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INCLUSION OF THE SECOND UMKEHR IN THE CONVENTIONAL UMKEHR RETRIEVAL ANALYSIS AS A MEANS OF IMPROVING OZONE RETRIEVALS IN THE UPPER STRATOSPHERE

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ABSTRACT

The Umkehr method for retrieving the gross features of the vertical ozone distribution requires measurements of the ratio of zenith-sky radiances at two wavelengths in the near-UV region while the solar zenith angle (SZA) changes from 60 to 90 degrees. A Brewer spectrophotometer was used for taking such measurements extending the SZA range down to 96 degrees.

Analyzed data from the Spring of 1991 imply that observations at twilight are of great significance in improving ozone retrievals in the upper stratosphere. Judged by the variance reduction for Umkehr layers 9 to 12 (25-30% for layer 11) and the increase in separation and amplitude of the averaging kernels for the relevant layers, the ozone retrievals in the upper stratosphere are shown to be in better agreement with climatological means.

1. BACKGROUND TO THE PROBLEM

The physical process of scattering, whether in diffuse transmission or in diffuse reflection, has long been investigated as a method of inferring the profile of ozone and those of other minor atmospheric constituents. The *Umkehr Effect*, first noticed by Götz, is a classical example of diffuse transmission where the vertical ozone distribution is deduced from measurements of the ratio of radiances measured at two wavelengths in the near-UV while the SZA varies near twilight.

Götz et al., (1934) discussed a method for calculating the gross features of the ozone profile and even attempted to report on possible profile distortion errors caused by the neglect of secondary scattering and aerosols.

A more accurate method for deriving ozone profiles from Umkehr measurements was given by Dütsch (1959); he linearized the problem in hand using a series expansion, correcting for second order terms with an iterative procedure.

In the last twenty years, profile inversion has undergone very rapid development. DeLuisi (1979) studied the possibility of shortening the time required for an Umkehr observation by incorporating more wavelength pairs in the measurement procedure and demonstrated that there is a 'trade-off' between the number of wavelength pairs and SZAs used, leading to almost the same information content about the ozone profile. More recent developments were based on a better set of standard profiles and their climatological covariance.

It has long been noticed that the Conventional Umkehr (CU), where the 60 to 90° range of SZA is used, delivers less ozone than normal for the area of the ozone maximum and the uppermost layers, and more ozone for the lowermost layers. Part of the error was found to be caused by atmospheric aerosols [DeLuisi et al., 1979]; it was evident that only stratospheric aerosols can cause significant profile distortions, especially for layers 7, 8 and 9 where the technique is most effective.

In this paper we present a method for improving ozone retrievals in the upper stratosphere by incorporating observations before sunrise or after sunset in the CU retrieval analysis; we will call that the Extended Umkehr (EU). The results for the random errors in the retrievals are also presented along with the averaging kernels and compared to the results of the CU analysis.

2. METHODOLOGY

A series of measurements of light scattered from the clear zenith-sky with SZA contains information about the vertical profile of an absorber, assuming that the absorber concentration remains constant during the observation period. If we were to look at the contribution to the total intensity received at the ground from light scattered at a thin layer centered at altitude z, then for monochromatic radiation we would be given

$$I_{z,sc} \propto I_z \, s_c \, [M]_z \tag{1}$$

where I_z is the radiation reaching altitude z, s_c is the scattering cross-section and $[M]_z$ is the air density at altitude z. (1) is highly non-linear for it depends on the atmospheric density profile and the amount of radiation reaching a particular altitude. Therefore, for each SZA the singly scattered radiation comes from a fairly well-defined layer, the *effective scattering layer* which moves higher up as the SZA increases. This *scanning effect* provides information about the vertical ozone distribution.

A retrieval problem can in general be stated as follows: given a set of experimental observations in which the unknown parameter (or set of parameters) is related to in a complicated way, find the optimum solution. In our case we have an independent virtual measurement x_0 with covariance S_x and a direct measurement y with error covariance S_y; then the optimum solution ($\hat{x}$) is the one which maximizes the conditional probability $P(\hat{x}|y,x_0)$. By means of Bayes theorem and under the assumption of independent Gaussian statistics [Martin, pp9-21, 1971], we obtain

$$\hat{x} = x_0 + S_x \left[\frac{\partial F(\hat{x})}{\partial x} \right]^T S_y^{-1} \left(y-F(\hat{x})\right) \qquad (2)$$

In the case of Umkehr analysis for ozone profiles, the forward calculation is not linear as already been discussed; linearizing then about a state x_n (a guessed value of the solution) yields

$$F(\hat{x}) = F(x_n) + K_n (\hat{x}-x_n) + 0 (\hat{x}-x_n)^2 \qquad (3)$$

where $K_n = \left.\frac{\partial F}{\partial x}\right|_{x_n}$.

Finally substituting (3) to (2), we obtain

$$x_{n+1}=x_0+S_xK_n^T\left(K_nS_xK_n^T + S_y \right)^{-1} \left[y-y_n-K_n\left(x_0- x_n\right)\right] \qquad (4)$$

$$\text{and } \hat{S} = S_x - S_xK_n^T \left(K_nS_xK_n^T + S_y \right)^{-1} K_nS_x \qquad (5)$$

where $\hat{x}$ has been replaced by x_{n+1} to show the iterative nature of the solution [Rodgers, 1976].

Equations (4) and (5) comprise the non-linear optimal estimation algorithm and in this form were used as the inverse model in this paper. When such an iterative method is used it is imperative to have a criterion for convergence. Throughout this analysis the process is stopped when the root-mean-square deviation of the solution vector from one iteration to the next is less than 1%. A quality check was also used based on a χ^2-test, namely in determining the confidence interval to within which the retrieved profile successfully reproduces the measurements.

3. APPLICATION OF THE METHOD TO OZONE PROFILES

Umkehr measurements were taken at London, Ontario using a Brewer spectrophotometer (#020), in the spring and summer of 1991.

Linear interpolation is used to derive the first-guess profile, using measured total ozone as predictor, from a set of eight standard ozone profiles [NOAA Tech. Memo., 1980].

A series of standard SZAs is used in the inversion algorithm (65, 70, 74, 77, 80, 83, 85, 86.5, 88 - 95) such that the Umkehr curve is represented well. The assumed error in the total ozone measurement is 1 matm-cm.

Total ozone measurements revealed that ozone was stable on day 108 under good observing conditions. Total SO_2 measurements with the same instrument showed small amounts, less than ~1-2 matm-cm; therefore, no serious SO_2 interference to Umkehr measurements is expected for that day [WMO, Report #18, p145, 1988]. Also polarization measurements performed with the same instrument showed no significant aerosol loading, thus avoiding any ozone profile distortions as their effects were not included in the forward calculation.

The elements of the measurement vector y are

$$N(\vartheta) = \log_{10}\left[\frac{I(\vartheta,\lambda_1)}{I(\vartheta,\lambda_2)} \right] + C_0 \qquad (6)$$

where ϑ is the SZA, $I(\vartheta,\lambda)$ is the zenith-sky radiance at wavelength λ, and C_0 is the *extraterrestrial constant* which combines solar spectrum and instrumental response. This unknown constant is removed by subtracting the N(60°) from each of the other N-values; this process also removes any solar variability with t>3.5 hours, the time required for a complete Umkehr observation.

The elements of the profile vector x are $\ln(x_i)$, where x_i is the ozone amount in Umkehr layer i.

Figure 1 shows the retrieved ozone profile and figure 2 the agreement between the measured Umkehr curve and that reconstructed from the retrieved profile. The fitting is good up to 93° of SZA whereas at 94 and 95° quite off, as indicated by the fitting residuals. It is known that during twilight the optical path increases dramatically with SZA and that most of the radiation attenuation occurs near the tangent point; therefore, any subvisible clouds near the horizon or even increased multiple scattering effects due to local aerosols might have affected the measurements. The quality check performed, indicates that for day 108 the retrieved ozone profile reproduces the measurements to within the 80% confidence interval.

Although any ozone changes in the upper stratosphere, due to rapid altering of the ozone photochemistry during twilight, are of concern to the inverse method, the *a priori* covariance matrix used allows for a 20% variability at the relevant layers (9-13); with the exception of layer 9, most of the information for these layers comes out of the *a priori* than the measurements.

4. ERROR ANALYSIS

An advantage of the Rodgers retrieval method is that it provides an estimate of the uncertainties in the retrieved profiles due to (a) measurement noise, (b) uncertain model parameters and inverse model bias, and (c) the inherent finite vertical resolution of the observing system. The observing system characterization can be carried out by studying the Transfer Function

$$T(x,b,x_a) = I\left(F(x,b) + \varepsilon_y, \hat{b}, x_a \right) = \hat{x} \qquad (7)$$

where I() is the inverse model, $\hat{b}$ the best estimate of model parameters b, ε_y the measurement error and x_a the best estimate of the true state x. Linearizing about $\hat{x}$ and, $\hat{b}$ and x_a yields

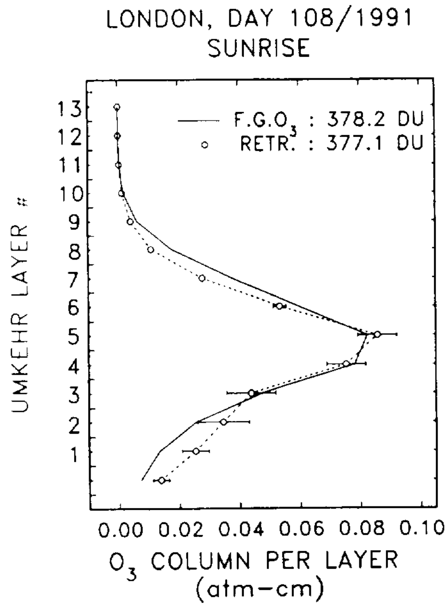

Figure 1

Retrieved height profile of ozone on day 108, 1991; the plots give the ozone reduced column (atm-cm) per Umkehr layer along with the total errors in the retrieval. The solid line corresponds to the first guess ozone profile. The total first guess (F.G.O_3) and retrieved amounts (RETR.) are also noted.

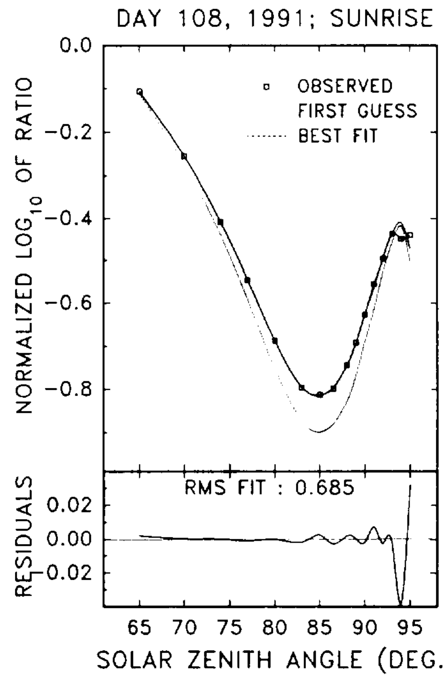

Figure 2

Reconstructed Umkehr curve based on the retrieved ozone profile on day 108, 1991. All the curves have been normalized to 60°, as discussed in the text. The fitting residuals are also shown in the bottom plots and the RMS fit number noted.

$$\hat{x}-x=\left(T(\hat{x},\hat{b},x_a)-\hat{x}\right)+(A-I)(x-\hat{x})+D_yK_b\varepsilon_b+D_y\varepsilon_y+D_a(x_a-\hat{x}) \quad (8)$$

for the total error in the retrieval.

Therefore, the overall error comprises:

Random errors $(A - I)(\hat{x} - x) + D_y\varepsilon_y$ and

Systematic errors $\left(T(\hat{x},\hat{b},x_a)-\hat{x}\right)+D_yK_b\varepsilon_b+D_a(x_a-\hat{x})$

[Rodgers, 1990]

The error analysis presented in this paper was carried out only for the random errors in the retrievals. The measurement process can be thought of as a mapping from profile space to measurement space. In this process, certain portions of the profile space cannot be measured (those corresponding to high frequency components or fine scale information about the profile) and this leads to an error called the null-space error, with covariance

$$S_N = (A - I)\, S_x\, (A - I)^T \quad (9)$$

Figure 3 shows the null-space error covariance for both the CU and the EU. The patterns presented (rows of matrix S_N) tend to have larger values at the top and bottom of the plot where there is little information about the true profile in the measurements. Note that inclusion of measurements before sunrise in the CU analysis reduced the amplitude of the errors for the uppermost layers 10 to 12, implying a greater information content of the EU.

Another useful diagnostic to look at is the averaging kernel of the retrieval

$$A = D_y K_x \quad (10)$$

which describes the retrieved profile as a weighted average of the true profile. The rows of A are peaked functions with FWHM characterizing the resolution of the observing system; their shape is an indication of anomalous retrievals (double peaks) [Rodgers, 1990].

The averaging kernels for the retrievals undertaken in this paper are shown in figure 4. As seen, inclusion of the second Umkehr increased the amplitude and separation of the averaging kernels for the uppermost layers compared with the CU analysis. In doing so the retrieval becomes more meaningful for layers 6 to 9 where the technique is mostly sensitive.

In figure 5, we present results for the CU, the EU and the first guess profile errors along with the variance reduction as a fraction of the first guess error variance (upper abscissa scale applies) for day 108; the EU reduced the variance by ~35% for layer 11, ~17% for layer 10, ~11% for layer 12 and only slightly for layers 5, 7 and 9 compared to the CU.

5. CONCLUSIONS

As was found before, the CU technique does not appear to provide any useful information below about 19 km but showed some potential in monitoring long-term changes in the upper stratospheric ozone; the same holds for the short Umkehr (SU) [DeLuisi et al., 1985].

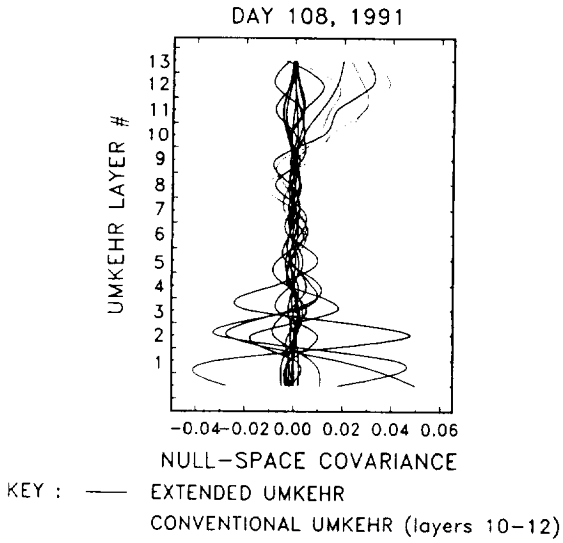

Figure 3

The rows of the null-space error covariance matrix of the EU retrievals are plotted along with similar patterns based on the CU analysis (layers 10-12, only). Note the reduction in null-space variance for the uppermost layers.

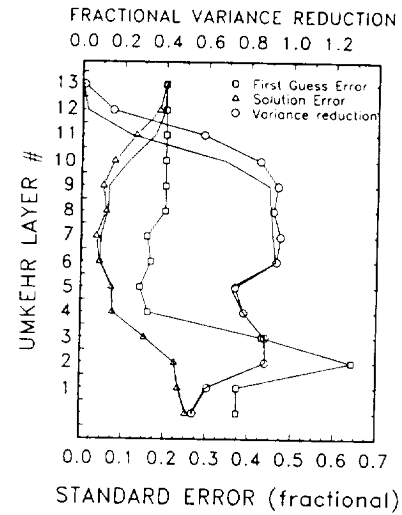

Figure 5

Results for the CU, EU and the first guess profile errors on day 108, 1991. The variance reduction is also plotted as a fraction of the first guess error variance where the upper abscissa scale applies. The solid line is based on the CU analysis. Note the variance reduction of the EU compared to the CU analysis.

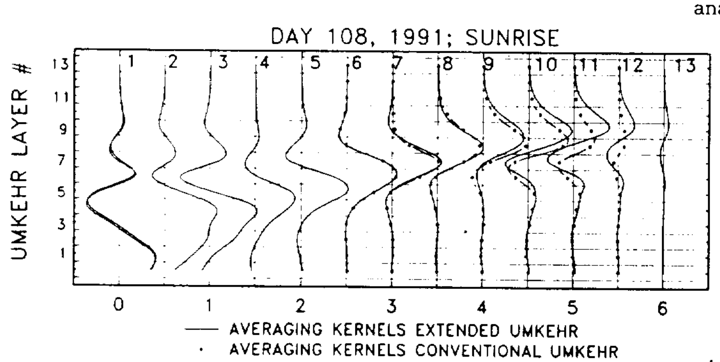

Figure 4

Averaging kernels for the ozone retrieval on day 108, 1991. Each kernel has been misplaced by 0.5 for clarity. The corresponding averaging kernels for the CU analysis (-*-) are also shown for layers 6 to 12.

The new EU which we have introduced for retrieving height profiles of ozone from Umkehr measurements, is potentially useful for correcting ozone retrievals in layers 7 to 12 by improving the information content of the technique and therefore contributing to a better understanding of the upper stratosphere global ozone trends in the future.

More refinement may be needed with respect to including the effects of multiple scattering which become important at SZA greater than 93°, and exploring the possibility of reducing the range of SZA to 80-95° by incorporating more wavelength pairs in the inversion procedure. One last comment is in order. The studies of Dave et al., 1979 and DeLuisi, 1979 made clear that Umkehr retrievals for the upper layers 7-9 are significantly affected by stratospheric aerosols and so corrections should always be applied for these scattering effects, especially after major volcanic eruptions.

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