Equivalence Method for Retrieving Stratospheric Constituent Profiles from Infrared Solar Occultation Data

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(Manuscript received 15 April 1985, in final form 28 September 1985)

ABSTRACT

Mixing ratios of stratospheric constituents can be inferred from satellite- or balloon-based infrared solar occultation measurements. The nonlinear system of equations that relates the measurements to the mixing ratios is often solved by the "onion-peeling" technique. We show how to implement onion-peeling with an algorithm in which limb paths are represented by equivalent homogeneous paths. The essential computations are confined to the tangent layers instead of the full multilayer limb paths. The algorithm yields the same solutions as conventional onion-peeling but requires significantly less computation time.

1. Introduction

In infrared solar occultation experiments, which are carried out from satellite or high altitude balloon platforms, the essential measurements are the transmittances of the atmosphere through limb paths. A cascading system of equations relates the measurements to the mixing ratios of the constituent being sounded. Such a system can be inverted by "onion-peeling" (Russell and Drayson, 1972), which is analogous to the well-known mathematical procedure of back-substitution (e.g., see Twomey, 1977, pp. 42–46). In this approach, the equations are solved one at a time, beginning with the equation corresponding to the measurement at the highest tangent point, and proceeding downwards. The *n*th equation relates the measured transmittance for the *n*th viewing angle to an expression for transmittance in which there is only one unknown, i.e., the mixing ratio in the *n*th layer of the atmosphere. Because they are nonlinear, the equations are usually solved iteratively, meaning that the mixing ratio is updated and the "forward" calculation of transmittance performed repetitively until agreement is reached between the measured transmittance and the calculated one.

This paper presents a more efficient method for implementing onion-peeling. The system of equations is solved by an algorithm originally devised for computing transmittances rapidly in slant paths (Weinreb and Neuendorffer, 1973). The algorithm is based on an equivalence established between the atmospheric path and a homogeneous path. This algorithm and its analog for limb radiance computations (Gordley and Russell, 1981) have already been used in retrievals of limb absorption data, but only for the "forward" transmittance or radiance calculations that are part of the usual iterative solution of each equation (Gordley and Russell, 1981; Weinreb et al., 1984). This paper demonstrates the utility of the equivalence method as a complete solution by itself. The equivalence method is well-suited to onion-peeling and is roughly an order of magnitude more efficient than the usual solution.

2. Limb absorption geometry

Observations can be made from a satellite or a balloon. Figure 1 illustrates an observing instrument, supported by a high-altitude balloon, viewing the sun through the limb of the atmosphere at sunrise or sunset. The data are expressed as atmospheric transmittances, in the absorption bands of the constituents being sounded, versus zenith angle or, equivalently, tangent height. In the data reduction, the atmosphere is treated as an onionlike composite of spherical shells, which in this work are taken to be 1 km thick. The pressure, temperature, and mixing ratio are constant in each layer. The boundaries of the layers are called levels, which are enumerated from zero to N, with zero at the top of the atmosphere and N at the bottom. The *n*th layer is bounded below by the *n*th level. The quantities τ_n and t_n are defined to be the modeled transmittances and the measured ones, respectively, for the line-of-sight tangent to the *n*th level. The variable that measures the quantity of the gas being sounded is q_n. This can be, e.g., the integrated absorber amount or the mean mixing ratio in layer n.

For simplicity we assume that the observer is high enough that absorption taking place in the layers above the balloon is negligible. The measurements are then described by the following system of equations:

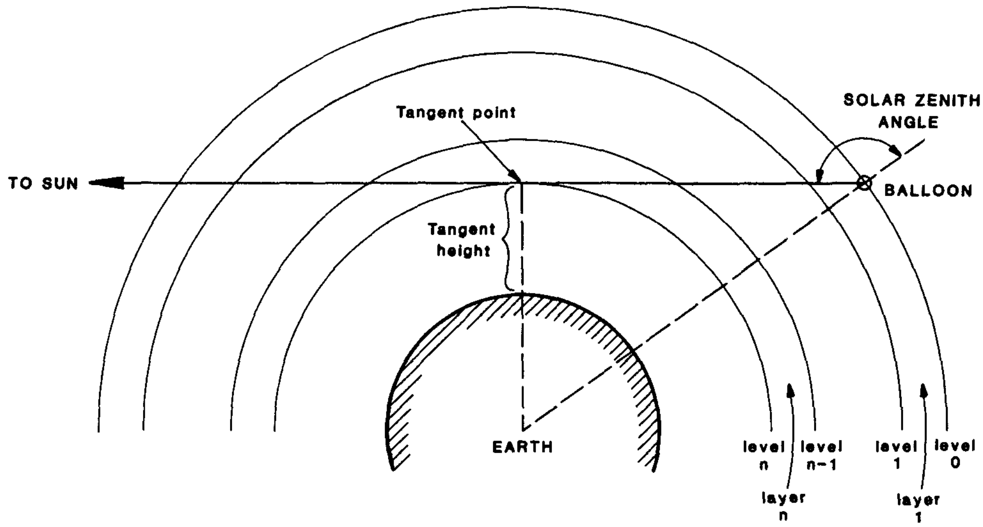

FIG. 1. Geometry of balloon-based solar occultation experiment.

$$\begin{aligned} \tau_1(q_1) &= t_1, \\ \tau_2(q_1, q_2) &= t_2, \\ &\vdots \\ \tau_N(q_1, q_2, \ldots q_N) &= t_N. \end{aligned} \tag{1}$$

As indicated in the left-hand sides of the equations, the transmittances are functions of the variable q in all the layers penetrated by the line of sight. They also depend on the pressure and temperature in these layers. In an occultation experiment, the pressure and temperature are assumed to be known a priori.

3. Onion-peeling approach

Equation (1) constitutes a system of N equations in N unknowns. In onion-peeling, the first equation is solved explicitly for q_1. The value of q_1 is then inserted into the second equation, leaving q_2 as the only unknown. The second equation can then be solved for q_2. This procedure continues until the Nth equation is solved for q_N.

The solution of each equation is usually obtained iteratively, because τ_n is generally a complicated and nonlinear function of q_n. For example, by Newton's method, the iterative equation is

$$q_n^{(k+1)} = q_n^{(k)} - (\tau_n^{(k)} - t_n)/(d\tau_n^{(k)}/dq_n^{(k)}) \qquad k = 1, 2, \cdots, \tag{2}$$

where the superscripts in parentheses refer to iteration number. The derivative is estimated from numerical differences. Therefore, in each iteration at least two, and probably three, forward calculations of transmittance over a multilayer limb path must be carried out.

4. Equivalence algorithm for transmittance calculations

The equivalence algorithm (Weinreb and Neuendorffer, 1973) was formulated for computing transmittances vertically through inhomogeneous atmospheres, given a homogeneous-path transmittance model. (A homogeneous path is one in which the pressure, temperature, and mixing ratio are constant.) We begin this section by describing that algorithm. Then we show how the method is applied for calculating transmittances with the more complicated geometry in limb paths. In the following section we will apply the method to retrieve absorber amounts by onion-peeling.

It is assumed that the mean pressure P, mean temperature T, and absorber amount ΔU are known in each layer. (ΔU is in such units as atm-cm or g cm^{-2}). One also has available a homogeneous-path transmittance model, represented by

$$\tau = f(P, T, U).$$

To calculate transmittances in inhomogeneous atmospheres, one works downward through the atmosphere, beginning at layer 1 (see Fig. 2). The transmittance through layer 1 is obtained directly from the homogeneous-path model, i.e.,

$$\tau_1 = f(P_1, T_1, \Delta U_1), \tag{3}$$

where ΔU_1 is the absorber amount in the layer. The algorithm continues downward, as follows: Assume that τ_{n-1}, the transmittance through layers $1, 2, \ldots, n-1$, has already been computed. To find τ_n, one proceeds in two steps, as illustrated by the arrows in Fig. 3. The first is to find the equivalent absorber amount U_{n-1} that will produce the transmittance τ_{n-1}

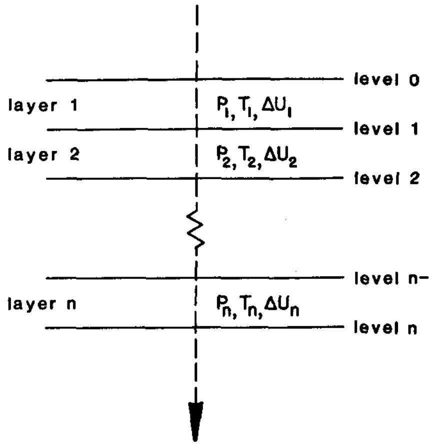

FIG. 2. Stratified atmosphere for transmittance calculations in the vertical direction.

in layer n, i.e., with pressure and temperature P_n and T_n, respectively. This choice of U_{n-1} will make the homogeneous path n equivalent to the inhomogeneous atmospheric path from layer 1 through $n-1$; i.e., both will have the same transmittance. The quantity U_{n-1} satisfies

$$\tau_{n-1} = f(P_n, T_n, U_{n-1}). \qquad (4)$$

Since τ_{n-1}, P_n and T_n are known, the only unknown in this equation is U_{n-1}. This allows one to solve for U_{n-1} by inverting (4). If the transmittance model allows, (4) can be inverted algebraically. If not, it can be inverted by, e.g., Newton's method.

Once U_{n-1} is evaluated, one proceeds to the second step, namely to evaluate τ_n from

$$\tau_n = f(P_n, T_n, U_n), \qquad (5)$$

where $U_n = U_{n-1} + \Delta U_n$, and ΔU_n is the known absorber amount in layer n.

The same algorithm can be used to calculate transmittances for limb paths. Now, however, the geometry is more complicated. The absorber amount in any layer depends on both mean mixing ratio and path length in the layer, and the latter depends on the choice of ray. Therefore, the absorber amounts and transmittances must be computed separately for each ray. Figure 4 illustrates the situation. Note that for the mth ray (i.e., the ray tangent to level m) there are two segments in each layer. One is in the anterior portion of the ray (between observer and tangent point), and the other is in the posterior portion (between the tangent point and the sun). For example, in layer n each segment is $\frac{1}{2}\Delta s(n, m)$ in length, so that the mth ray travels a total distance of $\Delta s(n, m)$ in layer n.

We define $\Delta U(n, m)$ to be the absorber amount along ray m in layer n. It includes equal contributions from posterior and anterior segments. It is computed from

$$\Delta U(n, m) = \rho(n)\Delta s(n, m), \qquad (6)$$

where $\rho(n)$ is the mean mass density in layer n. Because of the spherical symmetry assumed in the problem, $\rho(n)$ is the same in both anterior and posterior segments.

The lengths Δs can be computed directly from geometry if refraction is ignored. Since we do include refraction, however, the computation has to be done in an atmospheric ray trace, and knowledge of atmospheric pressures and temperatures is required.

The equivalence algorithm is applied separately for each ray. We define $\tau(n, m)$ to be the transmittance computed between the sun and level n along ray m. The calculation begins with layer 1, for which $\tau(1, m)$ is computed, and proceeds downward, until the tangent point is reached, the last computed transmittance being $\tau(m, m)$. Because the posterior and anterior segments are included in the absorber amount for each segment, $\tau(m, m)$ is the transmittance of the entire path between the sun and the observer along ray m.

By choosing to combine anterior and posterior segments, rather than treating them separately, we halve the number of computations. In addition, this approach allows the equivalence algorithm to be applied only in the direction of increasing rate of absorption, i.e., starting at layers with low density of absorbing gas and working towards layers with higher density. As the paper by Weinreb and Neuendorffer (1973) explains, the algorithm is generally most accurate when it is applied in that direction.

5. Equivalence algorithm for retrieving absorber amounts

A virtue of the equivalence algorithm, which contributes to its efficiency, is that once the transmittance has been computed for the path from the observer down to level m, the computation of transmittance to level $m+1$ involves only the single layer bounded by levels

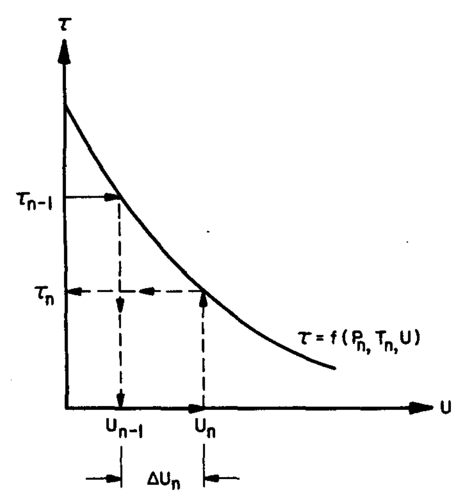

FIG. 3. Graphical representation of method for computing U_{n-1} from τ_{n-1}, then τ_n from U_n (after Weinreb and Neuendorffer, 1973).

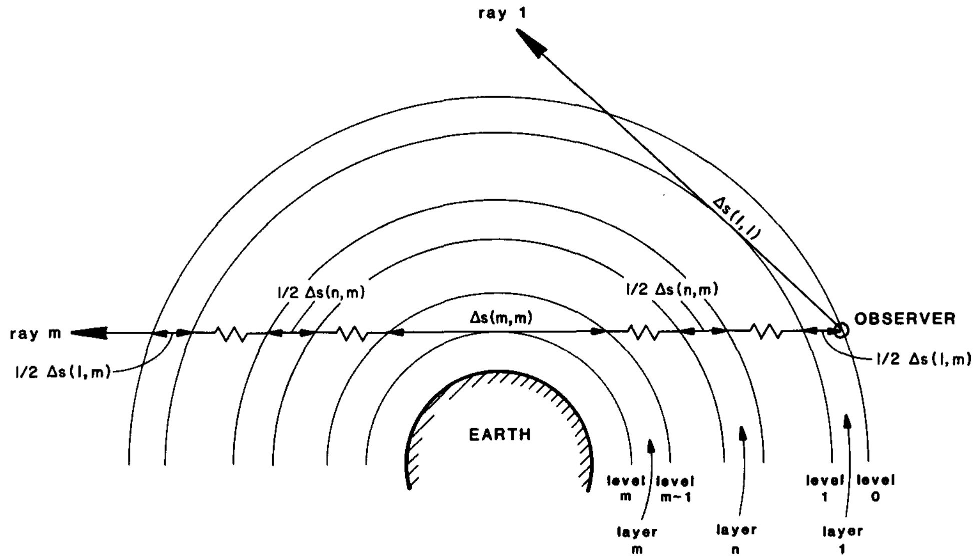

FIG. 4. Geometry of limb path, illustrating anterior and posterior segments in each layer.

m and $m + 1$. In this way, repeated multilayer integrations are avoided. In this and the following sections we show that the equivalence algorithm can also be applied to the retrieval of absorber amounts, and that it brings a similar efficiency to those retrievals.

To apply the equivalence algorithm to retrieving absorber amounts, we begin by following the ordinary onion-peeling approach. In layer 1 the analog of (3) for limb geometry applies, i.e.,

$$\tau(1, 1) = f[P_1, T_1, \Delta U(1, 1)], \qquad (7)$$

but now $\tau(1, 1)$ is known, because it equals t_1, the measured transmittance. On the other hand, $\Delta U(1, 1)$ is now the unknown. To solve for $\Delta U(1, 1)$, one inverts (7). The method then continues down through the atmosphere. Suppose that after the $(m - 1)\Delta t$ step we have solved for $\Delta U(1, \mathrm{m} - 1)$, $\Delta U(2, m - 1)$, . . . $\Delta U(m - 1, m - 1)$. In the mth step our aim is to invert the mth equation of (1) to infer $\Delta U(m, m)$, the absorber amount along ray m in the mth layer. However, to carry out computations along ray m, one must first modify the ΔU just derived for ray $m - 1$ so that they apply to ray m; i.e., one needs to compute $\Delta U(1, m)$, . . . $\Delta U(m - 1, m)$ from $\Delta U(1, m - 1)$, . . . $\Delta U(m - 1, m - 1)$. (This must be done with ordinary onion peeling as well as the equivalence method.) An efficient way to do this is to apply the "reslanting" relationships (Goldman and Saunders, 1979),

$$\Delta U(1, m) = \Delta U(1, m - 1)\Delta s(1, m)/\Delta s(1, m - 1)$$

$$\Delta U(2, m) = \Delta U(2, m - 1)\Delta s(2, m)/\Delta s(2, m - 1)$$

$$\vdots$$

$$\Delta U(m - 1, m) = \Delta U(m - 1, m - 1)\Delta s(m - 1, m)/\Delta s(m - 1, m - 1), \qquad (8)$$

which follow from (6).

At this point the equivalence method departs from ordinary onion-peeling. In ordinary onion-peeling, the mth equation of (1) is now solved for $\Delta U(m, m)$ by an iterative numerical algorithm such as (2). On the other hand, the equivalence method proceeds as follows: The transmittance $\tau(m - 1, m)$ along ray m from the top of the atmosphere down to level $m - 1$ is computed from $\Delta U(1, m)$, . . . , $\Delta U(m - 1, m)$ by the forward equivalence algorithm, as described in the previous section. Now we know both $\tau(m - 1, m)$ and $\tau(m, m)$, the latter being equal to t_m. To find $\Delta U(m, m)$, one proceeds in two steps, as illustrated by the arrows in Fig. 5. The first is to find the equivalent absorber amount $U(m - 1, m)$ that will produce the transmittance $\tau(m - 1, m)$ in layer m. With this choice of $U(m - 1, \mathrm{m})$, the homogeneous path with the pressure and temperature of layer m will become equivalent to the limb path from the top of the atmosphere through layer $m - 1$. The quantity $U(m - 1, m)$ satisfies the limb analog of (4), i.e.,

$$\tau(m - 1, m) = f[P_m, T_m, U(m - 1, m)]. \qquad (9)$$

We invert (9) to solve for $U(m - 1, m)$. This can be done by Newton's method, usually in a single iteration. The measured transmittance t_m now satisfies the limb analog of (5), i.e.,

$$t_m = f[P_m, T_m, U(m, m)], \qquad (10)$$

where $U(m, m) = U(m - 1, m) + \Delta U(m, m)$. In the second step one inverts (10) to obtain $U(m, m)$ and hence $\Delta U(m, m)$ itself.

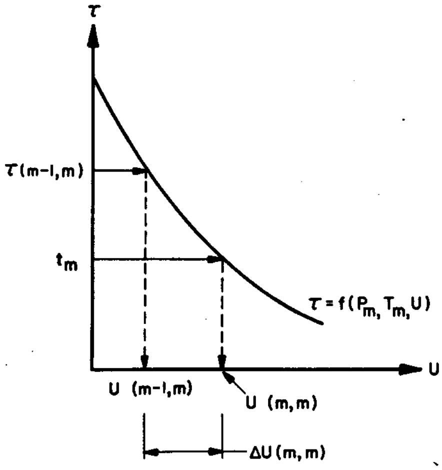

FIG. 5. Graphical representation of the method to compute $\Delta U(m, m)$ from $\tau(m-1, m)$ and t_m.

Note that in inverting (9) and (10), which are the key steps in the algorithm, we operate only on the transmittance function for a homogeneous path, the tangent layer. None of the other layers in the limb path are involved. This is why the method is so well suited to onion-peeling, and as demonstrated in the next section, it is why the method is so efficient.

The retrieval is complete when $\Delta U(N, N)$ is derived from the measurement t_N. (Recall that N is the index of the lowest layer.) At that point we have solved for $\Delta U(1, N)$, $\Delta U(2, N)$, . . . $\Delta U(N, N)$, the absorber amounts in all the layers along the Nth ray.

The choice of ΔU as the retrieved variable, although apparently dictated by the solution algorithm, is in fact a natural consequence of the integration along the line of sight that is inherent in limb observations. We have already noted that ΔU depends not only on the mixing ratio or concentration within a layer, but also on the length of the segment of the ray in that layer. We would prefer to convert the solution into units of an intensive quantity, such as mixing ratio. However, the integrated quantities ΔU are not easily converted to values for mixing ratio at discrete levels. There is a more natural correspondence between ΔU and the layer-mean mixing ratio, given by the approximation,

$$W_n \approx 10^3(R/M)(T_n/P_n)[\Delta U(n, N)/\Delta s(n, N)], \quad (11)$$

where W is layer-mean mixing ratio in ppmv; R the universal gas constant in cgs units; M is the molecular weight of the gas being sensed; T and P are layer-mean values of temperature (K) and pressure (mb), respectively; $\Delta U(n, N)$ is the absorber amount (in g cm^{-2}) in layer n along ray N, and $\Delta s(n, N)$ is the length of the line-of-sight segment in layer n along ray N. This choice of variable has the additional advantage of providing solutions that are smoother than those obtained when the solution is specified at discrete levels. Thus, after retrieving the profile in terms of ΔU, we apply (11) to express it in units of mean mixing ratio.

6. Application and discussion

Observations were simulated for one of the spectral intervals isolated by the balloon spectrometer described in Weinreb et al. (1984). This interval is used for sounding stratospheric water vapor. Its spectral response function is a triangle centered at 1507.0 cm^{-1} and having a half-power bandwidth of 3 cm^{-1}.

The simulations were based on the atmospheric profile listed in Table 1. It was assumed that the observing instrument was at an altitude of 46 km. Transmittances were calculated as described in section 4. The required homogeneous-path transmittance model, $\tau = f(P, T, U)$, was the polynomial of Smith (1968) as applied by Weinreb et al. (1984).

The simulated transmittance measurements (with no instrument noise added to them) are plotted in Fig. 6. The equivalence retrieval algorithm was applied to those simulated measurements. Figure 7 displays the

TABLE 1. Atmospheric profile.

Altitude (km)	Pressure (mb)	Temperature (K)	Water vapor (ppmv)
12	182.1	224.0	72.0
13	155.5	217.0	50.0
14	132.9	210.0	28.0
15	112.3	203.5	16.7
16	94.9	197.0	5.30
17	79.9	198.0	4.80
18	67.2	199.0	4.30
19	56.8	203.0	4.45
20	48.0	207.0	4.60
21	40.8	211.0	4.55
22	34.7	215.0	4.50
23	29.6	217.0	4.90
24	25.3	219.0	5.30
25	21.7	221.5	6.05
26	18.6	224.0	6.80
27	16.0	226.0	7.25
28	13.7	228.0	7.70
29	11.8	230.0	8.1
30	10.2	232.0	8.5
31	8.8	234.5	9.1
32	7.6	237.0	9.7
33	6.6	239.0	10.1
34	5.7	241.0	10.5
35	5.0	243.0	10.5
36	4.3	245.0	10.5
37	3.8	247.5	10.5
38	3.3	250.0	10.5
39	2.9	252.0	10.5
40	2.5	254.0	10.5
41	2.2	256.0	10.5
42	1.9	258.0	10.5
43	1.7	260.5	10.5
44	1.5	263.5	10.5
45	1.3	265.0	10.5
46	1.1	267.0	10.5

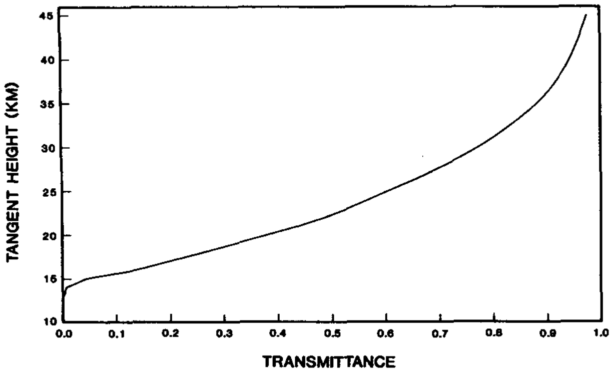

FIG. 6. Simulated transmittance measurements with no instrument noise.

"true" layer–mean mixing ratio profile and the results of the retrieval. The retrieval is nearly identical to the truth everywhere except at the 12–13 km layer. The reason for the error at 12–13 km is that the measured transmittance is zero for the ray with the 12-km tangent height; i.e., there is no signal from the 12–13 km layer. These results show that when the equivalence algorithm is consistent with the measured atmospheric transmittances, the retrieval is very accurate. However, if the algorithm is not consistent with the measured transmittance, the accuracy is less, as we show next.

We created an inconsistency between the measurements and the equivalence algorithm by adding simulated instrument noise to the transmittances in Fig. 6. The simulated noise was random and distributed normally with a zero mean and a standard deviation of $0.04t_n(1 - t_n)$. Its magnitude thus varied with the unperturbed transmittance t_n in such a way as to maximize the noise where the signal is roughly a maximum, i.e., near $t_n = 0.5$, which is typical in such an experiment. With these transmittances, the equivalence retrieval algorithm produced the retrieval plotted in Fig. 8. The retrieved profile oscillates about the true layer–mean mixing ratio profile with an amplitude of the order of 1 ppmv, or approximately 15% of the true layer–mean mixing ratios.

We also performed ordinary onion-peeling retrievals to compare them with the retrievals by the equivalence method. For the iterative equation we used (2). The retrieved variable was the absorber amount ΔU. Thus, the same variable was retrieved by both methods. Also, the results of the retrievals by both methods were converted to layer–mean mixing ratios W by the same equation, (11). In implementing the ordinary onion-peeling solutions, the initial estimate that is needed to begin the iterations was given for the mth equation by $\Delta U^{(1)}(m, m) = \Delta U(m - 1, m - 1)$; i.e., the initial estimate was the solution of the preceding equation. For each equation the solution converged in 4–7 iterations to the solution we had obtained with the equivalence method. Hence, ordinary onion peeling also produced the retrievals shown in Figs. 7 and 8. However, ordinary onion peeling consumed almost an order of magnitude more computer time than did the equivalence method. For example, execution time on a Digital Equipment Corporation MINC-11/23 minicomputer was 20 seconds for retrieving one 34-layer profile by the equivalence method. With the iterative method, it was 168 seconds, an increase by more than a factor of 8. This demonstrates that the equivalence method is significantly more efficient than ordinary onion-peeling.

The difference in efficiency between the two methods stems from the difference in the domains of the equations to be inverted in each. In ordinary onion-peeling one directly inverts (1) in which every equation actually represents a multistep algorithm for computing the transmittance over an entire multilayer limb path. In the equivalence method, one inverts the simpler function in (9) and (10) representing transmittance only of one homogeneous path, the tangent layer. In both methods the equations are inverted iteratively, but this requires less effort for the homogeneous paths of the equivalence method than for the multilayer paths of ordinary onion-peeling. Furthermore, as we have seen,

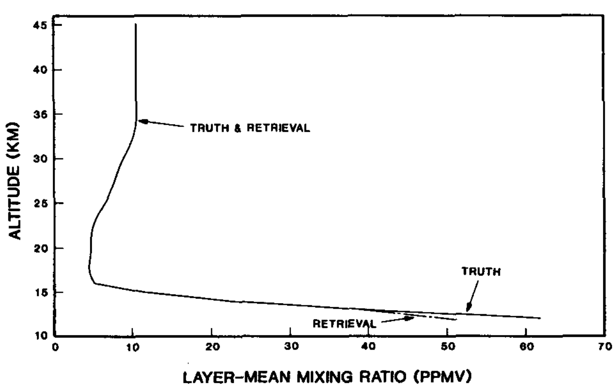

FIG. 7. Retrieval of layer–mean mixing ratio from noiseless simulated measurements, and true layer–mean mixing ratio profile.

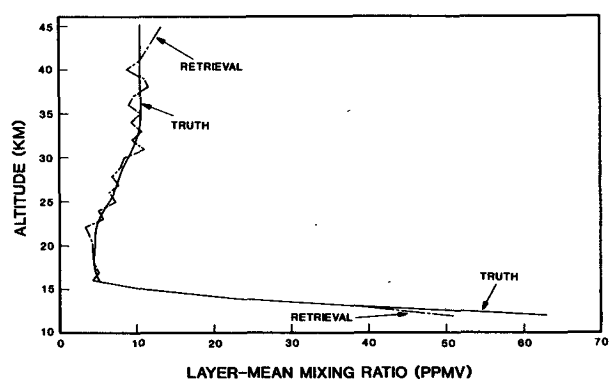

FIG. 8. As in Fig. 7 except that measurements include simulated instrument noise.

the inversions require a number of iterations in the multilayer case, but only one in the homogeneous path case. In short, the key to the efficiency of the equivalence method is that its main iterative steps are confined to a single layer, the tangent layer.

7. Summary

Onion-peeling is a commonly used method for deducing mixing-ratio profiles of stratospheric gases from solar occultation data. We have presented an equivalence algorithm for solving the equations that occur in onion-peeling. In simulation the equivalence algorithm produces the same retrievals as does the usual iterative method of solving the onion-peeling equations. However, the equivalence method is more efficient, because its main computations are confined to tangent layers instead of multilayer limb paths. As a result, execution time for the equivalence method is significantly less than that for ordinary onion-peeling.

Acknowledgments. The author is grateful to I-Lok Chang of The American University for offering helpful comments while this work was in progress. The author also thanks his colleagues at NOAA/NESDIS—Henry Fleming, Arthur Neuendorffer, James Lienesch, and Walter Planet—for reviewing the manuscript.

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