ON OPTIMAL MEASUREMENTS OF THE TRANSMISSION IN THE VISIBLE REGION ON TANGENTIAL PATHS

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The problem, of optimizing the measurements of transmissions of direct solar radiation in the visible region of the spectrum on tangential paths is studied. It is shown that the accuracy with which the optically active components of the stratosphere are reconstructed can be significantly improved with the help of an efficient arrangement of the measuring channels without an increase in the volume of measurements. The possibilities of the approach proposed are demonstrated for the example of the reconstruction of NO₂.

Introduction and formulation of the problem. One of the widely employed methods of remote determination of the vertical profiles of the content of optically active components in the earth's atmosphere is the method of inversion of the measurements of transmission of direct solar radiation on tangential paths in the visible and near infrared ranges.¹ With its help it is possible to reconstruct the content of gaseous components, such as O_3 , NO_2 , and H_2O , which are important for the radiation regime of the stratosphere, as well as the characteristics of the aerosol extinction.

An entire series of space instruments, which, though their spectral measurement range is close, differ significantly with respect to the number and position of the spectral measurement channels, has now been developed and is in operation. These instruments include the SAGE series,² and the MKS-M and MKS-6M apparatus.³ A similar instrument is the OZON-M apparatus, which makes it possible to perform measurements in the UV region of the spectrum, in addition to the visible and near-IR regions.⁴

The difference in the number and position of measuring channels in these instruments is determined either entirely by their constructional features or by the additional atmospheric problems set before the designers (MKS-M) or, as happened in the case of the SAGE apparatus, by considerations of simplicity of data processing.⁵ The accuracy and number of simultaneous measurements can significantly affect the error in the reconstruction of one or another component of the atmosphere.

Thus, based on a comparison of the accuracy of determination of NO_2 from the data obtained with the SAGE-I and OZONA-M apparatus, performed in Ref. 6, it was concluded that the accuracy of reconstruction with the help of OZONA-M is approximately 1.5 times higher. In addition, part of the gain in accuracy must be attributed to the use of the additional UV-range of measurements, while the rest of the gain in accuracy must be attributed to the fact that the number of spectral measurements is many times greater than in the case of the SAGE-I apparatus.

At the same time it should be borne in mind that a significant increase in the number of simultaneous measurements leads to just as significant an increase in the effort on data acquisition, transmission, and processing. In this connection it is of interest to investigate the possibility of efficient planning of a space experiment in which the position of each spectral channel is the solution of the problem of finding the minimum error in the reconstruction of the interesting data on the state of the atmosphere for a fixed number of channels within the given spectral range.

This work can be regarded as an illustration of the possibilities of such an approach for the example of reconstruction of NO_2 from measurements of the transmission in the visible range of the spectrum. This component was chosen as the object of study because the highest errors in reconstruction from measurements in the indicated region are obtained for it.

Mathematical model. We shall start from the following expression for the transmission of solar radiation on tangential paths for the sounding impact parameter h_1 at the wavelength λ_1 :

$$T_{ii} = \exp\left\{-2\sum_{j}\sum_{k=1}^{\infty} \alpha_{ij} x_{j} (z_{k}) \cdot G(z_{k}, h_{i})\right\}, \qquad (1)$$

where the quantity

$$G_{k1} = G(z_{k}, h_{1}) = \sqrt{(R_{E} + z_{k+1})^{2} - [n_{1}/n_{k+1}(R_{E} + h_{1})]^{2}} - \sqrt{(R_{E} + z_{k})^{2} - [n_{1}/n_{k} \cdot (R_{E} + h_{1})]^{2}};$$

describes the contribution of the spherical layer of the atmosphere with boundaries z_k and z_{k+1} to the total length of the path of a photon through a spherically symmetric atmosphere; n_k is the index of refraction of light in the *k*th layer; and, R_E is the radius of the earth. The quantities a_{1j} denote the volume extinction coefficient for the *j*th gaseous component (j = 1 denotes molecular scattering, j = 2is for ozone, and j = 3 is for nitrogen dioxide) or the value of the polynomial approximating the spectral behavior of the aerosol extinction at the wavelength λ_1 . Correspondingly, in the first case X_{jk} is the concentration of the *j*th component in the *k*th layer and in the second case X_{jk} is the coefficient in the corresponding polynomial.⁶

In writing Eq. (1) we neglected the wavelength dependence of the index of refraction in the spectral region under study $(0.4-1.02 \ \mu m)$.⁷ The structure of the obtained dependence of the transmission on the parameters of the medium makes it possible to obtain a linearized relation between the variations of the atmospheric composition and the transmission. It can be written in the following matrix form:

$$R = A\delta xG, \tag{2}$$

where

$$\{R_{11}\} = -\delta T_{11} / (2 \cdot T_{11}^{(0)}); \{A\}_{11} = \alpha_{11};$$

$$\{G\}_{k1} = G_{k1}; \{\delta x\}_{jk} = x_{jk} - x_{jk}^{(0)};$$

$$\delta T_{11} = T_{11} (x) - T_{11} (x^{(0)}),$$

where the index (0) denotes some approximation to the altitude distribution of the quantities of interest.

In Ref. 6 *a priori* statistics, obtained for the distribution of ozone in the atmosphere, was employed for solving an equation with an analogous meaning, but a different structure. It was shown that the iteration scheme of the solution converges.

For the purposes of our work the solution of Eq. (2) can be represented as follows:

$$\delta_{\mathbf{X}} = (\mathbf{A}^{\mathsf{T}}\mathbf{A})^{-1}\mathbf{A}^{\mathsf{T}}\mathbf{R}\mathbf{G}^{-1}, \tag{3}$$

which satisfies Eq. (2) in the sense of least squares.

It is obvious from the structure of the solution that the errors in the measurements can be significantly increased when they are converted into the reconstruction error, if the columns of the matrix Aare almost linearly dependent. In addition, the higher the degree of linear independence of the spectral channels, the better the reconstruction is. For this reason, the first desire is to arrange the channels so that some one component would dominate in the extinction at each wavelength. This corresponds to a diagonal matrix A. Apparently, this is the path taken in the design of the SAGE system. It makes it possible to employ the simple scheme described In Ref. 5 to invert the starting equation (1).

But the accuracy with which the atmospheric parameters sought are reconstructed is determined not only by the linear dependence of the columns of the matrix A, but also by the values of the extinction coefficients themselves. The existence of two

such factors that can, generally speaking, compete, makes the problem of choosing the optimal collection of channels nontrivial.

Assuming that the relative measurement error is independent of the altitude and wavelength it is not difficult to obtain an explicit expression for the variance of the errors in the reconstruction of the *j*th component at the *k*th altitude interval

$$\sigma_{ik}^2 = \frac{\sigma_T^2}{4} \sum_{i,1} \tilde{A}_{ji}^2 [G_{1k}^{-1}]^2, \qquad (4)$$

where $\tilde{A} = (A^T A)^{-1} A^{\tau}$ and σ_T^2 is the variance of the relative error in the measurements of the transmission. It is interesting to note that in this approximation the absolute accuracy of reconstruction does not depend on the atmospheric content of the components being reconstructed. Host often the reconstruction error summed over altitude is optimized:

$$S_{j} = \sum_{k} \sigma_{jk}^{2}.$$
 (5)

Numerical results and conclusions. To perform the calculations we employed an atmospheric model whose gaseous composition is closest to that employed for the numerical calculations described in Ref. 5. It consisted of uniform kilometer-thick layers from 10 to 75 km.

Information about the spectral dependence of the volume absorption coefficients was taken from Ref. 8 for NO_2 and Ref. 9 for O_3 .

The problem of minimizing *S* with respect to the position of the measuring channels in the given spectral interval $[\lambda_{\min}, \lambda_{\max}]$ is a problem of finding the minimum of a nonlinear function of many variables in the presence of simple bilateral limits of the type $\lambda_{\min} \leq \lambda_1 \leq \lambda_{\max}$.

It is well known that the SAGE-II variant is a seven-channel device, one channel of which is located at the center of the 0.94 μ m absorption band of H₂O. We fixed the position of this channel in the calculations, and we assumed that the H₂O content in the stratosphere was equal to zero. To solve the problem we employed the conjugate gradient method.¹⁰

We note that the obtained structure of the function to be minimized, described by the relations (4)— (5), makes it possible to perform the most difficult procedure of inverting the matrix G of large dimension once before performing the repeated calculations of Sand its gradient in the iterative search for a minimum.

The position of the measuring channels of SAGE-II was used as the starting approximation. The solution obtained is presented, together with the initial approximation, in Table I.

It turned out that by using the obtained channels instead of the SAGE-II channels it is possible to approximately triple the reconstruction accuracy. In the process the reconstruction of all other components of the atmosphere, which attenuate the radiation, is also improved, though not as much. As an illustration Fig. 1 shows the rms errors in the reconstruction of NO₂ and O₃ with $\sigma_T = 0.5\%$, which corresponds to Ref. 5.

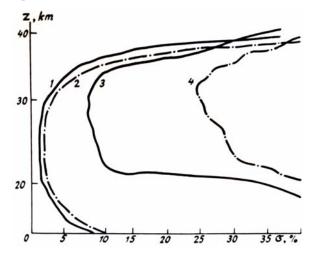


FIG. 1. The altitude profile of the theoretical relative error in the reconstruction of NO_2 and O_3 : 1), 2) for O_3 ; 3, 4) for NO_2 . The dotdashed lines correspond to the SAGE-11 variant and the solid lines correspond to the obtained solution.

Spectral channels of SAGE-II, μm		Obtained solution, µm	
1	0.385	1	0.408
2	0.448	2	0.413
3	0.453	3	0.425
4	0.525	4	0.448
5	0.600	5	0.545
6	0.94	6	0.596
7	1.020	7	0.94

TABLE I

Comparison of the data in Table I permits drawing the following conclusions.

1. For the employed parameterization of the aerosol extinction for determining NO_2 it is best to perform measurements not in the long-wavelength part of the region (near 1 μ m), where the aerosol extinction dominates, but rather in the short-wavelength part, where the extinction is stronger.

2. To increase the accuracy of reconstruction of NO₂ the additional measurements in the NO₂ band should be performed not in the pairs "maximum-minimum" (0.448 and 0.453 μ m in the SAGE-II variant) but rather at the additional maxima in the wavelength dependence of the volume absorption coefficient.

Figure 2 illustrates the second position well. (We note that a channel additional to the 0.448 μ m channel was introduced into SAGE for convenience of processing.²)

The function (5) being minimized has many extrema. This follows, in particular, from the complicated character of the spectral dependence of the absorption coefficient of NO₂. However, as follows from numerical experiments, the main gain in accuracy in the determination of NO₂ is achieved not by moving the position of the channels from one local maximum of this dependence to another, but rather by shifting the "aerosol" channel^S into a shorterwavelength region.

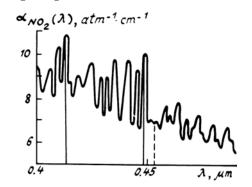


FIG. 2. The spectral dependence of the volume absorption coefficient of NO_2 . The broken vertical line shows the position of the additional channel introduced into the SAGE-II variant. The solid vertical lines mark the position of the channels obtained.

To verify that the system of channels obtained works, we performed a numerical experiment on the reconstruction of the composition of the atmosphere. For the starting approximation we employed an atmosphere with no aerosol, O_3 , and NO_2 , in which light is attenuated only as a result of the Rayleigh scattering. The errors in the reconstruction of NO_2 and O_3 after ten iterations are presented in Fig. 3.

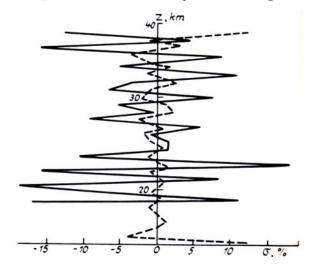


FIG. 3. The altitude profile of the relative errors in the reconstruction of NO_2 (solid lines and O_3 (broken lines), obtained in the numerical experiment using the optimal measuring channels.

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