A Technique for Estimating Atmospheric Moisture Profiles from Satellite Measurements

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ABSTRACT

In interpreting radiation data from the Vertical Temperature Profile Radiometers aboard the NOAA satellites, the following problem arose: given a satellite retrieval of the atmospheric temperature profile and a measurement of radiance from the earth's atmosphere in a single spectral interval (535 cm^{-1}) where water vapor is the principal optically active species, how can we estimate the atmospheric profile of water vapor mixing ratio? Our proposed solution has two steps. The first is to estimate the mixing-ratio profile by linear least-squares regression on the saturation mixing-ratio profile, the latter having been computed from the retrieved temperature profile. Associated with this estimate are residual errors. In the second step the measured radiance is used to reduce these errors, as follows: The covariance matrix of the errors is estimated and its principal eigenfunction is derived. The solution for the mixing-ratio profile is assumed to be a linear combination of this eigenfunction and the regression estimate of the mixing-ratio profile. The unknown coefficient in this solution is determined through a solution of the radiative transfer equation by Newton's method. In simulation, this method produced accurate solutions for mixing-ratio profiles and total precipitable water, the absolute error in the latter averaging 13% of the true value. This number increased to 26% when a uniform 2 K bias was introduced into the estimates of the temperature profiles.

1. Introduction

The Vertical Temperature Profile Radiometer (VTPR) (McMillin *et al.*, 1973) on each NOAA satellite sounds the atmosphere for temperature and water vapor profiles by measuring spectral radiance in eight intervals in the infrared. Measurements in one of the spectral intervals, near 12 μm in the atmospheric window, are used in a statistical procedure to eliminate the effects of clouds on the radiances measured in the other seven intervals. Profiles of atmospheric temperature are deduced from the "clear" radiances in the six intervals near 15 μm. There remain "clear" radiances in a single spectral interval near 18.7 μm in the rotational water vapor band, from which water vapor concentrations in the troposphere can be estimated.

The spectral response of the VTPR in the 18.7 μm interval, described fully by McMillin *et al.* (1973), approximates a Gaussian with center at 535 cm^{-1} and with a half-width of 20 cm^{-1}. In this interval the radiation R received at the satellite can be described by the following form of the equation of radiative transfer (Wark and Fleming, 1966):

$$R=B(T_s)\tau_s+\int_{x_s}^{x_0} B[T(x)][d\tau(x)/dx]dx. \quad (1)$$

In Eq. (1), x is a monotonic function of atmospheric pressure and is related to altitude, $T(x)$ is atmospheric temperature at the level x, B is the Planck radiance evaluated at the central wavenumber (535 cm^{-1}), $\tau(x)$ is the atmospheric transmittance in this spectral interval between the top of the atmosphere and the level x, and the subscripts s and 0 refer to the earth's surface and to the top of the atmosphere, respectively.

Water vapor enters Eq. (1) through $\tau(x)$, because $\tau(x)$ is a function, albeit complicated and nonlinear, of the water vapor mixing ratio profile. Clearly, from a single radiance measurement Eq. (1) cannot be solved for a unique water vapor profile. However, there is more information available to us. In particular, for each level x there is a relationship between mixing ratio W and temperature (and the latter is assumed to be known from the measurements in the first seven VTPR intervals). This relationship is expressed as

$$W(x)=V[T(x)]H(x), \quad (2)$$

where $V[T(x)]$, the mixing ratio at saturation, is a known function (Goff and Gratch, 1946) of the temperature and pressure at level x, and $H(x)$ is the relative humidity.[1] Unfortunately, Eq. (2) cannot be applied directly to produce $W(x)$, because $H(x)$ is unknown. How, then, can the information implicit in Eq. (2) be used to supplement the radiance measurement in solving Eq. (1)?

Our solution will be to apply the relationship expressed by Eq. (2) in a statistical manner. We proceed in two steps: First, we estimate $W(x)$ by linear least-squares regression on $V[T(x)]$. This produces a probable mixing ratio profile consistent with the temperature profile. Second, we apply the radiance measurement in an iterative solution of Eq. (1), using the estimated mixing-ratio profile as the initial estimate of the solution. In effect, we perturb the estimated profile until it satisfies the radiative transfer equation.

2. The initial estimate of mixing ratio

This section describes the procedure used to estimate the mixing ratio by regression on the saturation mixing ratio. The mixing ratio is specified at M levels in the atmosphere. The value of M should be large enough to permit accurate numerical quadrature of Eq. (1). For processing VTPR moisture data we use 40 levels ($M=40$) between 1000 and 190 mb. At each of those levels, the mixing ratio is estimated by the regression analysis as a linear combination of the saturation mixing ratios at L levels. In other words, we expect the mixing ratio at any level to be correlated not only with the saturation mixing ratio at the same level, but also with the saturation mixing ratios at other levels. By trial and error, the predictors were chosen to be the values of saturation mixing ratio at eleven levels between 1000 and 210 mb, i.e., $L=11$. With fewer levels the results were poorer; yet with more levels there was little improvement.

Mathematically the regression is done as follows: Let the saturation mixing ratio profile be represented by the vector $\mathbf{V}$ whose L elements are $V(x)$ specified at L levels, and let the mixing ratio profile be represented by the vector $\mathbf{W}$ whose M elements are $W(x)$ specified at M levels. The vector $\mathbf{V}$ is assumed to be random, with mean $\boldsymbol{\mu}_V$ and covariance matrix $\mathbf{S}_V$. Similarly, the vector $\mathbf{W}$ is assumed to be random with mean $\boldsymbol{\mu}_W$ and covariance matrix $\mathbf{S}_W$. If $\mathbf{S}_{WV}$ is the cross-covariance matrix of $\mathbf{W}$ and $\mathbf{V}$, the standard linear regression equation for the unbiased estimate $\hat{\mathbf{W}}$ is (Deutsch, 1965)

$$\hat{\mathbf{W}}=\mathbf{S}_{WV}\mathbf{S}_V^{-1}(\mathbf{V}-\boldsymbol{\mu}_V)+\boldsymbol{\mu}_W. \qquad (3)$$

The matrices $\mathbf{S}_{WV}$ and $\mathbf{S}_V$ and the vectors $\boldsymbol{\mu}_V$ and $\boldsymbol{\mu}_W$ are defined with ensemble averages performed over infinite populations. In this application they should be estimated from a large sample that is representative of sounding situations. The VTPR data have been utilized only over the oceans, so the matrices and vectors were constructed from a set of 1100 maritime radiosonde soundings of water vapor and temperature. The soundings in this dependent set are distributed nearly evenly in latitude and time of year. A similarly chosen group of 119 soundings was also accumulated for testing the retrieval procedure.

TABLE 1. Fractional reductions in mean-square error at eight atmospheric levels.

Pressure level (mb)	$r(x)$ [Eq. (3)]	$r(x)$ [Eq. (2)]
1000	0.93	0.91
900	0.85	0.83
800	0.73	0.53
700	0.52	0.19
600	0.47	0.22
500	0.52	0.32
400	0.44	0.38
300	0.53	0.42

In the test of the procedure, we applied the regression equation (3) to each of the 119 test soundings to produce profiles of $\hat{W}(x)$. From this we computed the mean-square error σ^2 of the solutions, defined at each level x by

$$\sigma^2(x)=(1/119)\sum_{i=1}^{119}[W_i(x)-\hat{W}_i(x)]^2,$$

where i is the index that enumerates the soundings and $W_i(x)$ is the true value of the mixing ratio.

If we had done no regression at all, we would still have an estimate of $W_i(x)$. This estimate is $\bar{W}_i(x)$, the mean mixing ratio for the dependent sample of 1100 soundings. Associated with this mean is the mean-square error σ_0^2 given by

$$\sigma_0^2(x)=(1/119)\sum_{i=1}^{119}[W_i(x)-\bar{W}(x)]^2.$$

The fractional reduction $r(x)$ in the mean-square error achieved when one estimates mixing ratio by Eq. (3) is defined as

$$r(x)=1-\sigma^2(x)/\sigma_0^2(x).$$

This quantity is listed in the second column of Table 1, which shows that the application of Eq. (3) reduces the mean-square error considerably.

An alternative approach to estimating the mixing ratio is to apply Eq. (2), where $H(x)$ is taken to be the mean profile of humidity for the dependent sample of 1100 soundings. This approach would be equivalent to Eq. (3) if the relative humidity were not correlated with the saturation mixing ratio. The reductions in mean-square error achieved by this approach are listed

[1] Strictly speaking, Eq. (2) holds for vapor pressures, not mixing ratios. However, as long as atmospheric pressure far exceeds the effective vapor pressure of water (and this is the usual atmospheric situation), Eq. (2) is a very good approximation.

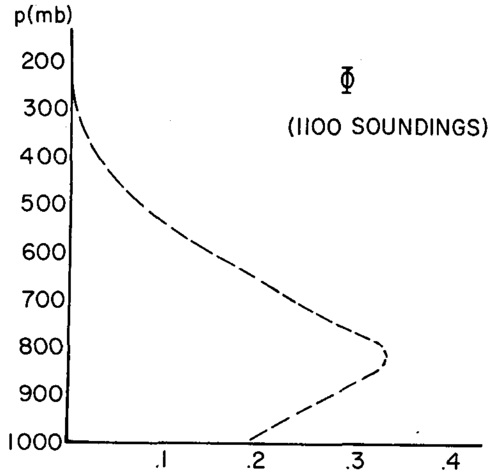

FIG. 1. The principal eigenvector of $\mathbf{S}_{\text{res}}$, the covariance matrix of the errors of $\hat{\mathbf{W}}$.

in the third column of Table 1. The table shows that Eq. (3) gives better estimates than Eq. (2), especially at the levels between 800 and 500 mb.

3. A one-parameter representation for mixing ratio

Now that the temperature-mixing ratio correlation has yielded the estimate $\hat{\mathbf{W}}$, it remains for us to utilize the radiance measurement. We seek a representation for the mixing ratio profile that depends on a single parameter, because that is all a single radiance measurement can determine uniquely.

Associated with the estimate $\hat{\mathbf{W}}$ is $\mathbf{S}_{\text{res}}$, the covariance matrix of the residual differences between $\hat{\mathbf{W}}$ and the true profile. In terms of the covariance matrices constructed earlier (Deutsch, 1965), $\mathbf{S}_{\text{res}}$ is given by

$$\mathbf{S}_{\text{res}} = \mathbf{S}_W - \mathbf{S}_{WV}\mathbf{S}_V^{-1}\mathbf{S}_{WV}^T.$$

Given $\hat{\mathbf{W}}$ and $\mathbf{S}_{\text{res}}$, it can be shown (e.g., Rodgers, 1972) that the most accurate one-parameter representation for the mixing ratio is

$$\mathbf{W} = \hat{\mathbf{W}} + c\boldsymbol{\phi}, \qquad (4)$$

where $\boldsymbol{\phi}$ is the eigenvector for the largest eigenvalue of $\mathbf{S}_{\text{res}}$. Like $\mathbf{W}$, the vector $\boldsymbol{\phi}$ is specified at M levels of the atmosphere. In applying Eq. (4), we note that c is the only parameter that has not yet been determined. The vector $\hat{\mathbf{W}}$ was determined by regression from the saturation mixing ratio, as described above. The vector $\boldsymbol{\phi}$ is known in advance, having been derived from the dependent sample of 1100 soundings, and it is displayed in Fig. 1. Consequently, we are now in a position to solve the radiative transfer equation for the parameter c.

It is worth noting that Eq. (4) expresses the profile of mixing ratio as the sum of two terms. The first is the estimated profile, which is consistent with the saturation mixing ratio (or temperature) profile. The second may be regarded as an adjustment, whose shape is shown in Fig. 1 and whose magnitude will be fixed by the measured radiance through a solution of the radiative transfer equation. Clearly, a solution based on a single measured radiance cannot recover the detailed structure of the mixing ratio profile. But because it incorporates atmospheric correlations as well as the measured radiance, the solution should reproduce the broad features of the profile.

Before proceeding with the solution of the radiative transfer equation, we briefly mention a related method of solution. It is possible to apply a one-step solution which is formally the same as Eq. (4), $\mathbf{W} = \overline{\mathbf{W}} + c\boldsymbol{\theta}$. However, now $\overline{\mathbf{W}}$ is the mean profile for the 1100 soundings, and $\boldsymbol{\theta}$ is the principal eigenvector of $\mathbf{S}_W$, not $\mathbf{S}_{\text{res}}$. Such a solution was used by Prabhakara *et al.* (1970) for the remote sensing of atmospheric ozone. This solution differs from ours in that it lacks the first step—the regression—which utilizes correlations between mixing ratio and temperature to produce the estimate $\hat{\mathbf{W}}$ and the vector $\boldsymbol{\phi}$. In other words, the advantage of our Eq. (4) is that it is based on $\hat{\mathbf{W}}$, and $\hat{\mathbf{W}}$ is a better estimate of the solution than $\overline{\mathbf{W}}$, as a glance at Table 1 will show.

4. Solution of the radiative transfer equation

The integrand of Eq. (1), $Bd\tau/dx$ (where x is proportional to $p^{2/7}$), is plotted in Fig. 2 as a function of atmospheric pressure for two atmospheres, one moist, one dry. This function, which measures the contribution

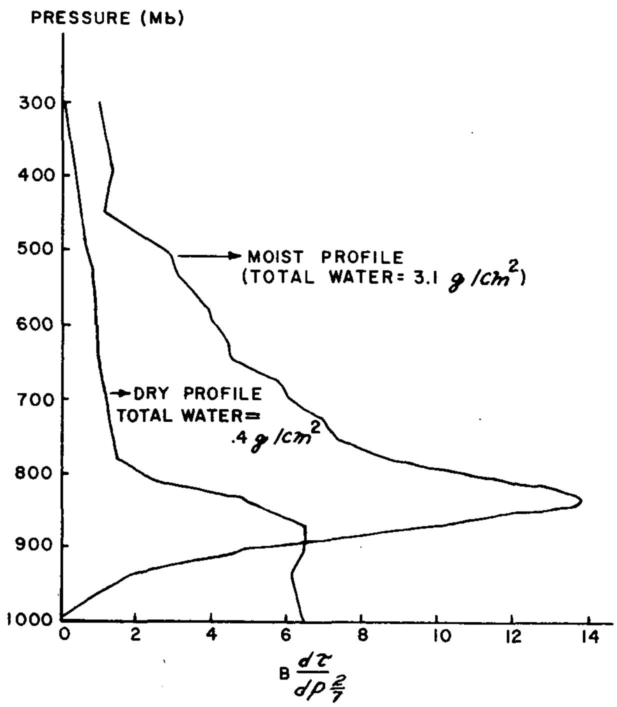

FIG. 2. Relative contributions of atmospheric levels to radiance.

of each level in the atmosphere to the radiance received in the 535 cm^{-1} spectral interval, is highly responsive to changes in atmospheric moisture content. For a moist atmosphere, the radiance originates from higher levels than for a dry atmosphere. Thus, barring large temperature inversions, moist profiles produce lower values of radiance.

Integrating Eq. (1) by parts, and assuming that the temperature of the surface equals the atmospheric temperature at level x_s, one gets

$$R=B[T(x_0)]+\int_{x_0}^{x_s}\tau(x)\{dB[T(x)]/dx\}dx. \quad (5)$$

As mentioned earlier, $\tau(x)$ is a nonlinear function of water vapor mixing ratio. Moreover, τ at level x not only depends on the mixing ratio at x, but also depends strongly on the mixing ratios at levels above x (see, e.g., Goody, 1964). Therefore, it is inaccurate to approximate $\tau(x)$ with the first term in a Taylor series in the single variable $W(x)$. Instead, either Eq. (1) or Eq. (5) can be solved for the constant c as follows: We let the right-hand side of Eq. (1) or Eq. (5) be designated $I(c)$ so that

$$R-I(c)=0.$$

The function $I(c)$ can be calculated from c (and the temperature profile), because τ can be calculated from $W(x)$, and $W(x)$ is a known function of c [Eq. (4)]. Because I is a complicated function of c, the simplest solution of such an equation is by Newton's method, i.e.,

$$c^{j+1}=c^j+[R-I(c^j)]/I'(c^j), \quad (6)$$

where c^j is the solution for c in the jth iteration, R is the measured radiance, and $I'(c^j)$ is dI/dc evaluated for $c=c^j$. In the application of Eq. (6), the iterations begin with $c^0=0$ and stop when the residual $|R-I(c^j)|$ is less than ϵ, the expected uncertainty in the measurement of R. Given c^j, the next iteration proceeds as follows:

1) Calculate the mixing ratio profile $\mathbf{W}^j$ by Eq. (4).
2) At each level of the atmosphere, restrict the mixing ratio to values greater than zero and less than saturation. (In actual practice these constraints were seldom used, being invoked only in extremely moist atmospheres.)
3) From $\mathbf{W}^j$ and the temperature profile, calculate the transmittances. In the examples described below, τ was calculated by methods described in Wark *et al.* (1974) and in Weinreb and Neuendorffer (1973).
4) Apply Eq. (1) to produce $I(c^j)$, and take the derivative I' by finite differences.
5) If $|R-I(c^j)|\leqslant\epsilon$, we are done, and $\mathbf{W}^j$ is the solution. If not, continue.
6) Apply Eq. (6) to produce c^{j+1}.

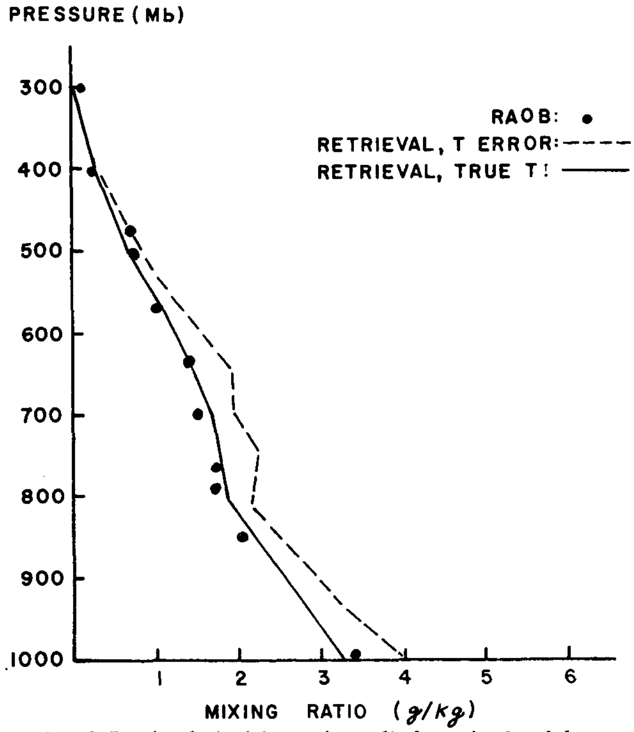

FIG. 3. Retrieval of mixing-ratio profile from simulated data for the dry case. Precipitable water = 1.0 cm.

We emphasize that the single measured radiance alone cannot determine unique values of the total precipitable water or the mixing ratio profile. Many reasonable mixing ratio profiles, each with a different total precipitable water, can produce the same value of radiance. The technique of this paper first restricts the range of possible mixing ratio profiles to a set of probable profiles, consistent with the temperature, whereupon the radiance measurement fixes the profile and the total precipitable water.

5. Results, assuming the temperature is known

Retrievals were performed on the 119 test profiles, for which simulated radiances were computed in advance from the true temperature and mixing ratio profiles by Eq. (1). The retrieval procedure was an application of Eq. (3), followed by the iterative solution described in the preceding section. In these retrievals it was assumed that the true temperature profile was known. Results for two of the profiles (solid curves) along with the true mixing ratio profiles (dots) are displayed in Figs. 3 and 4. For both solutions three iterations of Eq. (6) were required. The values of total precipitable water calculated from the retrieved profiles in Figs. 3 and 4 were 1.0 and 1.8 cm, respectively. These were in agreement with the values calculated from the true profiles. Over the test sample of 119 profiles, the average absolute error in total precipitable water was 13%, indicating that this quantity was accurately retrieved.

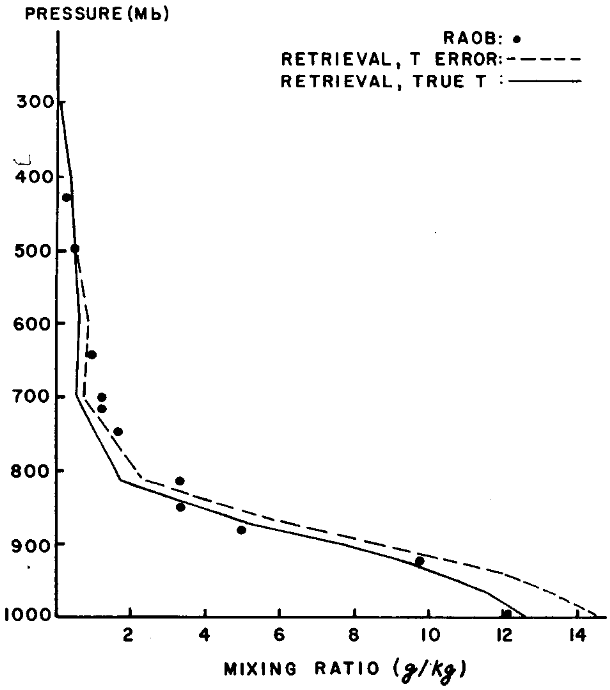

FIG. 4. As in Fig. 3 except for the moist case. Precipitable water = 1.8 cm.

6. Effect of temperature errors

In the actual sounding situation the moisture retrieval is based on the results of the temperature retrieval; yet temperature retrievals usually are accurate only to within several degrees. The effect of errors in the temperature profile used in the moisture retrieval is twofold. First, inserting an incorrect temperature profile in the regression [Eq. (3)] yields a less-than-optimal estimate $\hat{\mathbf{W}}$. Ideally, one could minimize this error by replacing $\mathbf{S}_V$ and $\mathbf{S}_{WV}$ in Eq. (3) with covariance matrices involving the statistics of the saturation mixing ratios derived from VTPR temperature retrievals. However, no such statistics have been accumulated for VTPR retrievals. Second, the calculation of $I(c)$ in Eq. (6) involves temperature and consequently will be incorrect. A temperature profile that is too hot usually produces a retrieved moisture profile that is too wet. In Figs. 3 and 4 the dashed curves show what happens when the moisture retrieval uses a temperature profile too warm at all levels by 2 K, a value that produces an error in $I(c)$ perhaps typical of errors encountered in actual sounding situations. As before, simulated radiances were computed in advance from the true temperature and mixing ratio profiles. In solving for the mixing ratio profiles the number of iterations of Eq. (6) was 4 and 2 for the profiles of Figs. 3 and 4, respectively. On the average, the required number of iterations in the 119 retrievals did not increase over the number required with no temperature error. However, the retrieved profile of Fig. 3 is definitely degraded at all levels below 450 mb. For Fig. 4 the retrieval was worse below 850 mb, but actually was improved between 850 and 500 mb. Generally, as expected, the 2 K temperature error introduced an overly moist tendency in the solutions. For the total precipitable water, values of 1.2 and 2.1 cm were obtained for Figs. 3 and 4, respectively. These values are 0.2 and 0.3 cm too high, although they would probably be satisfactory in an actual sounding. Over the test sample of 119 soundings the average absolute error in the total precipitable water increased to 26%, with a strong tendency toward too much moisture. Retrieving with a temperature profile that fluctuates about the true profile, which is more typical of the VTPR soundings, will be less likely to induce a moist or dry tendency in the retrieval, because such a temperature profile is likely to produce a smaller error in $I(c)$; however, problems may arise with the shape of the retrieved profiles through the regression equation (3).

7. Conclusion

The procedure to deduce the atmospheric moisture profile from a single measured radiance in the H_2O rotational bands has been described. First, an estimate of the mixing ratio is obtained by linear regression on the saturation mixing ratio. Then the solution, which was expressed as a linear combination of this estimate and an empirical orthogonal function, is specified by the requirement that the radiance calculated from the radiative transfer equation agree with the satellite measurement. Because much information on the moisture profile can be derived from the temperature profile, the method in simulation provides accurate retrievals of the mixing ratio profile and total precipitable water. Success of this retrieval technique will depend to a large extent on the accuracy of the temperature profile retrieved from the measurements in the other VTPR spectral intervals.

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