

THE UPDATED STATISTICAL INVERSION TECHNIQUE
TO THE EVALUATION OF UMKEHR OBSERVATIONS.

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ABSTRACT

In the present study the standard retrieval Umkehr method to estimate the vertical distribution of ozone was updated using statistical approach to the mathematical inversion scheme. The vertical ozone profile covariance matrix were used as a priori information for the inverse problem. A new method of the ozonesonde data organization according to air mass types helped to improve the covariance matrix quality. A retrieval method was developed using eigen vector technique. An optimal vertical ozone profile resolution was determined from the mathematical inversion scheme analyze based on the same technic. The sun radiation transfer was accounted for multiple scattering and atmospheric sphericity in this calculations. The retrievals using actual Umkehr Dobson spectrophotometer observations were also performed to provide the comparison of the standard and updated methods with concurrent ozone sound data at Boulder U.S. The comparison have revealed that the present method has some advantages in both resolution and accuracy, as compared to the standard one, especially for the atmospheric layers below ozone maximum.

1. THE INVERSION TECHNIQUE.

In order to determine the VOD from the Umkehr effect, the ratio of the fluxes of solar UV radiation scattered at the zenith at three pairs of wavelengths are recorded with a Dobson spectrophotometer at different solar zenith angles. The Umkehr effect can be described by an integral Fredgholm equation, which in operator form is

$$\mathbf{A}\mathbf{x} = \mathbf{U} + \mathbf{e} \quad (1)$$

where \mathbf{A} attenuation of solar UV radiation in the atmosphere. \mathbf{e} is the measurement error

vector, \mathbf{x} is the VOD vector, and the values of the vector \mathbf{U} are the logarithms of the ratios between pairs of spectrophotometer readings. The direct operator \mathbf{A} was evaluated for multiple scattering spherical atmosphere, taking into consideration all scattering orders.

Equation (1) is a nonlinear integral equation, whose solution for \mathbf{x} is a typical ill-posed inverse problem. The statistical approach to solving the problem is the most nearly optimal. As usual, the problem is readily linearized, if we seek a solution of Eq.(1) as a variation from the mean :

$$\Delta \mathbf{x} = \mathbf{x} - \bar{\mathbf{x}} \quad (2)$$

where $\bar{\mathbf{x}}$ is the mean VOD for given air mass and month.

Replacing vertical integration in the operator \mathbf{A} by layer wise summation and replacing the integral with respect to the wavelength by the corresponding sum, we obtain a system of linear algebraic to determine $\Delta \mathbf{x}$

$$\mathbf{B}\Delta \mathbf{x} = \Delta \mathbf{U} + \mathbf{e} \quad (3)$$

where \mathbf{B} is a linear operator (or matrix) operating on the VOD variation vector, and $\Delta \mathbf{U}$ are the variations in the ratios of the Dobson readings.

The number of rows m in matrix \mathbf{B} depends on the number of observations that differ by the solar zenith angle or spectral pair used, whereas the number of columns n depends on the number of the layers used in the atmospheric model from which the VOD is retrieved. In general, $m = n$, and in the present case $m > n$, i.e., the system of equations is over determined and subsequently the solution of Eq. (3) is understood in the sense of the least-squares method.

Following the method developed by Kozlov [1], we construct an information operator \mathcal{W} of the form

$$\mathcal{W} = \mathcal{C}^* \Sigma^{-1} \mathcal{B} \quad (4)$$

where \mathcal{C} is the covariance matrix of the VOD, \mathcal{B}^* is the transpose of matrix \mathcal{C} , and Σ^{-1} is the inverse of the error matrix.

We'll search a solution of system of linear algebraic equations (3) as an expansion in a system of eigenvectors $\{ \mathbf{f}_n \}$ of operator \mathcal{W} in Eq. (4), forming the orthogonal basis:

$$\Delta \mathbf{f} = \sum_n \xi_n \mathbf{f}_n \quad (5)$$

where ξ_n are the components of the projection on the bases [2] and have the form

$$\xi_n = \frac{\lambda_n}{\lambda_n + 1} (\mathcal{B}^* \Sigma^{-1} \Delta \mathbf{v}, \mathbf{f}_n) \quad (6)$$

Thus the solution of system (3) reduces to a computational far simpler problem of finding eigenvalues and eigenvectors of information operator \mathcal{W} in Eq. (4). By virtue of rapid decline in the function $\lambda_n / (\lambda_n + 1)$ with decreasing eigenvalues λ_n , the contribution of the terms with $\lambda_n \ll 1$ to sum (5) may be neglected; it therefore becomes possible to use simple, stable iteration algorithms to find the eigenvalues and vectors.

The information volume \mathcal{W} is given by the equation

$$\mathcal{W} = \prod_n \lambda_n \quad (7)$$

where the factors λ_n are the eigenvalues of the information operator \mathcal{W}

that exceed unity. \mathcal{W} is a measure of the information content of the problem and is a convenient criterion of optimization. It may be interpreted as the number of distinguishable VOD profiles for a given information operator \mathcal{W} .

2. A PRIORI INFORMATION ABOUT THE SOLUTION.

The key factor in statistical regularization of the solution of the inverse problem is the use of statistically realistic a priori information about the solution. When constructing the

covariance matrices of the VOD in the present mode, we grouped data from the world sounding network in terms of its association with three types of air masses, arctic, temperate and tropical, separated by jet streams. This classification made use of the division of the ozone field into zones with different ozone concentrations, coinciding with the distribution of air masses in the upper troposphere, made by Shalamiansky and Romashkina [3].

Ozone sounding data from 14 stations in the northern hemisphere made in the same air mass between 1975 and 1987 were used to calculate the covariance matrices and the mean ozone and temperature profiles. It was used a simple and reliable algorithm for detection of the air mass type, based on an analysis sounding data at 200 mba and 300 mba atmospheric levels [4].

Partitioning the VOD data in terms of air mass type yielded three types of mean profiles, which differed strongly from each other. Each of them is stable and homogeneous, with relatively little variability, but with a pronounced characteristic seasonal variation for each height. These mean profiles and the corresponding covariance matrices calculated for each month were used as a priori statistical information, when solving the inverse problem (1).

The covariance matrices obtained from ozone sounding were artificially extended to a height of 70 km. As will be shown, this method is most sensitive to layers above the ozone maximum, and we may therefore relax the requirements regarding a priori information at this altitudes. Thus, assuming that the correlations between the ozone concentrations in the upper layers of the atmosphere (40-70 km) will be the same as at the maximum ozone sounding heights (35-40 km), when modeling the covariance matrix for each layer of the upper atmosphere we considered correlations only with the adjoining layers. These correlations were assumed to be independent of layer number and to be the same as in the topmost ozonesonde layers. The ozone profile models used in the calculations were extended with help averaged satellite data [5]. The data were grouped in the month and latitude arrays, there is no ozone field separation on air masses at these atmospheric levels.

3. THE DIRECT OPERATOR.

The direct operator \mathcal{A} of the problem (1) was calculated for a multiple scattering spherical model of the atmosphere with allowance for atmospheric refraction, aerosol extinction, and the temperature dependence of the ozone absorption coefficients in an atmospheric model consisting of 70 uniform 1-km layers. It was used the successive calculation of the scattering order method, that was adopted to the Umkehr problem. It requires about 10 minutes of the PC AT computer time to calculate the operator \mathcal{A} for standard set of zenith angles and for the three Dobson pairs.

The stratospheric and tropospheric aerosol models [6] were used in the calculations. It was confirmed numerically the relatively slight influence of the tropospheric aerosol extinction on the Umkehr observations, but the stratospheric aerosol extinction affects dramatically on the Umkehr curve.

We used the base aerosol model of clear stratosphere in the calculations.

To test our algorithms and programs we received during the 8th soviet-american Working group the Umkehr data, which were accompanied by concurrent direct measurements of the ozone and temperature profiles with ozone sounds in Bolder [7]. The Umkehr data were obtained using Dobson automatic spectrophotometer.

Figure 1 compares the calculated Umkehr counts using concurrent ozone sound data and the real experimental Umkehr observations.

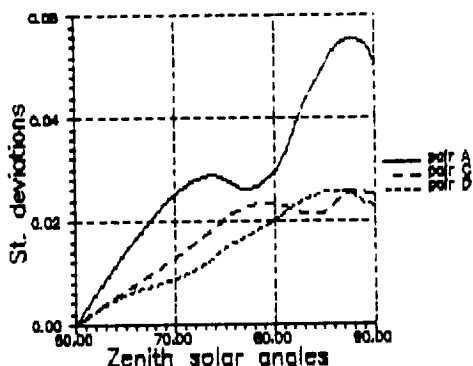


Fig.1 The standard deviations of the calculated Dobson counts from the real Umkehr data for 20 realizations.

The deviations have a tendency to increase with zenith angle and its are slightly larger for the pair A. The values of these deviations were used in the solution of the inverse problem (3), as a measurement error vector ϵ . Unfortunately, we have no real experimental information about VOD for the heights above 40 km except averaged satellite data [5], but the Umkehr measurement are sensible to the VOD for heights up to 50 km. There is some uncertainty in results of the comparison, due to this circumstance.

4. OPTIMIZATION OF THE ATMOSPHERIC LAYERS.

A preliminary selection of the optimum number of layers and their thickness in the atmospheric model used for reconstruction of the VOD may be made by analyzing the form of the operator B in Eq.(3). The retrieval method has little sensitivity to the lower layers of the atmosphere and is most sensitive in the layers above the maximum of the ozone layer (20-30 km). Thus, to maintain the stability of the Umkehr procedure, we need to make the lower layers of the

atmosphere relative to those that maximized the sensitivity of the method. Figure 2 shows the weight function of the operator B , which was calculated for the Dobson pair C.

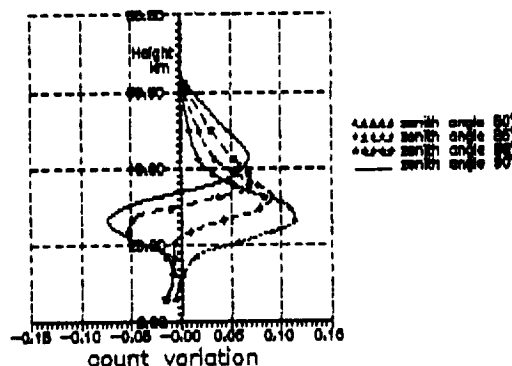


Fig.2 The weight function of the Umkehr observation for pair C.

The maximums of the weight functions for the pairs A and D are settled over and lower of the pair C maximum accordingly. It means, that every pair has its own maximum of sensitivity to the VOD, so every pair adds the information about ozone profile.

The final choice of the layers in the atmospheric model, that give the maximum vertical resolution in retrieved ozone profiles, while maintaining the stability of the Umkehr procedure was found and verified by information analysis of inverse problem (3). The information content \mathcal{H} for a fixed measurement error ϵ and the deviation of the specified VOD variation vector Δx , and the retrieved variation vector Δz were used as measures of the VOD retrieval. We were able to increase the total number of layers, in which the VOD was retrieved considerably, relative to the standard method (9 layers in the standard method and 20 in our method), and in general the reconstructed ozone profiles had high resolution. The possibility of achieving such an increase in resolution apparently results from the higher quality of the a priori information about the solution used in our method relative to that used in the short method.

5. THE RETRIEVING PROCEDURE.

To demonstrate the capabilities of the above method of retrieving the VOD from Umkehr data, we made trial retrievals of the VOD from experimental data provided by U.S. scientists. To reconstruct the VOD by our method for a specific day and

observation site, first of all we have to determine the ozone air mass in situ. Using a special approach [5], based on aerological data or charts of 200 and 300 mba isobaric surfaces we can determine the type of air mass at the station on the day of the observations. An ozonesonde database is then used to calculate the mean VOD vector \bar{z} , the temperature profile, and the covariance matrix C from Eq. (4) for the month of the observations and the air mass type.

With help direct operator A from Eq.(1), the vector \bar{v} of the logarithms of the ratios of the readings could be obtained using the calculated mean profiles of temperature and ozone. Subtracting the values of the vector \bar{v} from the corresponding values of the observation vector v_{obs} , we obtained the right-hand side Δv of Eq. (3), which the desired variation vector Δz can be found from Eq.(6) by the method described.

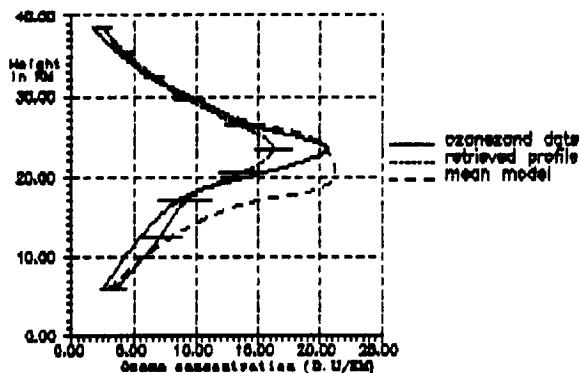


Fig.3 The comparisons of retrieved ozone profile with ozonesond data and the mean month model of ozone profile, 02.13.87 Boulder.

The figure 3 demonstrates the example of the VOD derived from Umkehr measurements at Boulder in 02.13.87. Horizontal bars display the theoretically estimated errors of the VOD reconstruction. The mean model ozone profile corresponds to a February temporal air mass.

Usually, for a real level of the experimental errors (see Fig.1), we have 3-4 eigenvectors with $\lambda_n > 1$, that give the improvement of a priori ozone profile information due to Umkehr measurements approximately in two times.

6. CONCLUSIONS.

Our conclusion regarding the relative quality

of the method is still preliminary, the body of statistics for comparison is still small and needs further expansion. But it will be noted, that the proposed statistical method increases the resolution of the ozone profiles while maintaining the stability of the computation procedure and improving the accuracy of retrieval, particularly in the lower layers of the ozone profile.

All algorithms, ozone profile database, and calculating procedures were integrated in the IBM PC compatible software. Using this software the Umkehr data could be developed on any ozone network station in the real time scale.

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