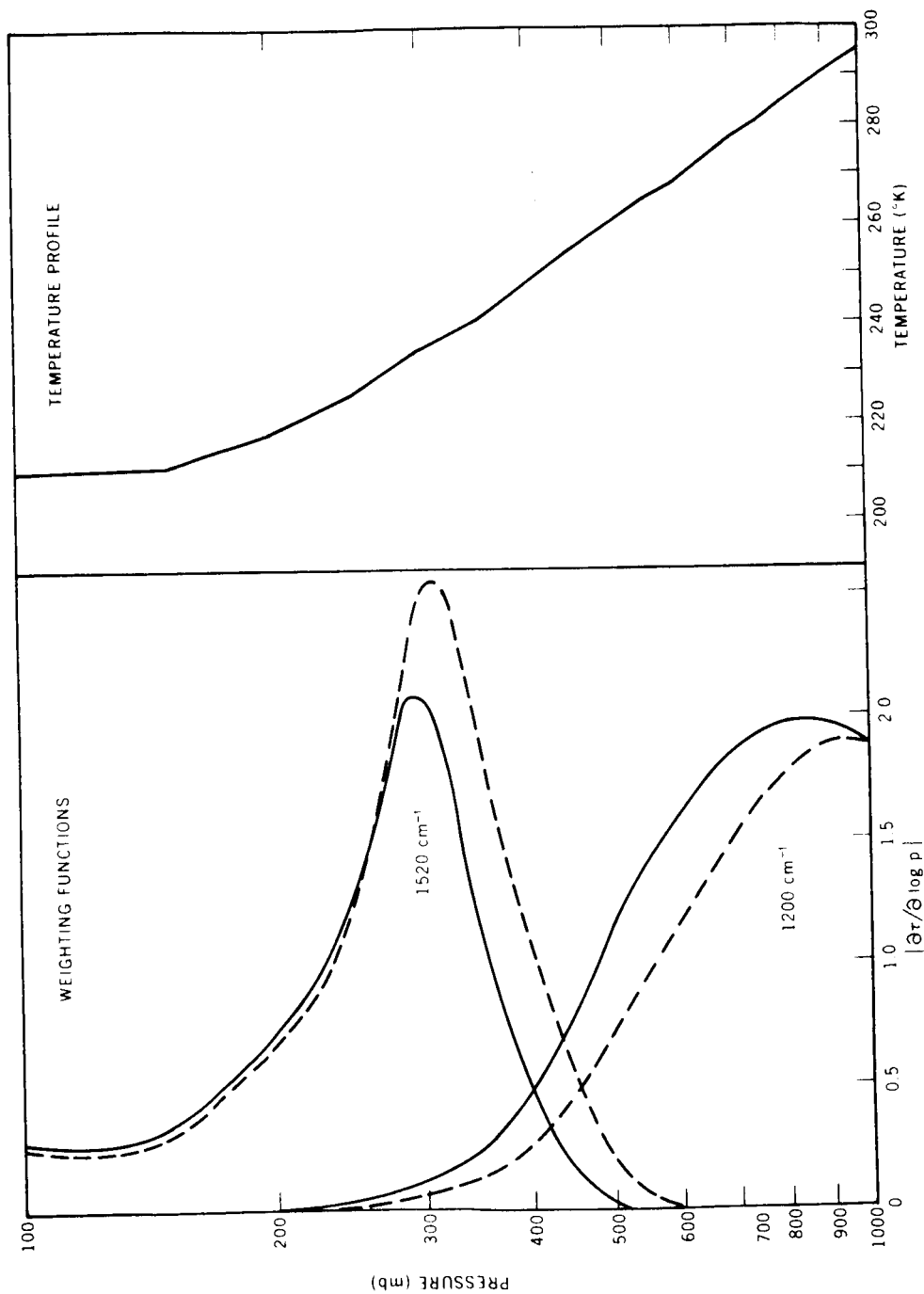


Figure 2—Weighting functions and temperature profile for model atmospheres used to illustrate the principles of inferring information on tropospheric water vapor from remote measurements of spectral intensities. The solid lines refer to a model with a relative humidity of 80% at all levels while the broken lines refer to a model with a 40% relative humidity at all levels.

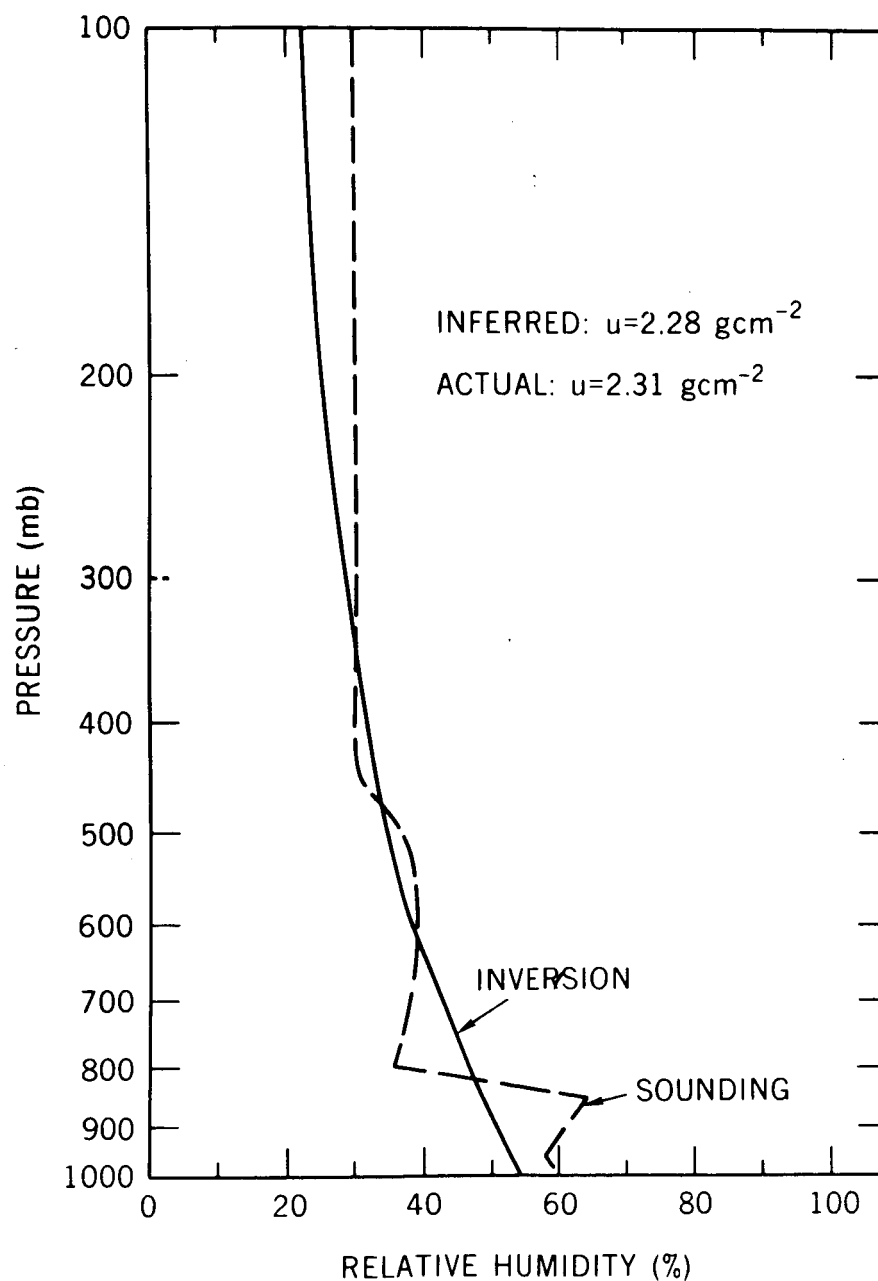


Figure 3—Inversion of synthetic data from a mid-latitude model atmosphere. A 3-parameter representation consisting of two ramps linear in pressure was employed.

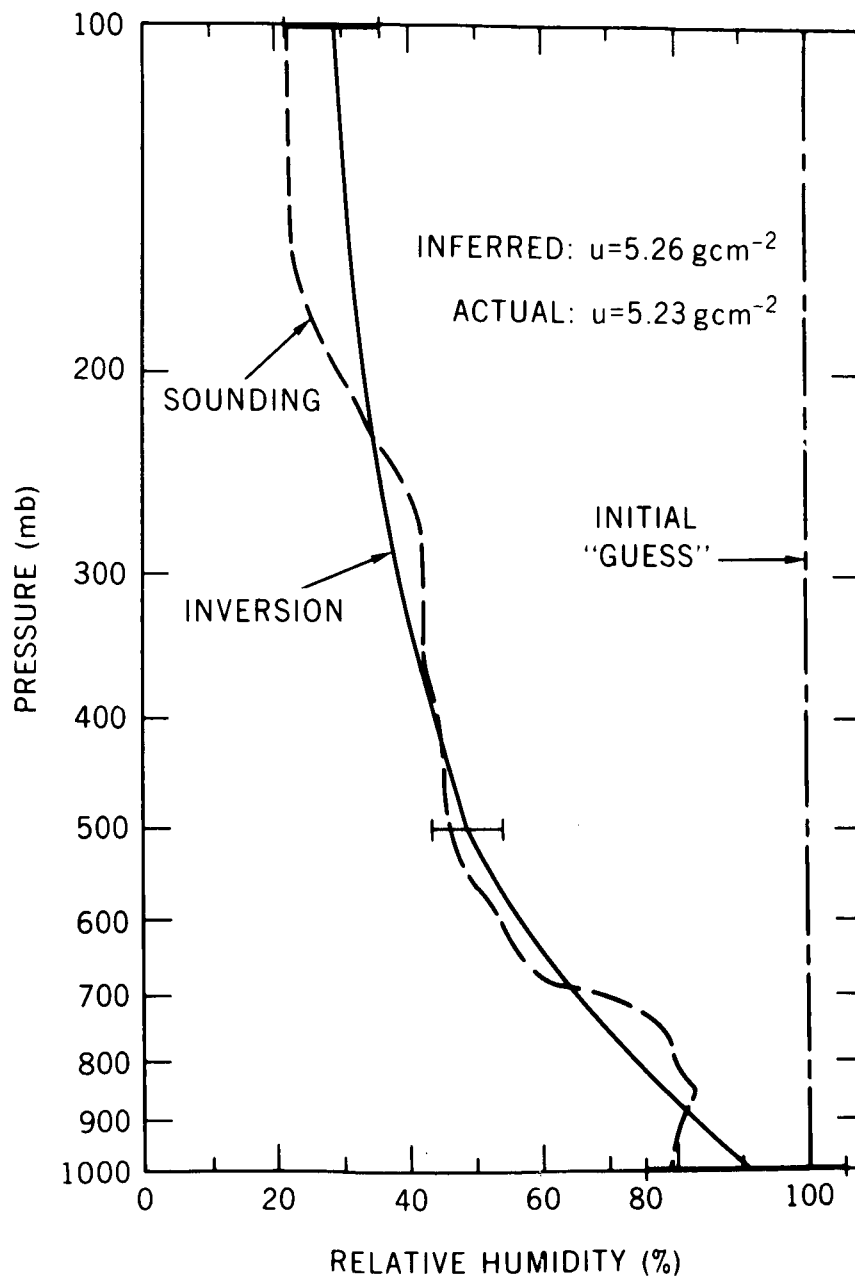


Figure 4—A 2-ramp inversion of synthetic data from a tropical model atmosphere. The error bars indicate the rms dispersion in the inferred profile due to noise in the intensities with an rms value typical of that expected from satellite borne instruments.

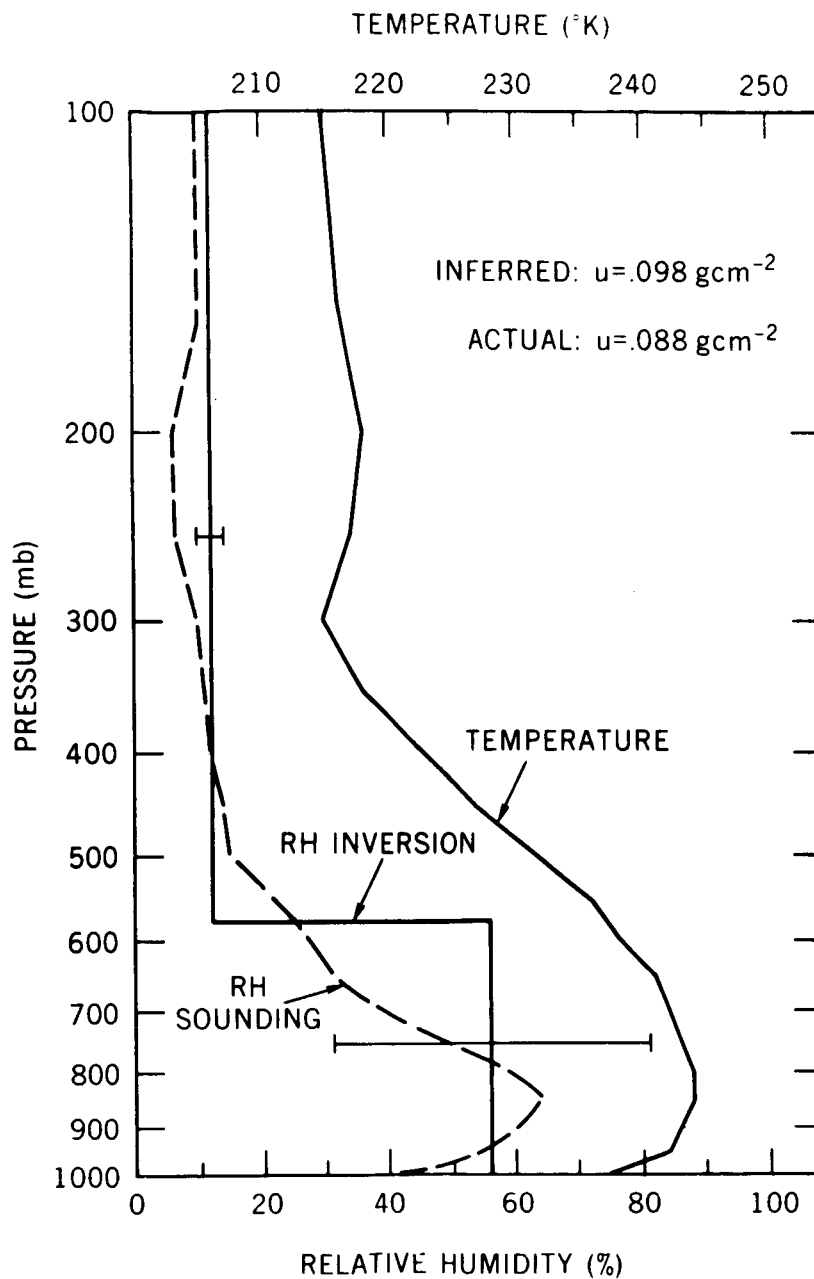


Figure 5—A 2-layer inversion of synthetic data from a model polar winter atmosphere. The error bars have the same significance as in Fig. 4. The temperature profile employed in the model is also shown.

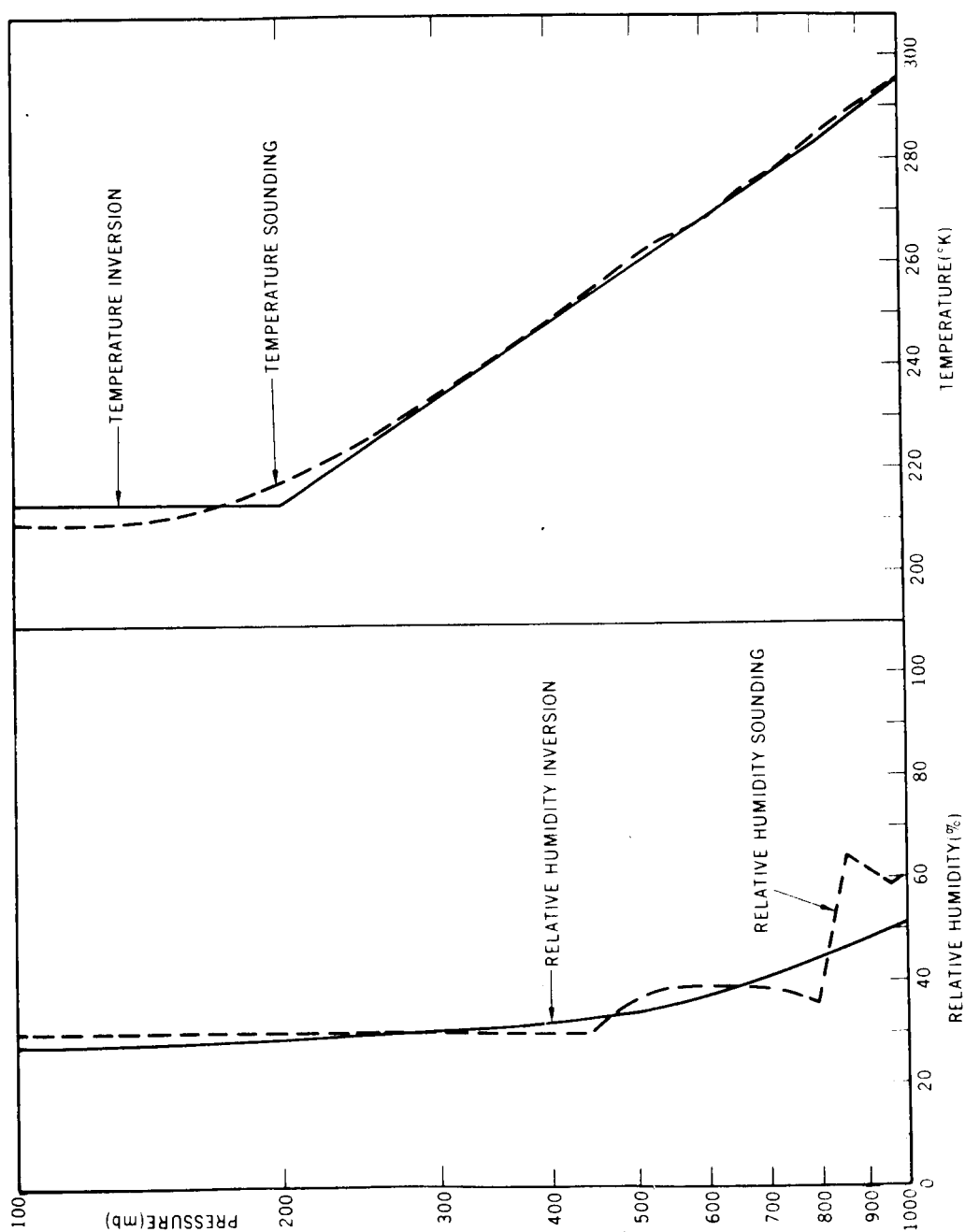


Figure 6—Combined temperature and relative humidity inversion using synthetic data from a mid-latitude model atmosphere. Three-parameter representations were employed for both the temperature and relative humidity profiles.

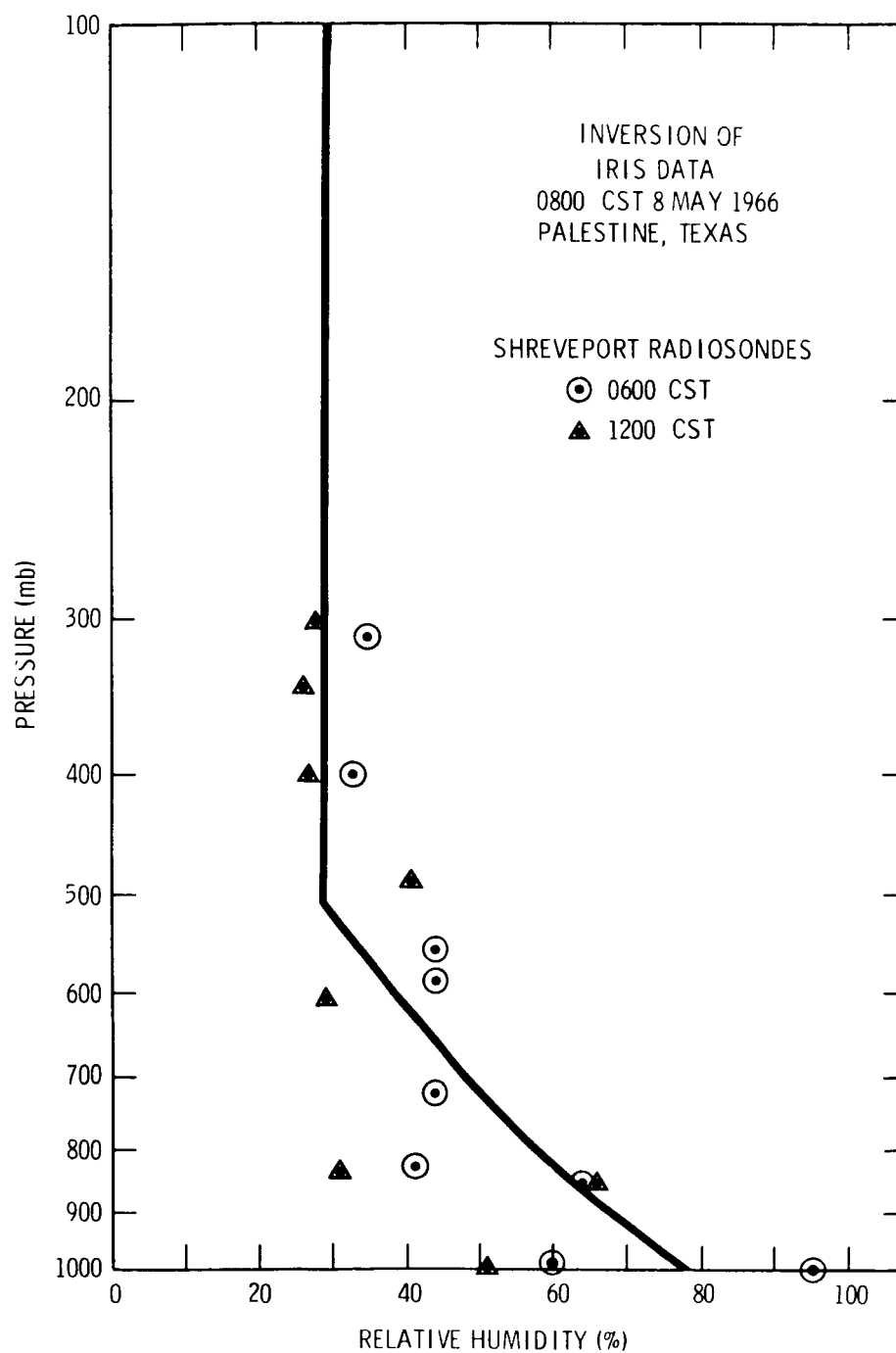


Figure 7—Inversion of data from the IRIS balloon flight shown in Fig. 1.
Data from a nearby radiosonde station are shown for comparison.

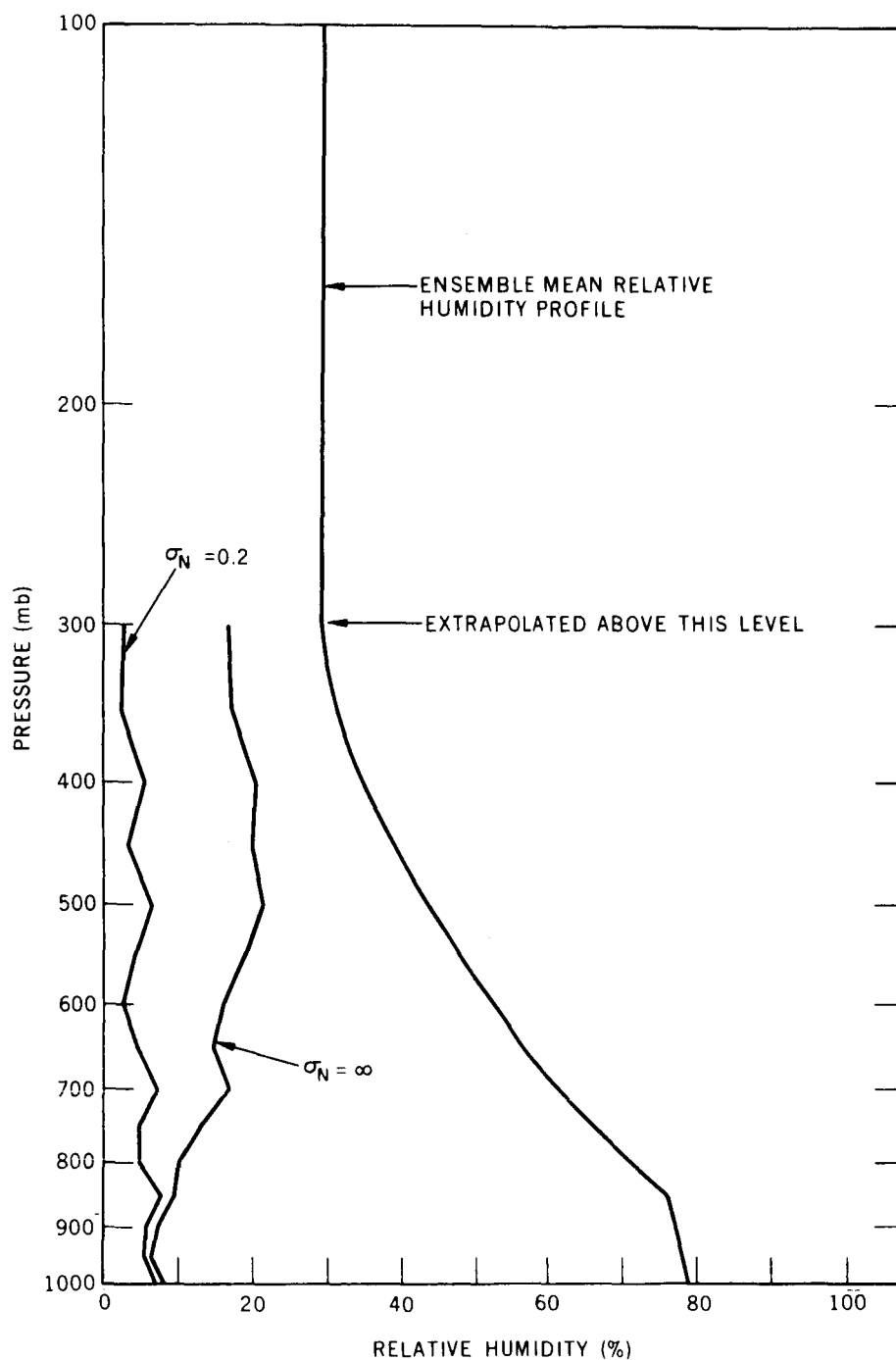


Figure 8—Mean relative humidity profile and standard deviations for a tropical ensemble. The curve marked $\sigma_N = \infty$ is the standard deviation for the ensemble and that marked $\sigma_N = 0.20$ is the standard deviation resulting when spectral intensity measurements with an rms error of $0.20 \text{ erg cm}^{-2} \text{ sec}^{-1} \text{ ster}^{-1} \text{ cm}$ are employed.

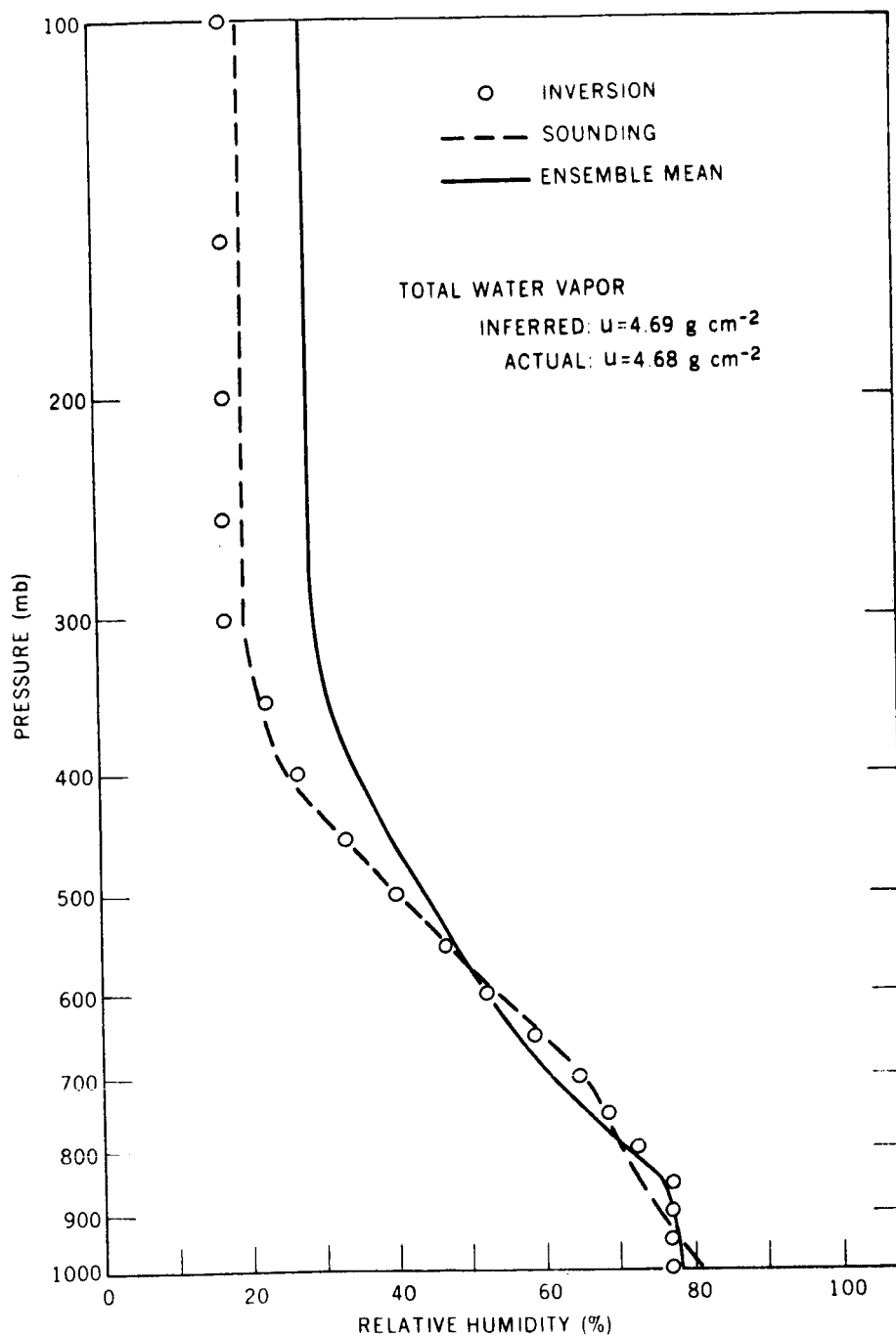


Figure 9—Statistical estimation of a relative humidity profile using synthetic data from a model atmosphere. A member of the ensemble which did not depart greatly from the ensemble mean was employed as the sounding.

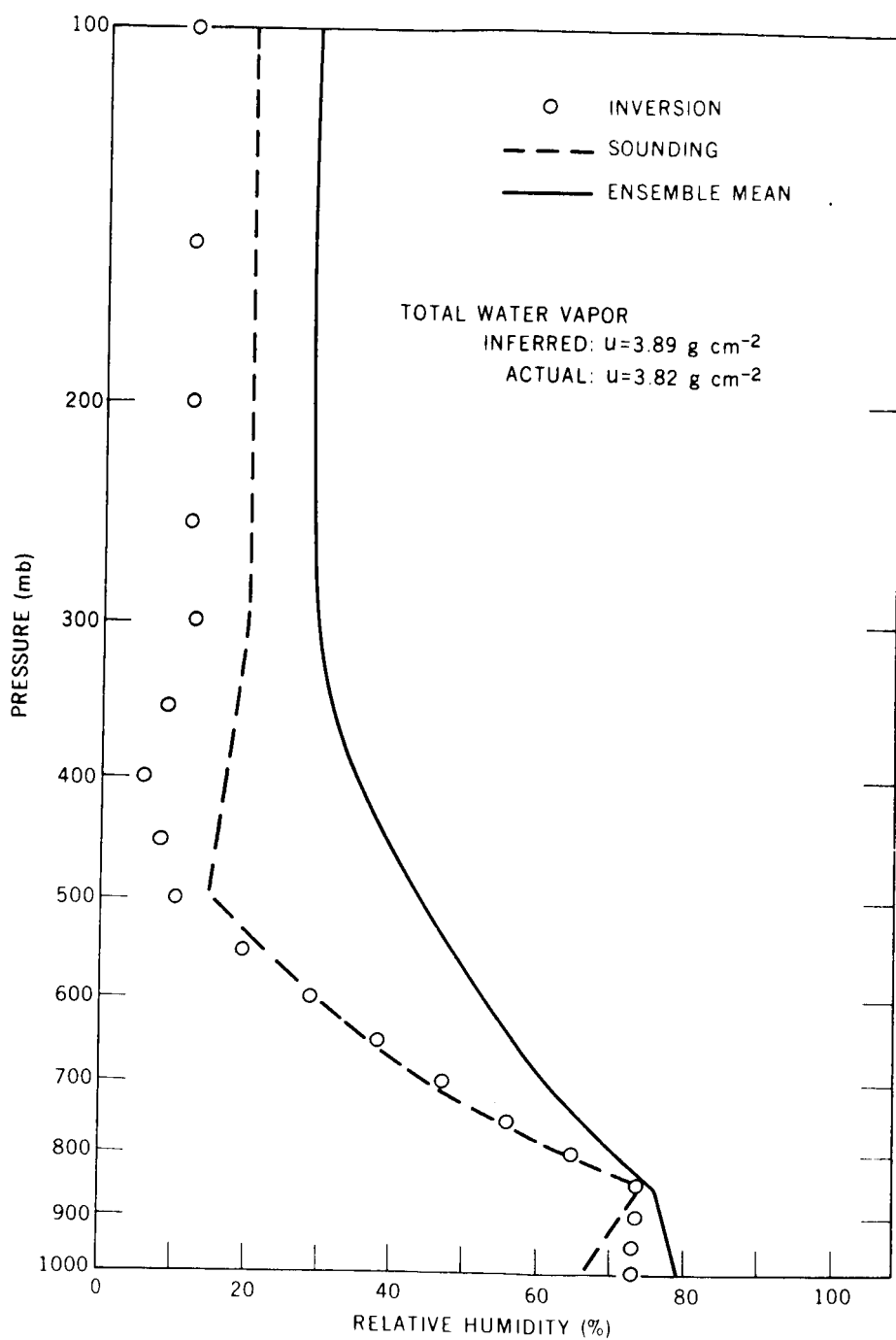


Figure 10—Statistical estimation of a relative humidity profile using synthetic data from a model atmosphere. A member of the ensemble showing considerable deviation from the ensemble mean was employed as the sounding.

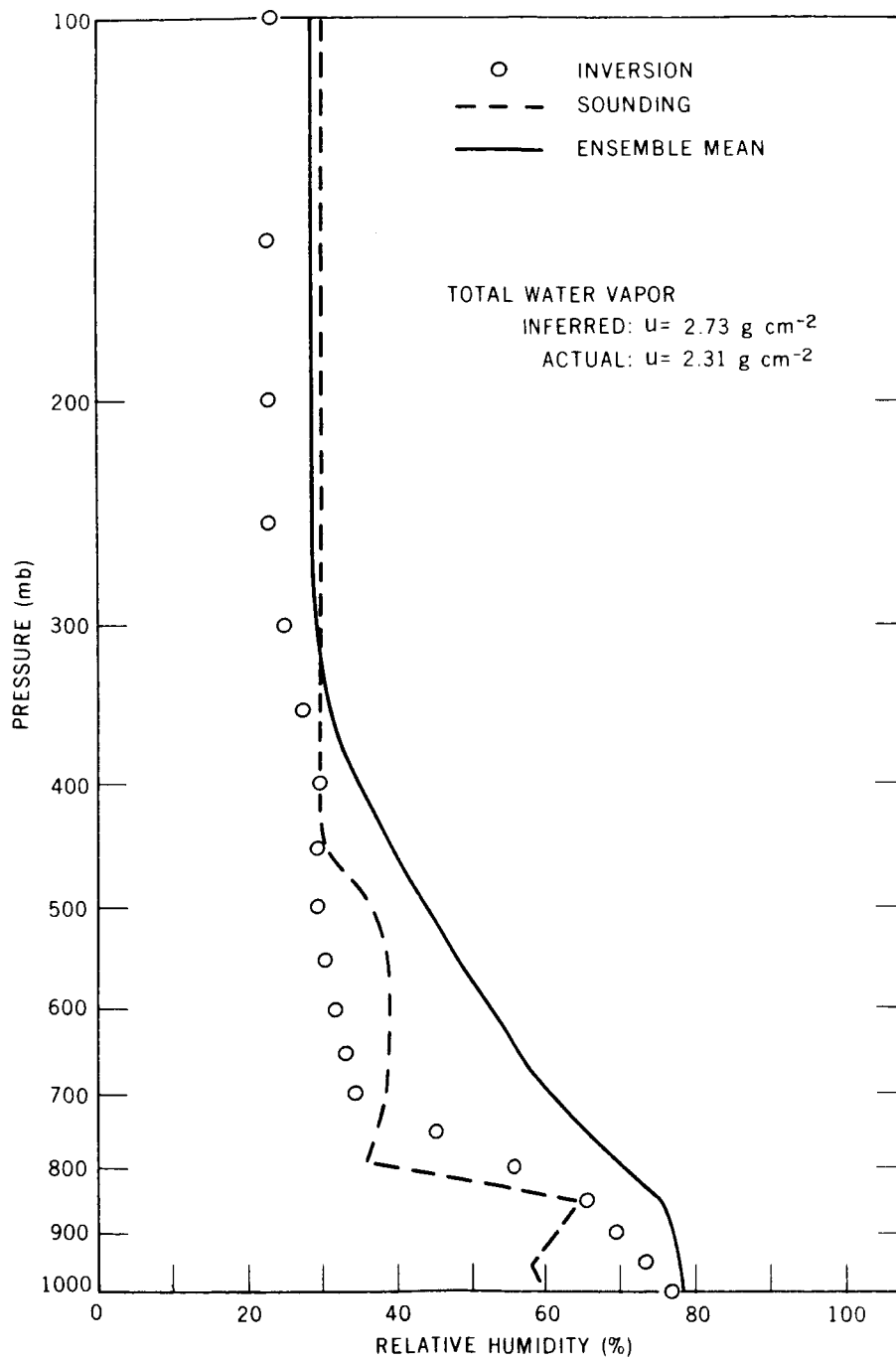


Figure 11—Statistical estimation of a relative humidity profile using synthetic data from a model atmosphere. The mid-latitude sounding employed was not a member of the ensemble on which the statistical parameters of the estimation were based.