New Umkehr ozone profile retrieval algorithm optimized for climatological studies

I. Petropavlovskikh,[1] P. K. Bhartia,[2] and J. DeLuisi[1]

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[1] We present a new Umkehr ozone profile retrieval algorithm (UMK04) that has been optimized for the study of monthly mean anomalies (MMA) to assess climate variability in multi-year time series. Although the Umkehr technique is too noisy to monitor short-term variability in atmospheric ozone, it is capable of monitoring long-term changes in MMA with less then 5% uncertainty in the stratosphere, and with no influence from a priori information. By examining the information content of UMK04 we conclude that Umkehr data contain useful information about long-term ozone trend down to the surface, provided the data are analyzed as column ozone amounts in 8-layers, consisting of two ~9.6 km layers in the lower atmosphere (253–1013, 63–253 hPa), five ~4.8 km layers (32–63, 16–32, 8–16, 4–8, 2–4 hPa) in the stratosphere, plus a broad top layer spanning from 0–4 hPa. **Citation:** Petropavlovskikh, I., P. K. Bhartia, and J. DeLuisi (2005), New Umkehr ozone profile retrieval algorithm optimized for climatological studies, *Geophys. Res. Lett.*, *32*, L16808, doi:10.1029/2005GL023323.

1. Introduction

[2] The Umkehr technique has been used since the 1930s [*Götz et al.*, 1934] to estimate the vertical ozone profile from zenith sky measurements taken at a pair of wavelengths in ultraviolet (311.5 and 332.5 nm) using the Dobson spectrophotometer [*Dütsch*, 1959]. Since 1984 Brewer instruments have also taken similar measurements at 6 discrete wavelengths [*McElroy and Kerr*, 1995; *World Meteorological Organization*, 2000]. Since these measurements are made routinely by some 78 Dobson stations and about 66 Brewer instruments around the world (WOUDC, Canada), they provide an inexpensive way of monitoring long-term changes in the ozone layer. Moreover, the Umkehr technique is similar to satellite solar occultation techniques, having the unique advantage that the ozone profile retrieval doesn't require absolute radiometric calibration, a problem that has plagued the satellite backscatter ultraviolet (BUV) instruments since its inception in 1970. Indeed, the Umkehr technique is the only ground-based technique that provides information that closely matches that provided by the BUV technique in vertical resolution and information content. This capability makes the Umkehr retrievals very valuable for monitoring the drift of the BUV instruments and for cross-calibrating between data gaps. With the recent adoption of the BUV technique as the primary ozone-monitoring sensor on meteorological satellites of both the US (NPOESS) and of Europe (METOP), continuing the Umkehr time series using an improved algorithm has become extremely important.

[3] Umkehr data from the Dobson instruments are currently processed using the UMK92 algorithm developed by *Mateer and DeLuisi* [1992]. This algorithm shares many common features with the BUV (version 6) algorithm [*Bhartia et al.*, 1996] that was used to process the BUV data collected since 1970 by instruments on several NASA and NOAA satellites. The V6 BUV algorithm was recently replaced with a new version V8 [*Bhartia et al.*, 2004], and 25 years of reprocessed data were recently released at the 2004 Quadrennial Ozone Symposium (Kos, Greece, 2004). In this paper we describe a parallel development of a new Umkehr algorithm (UMK04) that shares many common features with the V8 BUV algorithm. Both algorithms are designed to optimally retrieve monthly mean anomalies (MMA) from the data. The MMAs, commonly used for climate studies, are obtained by removing long-term monthly means from a multi-year time series. Although UMK04 incorporates several other improvements to the forward and inverse models used in the retrieval, in this paper we limit our discussion to those features of the algorithm that affect the estimation of MMAs. The website http://www.srrb.noaa.gov/research/umkehr provides a more complete description of all the features that have been incorporated into UMK04.

[4] In section 2 of this paper we describe three key features of UMK04 that affect MMAs. Section 3 discusses the Averaging Kernels (AK) [*Rodgers*, 2000], which provide a measure of the vertical resolution and information content of the retrieved profiles. AKs are also used to determine how changing the range of solar zenith angles for data collection affects the information content. Finally, in section 4, we compare how well UMK92 and UMK04 reproduce a model-estimated trend in the ozone profile, and compare the MMAs derived from actual data. Section 4 also describes typical sources of errors in the Dobson C-pair Umkehr retrieval, and provides estimates for stratospheric aerosol errors.

2. Key Features of UMK04

2.1. A Priori Profiles

[5] UMK04 is based on the optimal estimation technique described by *Rodgers* [2000]. We can rewrite Rodgers' equation (12.10) to demonstrate how time-dependence in the a priori information can propagate to the monthly mean anomalies (MMA) in retrieved ozone:

$$\hat{M} = A \times M_T + (I - A) \times M_A + G_y \times (\bar{\varepsilon} - \varepsilon_0), \qquad (1)$$

[1]Cooperative Institute for Research in Environmental Sciences, National Ocean and Atmospheric Administration, Boulder, Colorado, USA.

[2]NASA Goddard Space Flight Center, Greenbelt, Maryland, USA.

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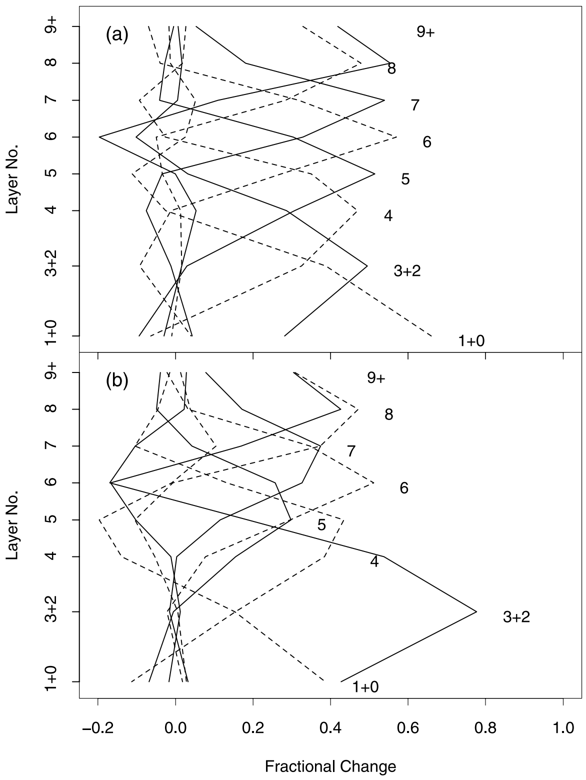

Figure 1. Each line shows algorithm's response (AK) to a 1 percent ozone change in 8 coarse layers (see Table 1 for details on layer system. (a) AKs are calculated using Rodgers covariance matrix with 0.2 coefficient and 60-degrees SZA for normalization. (b) The same as (a), but using climatological information about covariance between layers.

where $M = \frac{\bar{x}-\bar{x}_0}{\bar{x}_0}$ is the mean monthly ozone anomaly (subscripts T and A denote the true and a priori values of M respectively, x the monthly mean layer ozone, and x_0 the long-term mean of x), A is the averaging kernel [*Rodgers*, 2000, equation 3.28], G_y is the retrieval gain matrix [*Rodgers*, 2000, equation 3.27], and $(\varepsilon - \varepsilon_0)$ represents the MMA in the calibration drift of the instrument. The first term on the right side of the Equation 2 shows that A acts as low-pass filter to smooth out high vertical resolution features from the true anomaly. The trend information is contained in this term. The second term is unique to remote sensing problems. It shows that time dependent changes in the a priori could also affect the retrieved M, if they pass through the high-pass filter $(I - A)$, i.e., if they have vertical structures finer than the inherent vertical resolution of the measurement represented by A.

[6] UMK92 uses total ozone-dependent a priori profiles to constrain the retrieval, which introduce high frequency structures in a priori that can produce undesirable non-zero contributions from the second term. In UMK04 algorithm we avoid this problem by keeping the a priori fixed from one year to next. Thus any long-term variability seen in the UMK04 retrieved data is truly independent of the a priori information.

[7] The third term captures the effect of any long-term instrument drift on the retrieved M. Since total ozone (measured by the direct sun technique) is part of our measurement vector, any errors in total ozone are also contained in the third term. We use the re-evaluated total ozone dataset developed as a part of the REVUE project [*Bojkov et al.*, 2002] to minimize this error.

2.2. State Vector

[8] In UMK04 algorithm we define the state vector ($\boldsymbol{x}$ in Rodgers' notation) as the layer ozone amount, ω, rather than $\log(\omega)$ as in UMK92. Although the use of $\log(\omega)$ as state vector ensures a positive-definite value of retrieved ω, it has the undesirable property that it distorts the layer ozone statistics by making it harder for the algorithm to retrieve very low ozone values in a layer where the a priori ozone values are large. Indeed, even negative values of ω must be included in computing means when ω differs from zero by less than the measurement uncertainty. UMK04 preserves the probability distribution function of ω, and ensures that the monthly mean of $\bar{\omega}$ is an unbiased arithmetic mean.

2.3. Measurement Error

[9] In a classic paper, *Backus and Gilbert* [1970] showed that (up to a point) the vertical resolution of a remote-sensing technique, such as Umkehr, can be improved by reducing the measurement noise. The basic measurement of Dobson is the N-value (1N = 2.3% of radiance). UMK92 assumes a rather large measurement error (σ = 1N). Since the measurement vector uses normalized N-values [$N(\theta) - N(\theta_0)$, where θ_0 are the SZAs and subscript 0 refers to the minimum value of θ], these errors increase to 1.4N (3.2%). Based on careful examination of the Umkehr data simultaneously collected from two automated Dobson instruments located at Arosa, Switzerland (R. Stübi and E. Maillard, private communication, 2003) we believe that the Umkehr noise is considerably smaller than 1N at smaller solar zenith angles. In UMK04, we assume a solar zenith angle-dependent noise estimate (see the website) that improves the vertical resolution of retrieved profiles, particularly in the lower layers.

3. Information Content

3.1. Vertical Resolution

[10] To minimize representation errors (i.e., error in calculating the N-values) UMK04 divides the atmosphere in 61 layers, which are obtained by dividing the standard ~4.8 km thick Umkehr layers into 4 layers. From the analysis of the 61-layer Averaging Kernels (AK) we find that the vertical resolution of UMK04 is about 10 km above ~20 km, and worse below. Therefore the standard Umkehr layering scheme is optimum for analyzing the data in layers 4 and above (by providing two layers per resolution element), but it is too fine for the lower layers. Figure 1 shows how the layers could be combined to keep the information content very nearly the same in all layers. This results in 7 layers, in which layers 2 and 3 are combined to form ~9.6 km thick layers, whereas layer 1 is traditionally ~10 km wide.

[11] Like UMK92, UMK04 provides no useful information in Layer 9. However, the column ozone in layer 8+, (representing layer 8 plus the atmosphere above it), is of high quality. This information is useful for comparing Umkehr data with similar data provided by the BUV

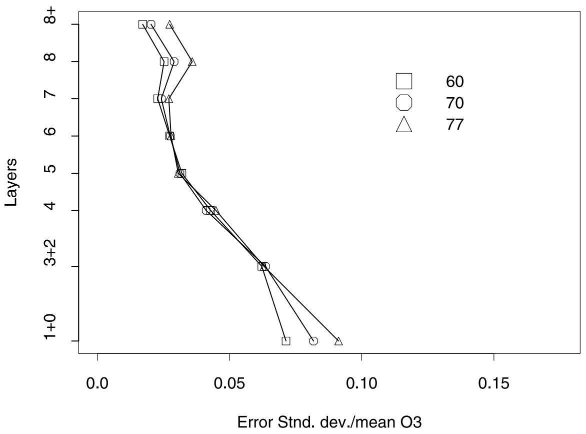

Figure 2. Relative error of the retrieval as function of layers: standard deviation in monthly averaged ozone divided by mean ozone. Effect of minimum SZA is shown by three lines representing three scenarios (60, 70 and 77 degree normalization SZA).

instruments. Therefore we recommend that layer 8+ values should also be reported.

[12] Figure 1 shows the response of the algorithm to a change in ozone in a given layer (obtained from the 61-layer AK matrix) for two different assumptions about the a priori covariance matrix (S_x in Rodgers' notation). For Figure 1a, we assume that the (fractional) standard deviation of layer ozone is large (0.1) and independent of height, and the inter-layer correlations drop-off exponentially with distance between the layers (see the website for more detail). For Figure 1b, we use the covariance matrix derived using data collected from middle latitude sondes (Hohenpeissenberg) and satellite instruments (primarily SAGE). Since it is important to have undistorted response functions for the analysis of trends we have adopted the former S_x matrix for UMK04. (Although, this may seem to violate the basic tenet of maximum likelihood estimation, one should note that the covariance matrices derived from actual data are dominated by short-term variability; they are not necessarily optimal for deriving MMAs.)

3.2. Effect of Minimum Solar Zenith Angle (θ_0)

[13] Traditionally, C-pair Umkehr measurements are taken between 60° and 90° SZAs. Even in lower latitudes it takes 2–3 hours to take these measurements. At higher latitudes, measurements at 60° are not even possible near the winter solstice. To reduce the observation time, the so-called "short-Umkehr" technique was proposed some years ago [*DeLuisi et al.*, 1985]. In this technique, one increases the number of pairs to 3, which presumably allows one to collect data between 70° and 90° SZA without loss of information. Though many Dobson stations (called automated Dobsons) collect such data, there is currently no operational algorithm to process the short-Umkehr data. Surprisingly, loss of information in the standard C-pair Umkehr technique as a function of θ_0 has not been studied previously to determine the added value of the short-Umkehr. Figure 2 shows that even for the standard Umkehr there is very little loss of information when one changes θ_0 from 60° to 70°, except in the tropospheric (0+1) layer. Indeed, even for θ_0 = 77° there is very little loss of information in the upper layers. Although the triple pair Umkehr may do better, this is yet to be demonstrated using real data. Therefore, we recommend that the Dobson stations that cannot or do not want to make measurements at 3 separate pairs, or want to cut down their observation time, take just the C-pair measurements between 70° and 90° SZA. Cloud-free data taken over a SZA interval as short as 77° to 90° would provide useful information in the upper layers where no ozonesonde data are available. On the other hand, the AK analysis also shows that there is useful information in layer 1 (256–1013 hPa), provided the measurements start at 60° SZA. Therefore, it is highly recommended that low latitude Dobson and Brewer stations take Umkehr measurements regularly starting at 60° SZA.

4. Error in Derived Trends

[14] There are 4 types of errors associated with the MMAs and trends derived from the Umkehr method. Three of these are related to the algorithm, and fourth is related to the instrument. These errors are briefly described below.

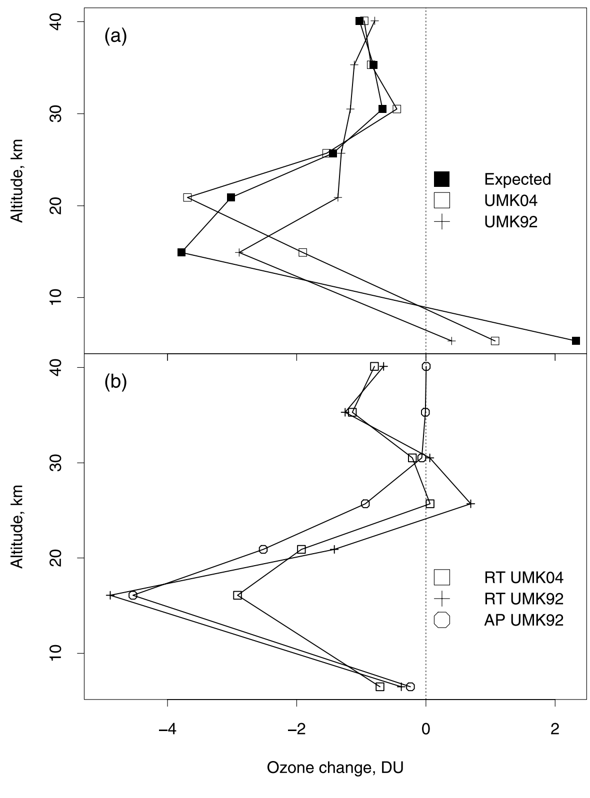

Figure 3. A vertical distribution of ozone profile changes (in DU per decade). The estimated trend in the ozone profile (solid squares) is compared with results of the two Umkehr algorithm retrievals: the UMK04 (open squares) and the UMK92 (pluses). (b) Example of linear trends derived from Dobson Umkehr data at NOAA/CMDL Boulder over 1979–1997 time-period (aerosol corrections applied). Trends derived from the UMK92 (pluses) and the UMK04 (open squares) retrieved data are compared to trends in UMK92 (open circles) and UMK04 a priori ozone (vertical line at zero point).

Table 1. Change in Eight Umkehr Layers (percent) Corresponding to Stratospheric Aerosol Interference for 350 DU Standard Ozone Profile[a]

	8+	8	7	6	5	4	2+3	1
10-km	−3.2	−3.9	−4.7	−3.2	−1.2	−0.9	0.3	3.0
15-km	−15.8	−17.7	−11.3	−1.5	−1.2	−4.1	1.1	7.8
20-km	−42.9	−46.0	−11.2	3.1	−19.3	−18.3	14.1	26.1
25-km	−67.5	−73.0	−7.5	−6.5	−58.0	−39.3	48.4	56.0
P (hPa)	3.9	3.9	7.8	15.6	31.2	62.5	250	1000

[a]Optical depth is 0.1. The last row states atmospheric pressure at the bottom of the Umkehr layer.

4.1. Error Due to Limited Vertical Resolution

[15] Given the low vertical resolution of the technique, it is clear that Umkehr will miss many subtle vertical features in the MMAs of ozone profiles. To see how this loss of information might affect trends, in Figure 3a we show how well the technique can retrieve a postulated long-term trend in mid latitude ozone profile [*Miller et al.*, 1997] based on high resolution satellite and ground-based data. This case represents a somewhat extreme test of the Umkehr technique, for the sign of the trend changes sharply at an altitude where the technique has the worst vertical resolution. Yet, UMK04 is able to capture much of the relevant information, for example, separation of negative trends in the stratosphere from positive trend in the troposphere, and does significantly better than UMK92.

4.2. Error Due to A Priori

[16] Figure 3b shows the ozone trends derived from the two algorithms using the Umkehr data from the Boulder Dobson station. The two algorithms differ considerably in the lower layers. As discussed earlier, trend derived by UMK92 is strongly influenced by the trend in the a priori profiles used by the UMK92 algorithm. This error doesn't occur for UMK04 since the a priori profiles do not have any trend.

4.3. Error Due to Stratospheric Aerosol

[17] It is well known that the stratospheric aerosols produced from SO_2 injected by strong volcanic eruptions can produce large errors in the ozone profile retrieved by the Umkehr technique [*Mateer and DeLuisi*, 1992]. The algorithm does not account for aerosol interference in Umkehr measurement, thus measurement changes are interpreted as ozone changes. Table 1 provides an estimate of these errors for UMK04. As in UMK92, the errors are a strong function of aerosol altitude and are largest for the uppermost and lowermost layers.

4.4. Instrumental Errors

[18] Since normalized N-values (and direct-sun total ozone) are used as measurement in Umkehr retrieval, the technique is not sensitive to absolute radiometric calibration of the instrument. However, it is well known that the Dobson instruments suffer from internal scattered light problem that becomes significant at large solar zenith angles. This is probably the reason why the mean ozone derived from the Umkehr technique is too low in layer 8 by ~5% compared to all other measurements [*World Meteorological Organization*, 1998]. Since this error may change when an instrument is replaced or refurbished, one can get discontinuities in the retrieved time series. To reduce the impact of this error it is highly desirable that data from several independent stations are available for trend calculation, highlighting the need for the Dobson and Brewer stations to collect such data as often as possible.

5. Summary and Future Plans

[19] We have shown that UMK04 is a significant improvement over the current operational algorithm (UMK92) for the estimation of long-term trends. It differs from the UMK92 in 3 key respects: 1) The a priori profiles have no impact on the MMA, which are influenced only by the MMA of the radiances; 2) The algorithm is more linear, hence it preserves the probability distribution function of the layer ozone which could otherwise bias the monthly means; and 3) The measurements in the UMK04 are given more weight than in the UMK92, while considering total ozone information as part of the measuring system, rather than a part of a priori as in the UMK92. Therefore, information content of the lower layers in UMK04 becomes similar to other layers, thus improving lower layer retrieval. We also show that information in the upper layers is not degraded by changing the starting SZA to 70°. We hope that these results would encourage more stations to collect Umkehr data for long-term monitoring of the health of the ozone layer and for validation of operational satellite instruments based on the BUV technique.

[20] We have used UMK04 to process all available data from both the old type of Dobson instruments that collect only the C-pair Umkehr data as well as from the automated Dobsons that collect data for 3 pairs (though we use only the C-pair data). We also plan to apply UMK04 to data collected by the Brewer instruments by selecting two wavelengths that are closest to the Dobson C-pair wavelengths. This will produce a consistent long-term dataset from all 3 types of instruments for trend studies. Simple extension of UMK04 can be made to use all 3 Dobson pairs or all 6 individual Brewer wavelengths. However, our preliminary analysis (using AKs) indicates that use of additional pairs or wavelengths would produce only marginal benefit, so we have given this effort a lower priority. We encourage others to test this contention by comparing the results of their algorithms with UMK04.

[21] **Acknowledgments.** Umkehr data used in this publication are archived at the WMO ozone and UV data center (WOUDC) in Toronto, Canada, and were collected in Boulder, USA (NOAA/CMDL). This work was funded by OMI Satellite Science Team Project (EOS/AURA satellite) from NASA/Goddard.

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P. K. Bhartia, NASA Goddard Space Flight Center, Code 916, Greenbelt, MD 20771, USA.

J. DeLuisi and I. Petropavlovskikh, Cooperative Institute for Research in Environmental Sciences, NOAA/ARL R/E/AR*1, 325 Broadway, Boulder, CO 80303, USA. (irini.petro@noaa.gov)