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Potential Accuracies of Retrieving the Vertical Profiles of Atmospheric Parameters (Satellite-Based Transmittance Method): 1. Ozone and Nitrogen Dioxide Contents

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Abstract—Potential accuracies of retrieving the ozone and nitrogen dioxide vertical profiles from slant-path atmospheric transmittance measurements with the SAGE-III spectrometer launched aboard the Meteor-3M satellite are analyzed on the basis of closed-loop numerical experiments. All conditions of the numerical experiments, namely, the initial data set, methods of interpretation and parametrization of the spectral dependence of the aerosol extinction coefficient, are described. It is shown that the potential accuracies of retrieval of the ozone and nitrogen dioxide vertical profiles depend significantly on the description of the spectral dependence of the atmospheric aerosol extinction coefficient. The mean error of ozone retrieval at heights between 12 and 75 km ranges from 0.27 to 0.75%, depending on the parametrization type. The ultimate accuracy of nitrogen dioxide retrieval in the height range between 20 and 45 km is 0.3–4.6%. The retrieval errors are minimal when optimal parametrizations of aerosol extinction are used, namely, when the aerosol extinction coefficient variations are expanded into four or five eigenvectors of the quasi-empirical basis. The retrieval errors obtained on the basis of the optimal parametrizations are lower than those obtained on the basis of the parametrization proposed by Lumpe *et al.* by a factor ranging from two to three for ozone and by a factor of about ten for nitrogen dioxide.

INTRODUCTION

In recent years, the global aerosol and gas compositions of the atmosphere have been intensively studied by using satellite measuring techniques [1, 2]. These techniques make it possible to monitor space–time variations and long-term trends in the atmospheric contents of aerosols and minor gases, to reveal the interconnections of the minor-gas and aerosol contents with solar activity, and to improve and validate various numerical models of the atmosphere.

The method based on slant-path measurements of the atmospheric extinction of solar (and also lunar and stellar) radiation can be regarded as the most exact satellite method [3–8]. The advantages of this method are due to its simplicity (Bouguer's law), high informativeness, high accuracy (no worse than 0.1%) of solar radiation measurements, and ease of solving the inverse problem.

The errors of determining the vertical profiles of different gases and aerosol extinction by this method depend on many factors: the instrumentation performance (signal-to-noise ratio, angular aperture, numbers and positions of spectral channels, etc.); errors in specifying prior data (mainly, the absorption coefficients of the gases); and the procedure of profile retrieval. The errors are instrumentation-dependent and are thoroughly controlled prior to and during satellite measurements.

The method of solving the inverse problem can significantly affect the accuracy of the satellite method (depending on algorithms of measured-data inversion, methods of aiming-height determination, consideration of the Sun's limb darkening). In [9–11], it is shown that the parametrization of the aerosol extinction spectral behavior is necessary for any retrieval procedure and that the parametrization type can significantly influence the accuracy of vertical ozone profile retrieval, especially for the lower stratosphere and the upper troposphere. Obviously, the parametrization also controls the accuracy of determining the spectral dependence of the aerosol extinction coefficient, which can vary dramatically in the stratosphere, and, as a consequence, determines the accuracy of the solution of the subsequent inverse problem relating to the retrieval of aerosol microphysical characteristics in the stratosphere. In [12], different approaches to this problem were analyzed, and a method of optimal parametrization of the spectral aerosol extinction behavior was proposed. This method is based on the A.M. Oboukhov method of the expansion of a random function in terms of a quasi-empirical orthogonal basis [13].

In this work, the limiting possibilities of the transmittance method are analyzed through numerical experiments based on the aerosol extinction spectral behavior preset in different forms. To isolate and study the effect of the aerosol-extinction parametrization on the accuracy of determining gas concentrations, exact input data are used for the retrieval procedure. The estimates thus obtained characterize the minimum errors of the transmittance method. This work describes the characteristic features of the numerical simulation of the joint Russian–American satellite experiment with the SAGE-III instrumentation installed aboard the Russian satellite Meteor-3M, launched on December 10, 2001. The potential accuracies of retrieving the vertical profiles of ozone and nitrogen dioxide are analyzed for different parametrizations of the aerosol extinction spectral behavior. In [14], the potential accuracies of retrieving the vertical profiles and the spectral behavior of the aerosol extinction coefficient are examined.

METHOD OF NUMERICAL EXPERIMENTS

Model Profiles

The vertical profiles were preset in the numerical experiment as random functions with specified mean and covariance matrices. The climatically mean midlatitudinal winter O_3 profile and the global mean NO_2 profile were taken as the mean O_3 and NO_2 profiles, respectively. The model covariance matrices were characterized by a correlation radius of 5 km and relative rms deviations of 60 and 100% for O_3 and NO_2, respectively. The spectral and height behaviors of the aerosol extinction coefficient were taken in accordance with the stratospheric aerosol statistical model presented in [12]. We note that this model is characterized by a high variability (by several orders of magnitude) of the aerosol extinction coefficient and by different types of the spectral behavior of this coefficient. The atmospheric molecular radiative model used in this work is described in [8]. The numerical experiments included 500 random realizations of the parameters indicated above.

Parametrization of the Spectral Dependence of the Aerosol Extinction Coefficient

In this work, three following parametrizations are considered (see [12] for details):

(1) linear optimal parametrization:

$$\sigma(\lambda) = \langle\sigma(\lambda)\rangle + \sum_{p=1,n} a_p f_p(\lambda), \qquad (1)$$

(2) logarithmic optimal parametrization:

$$\ln\sigma(\lambda) = \langle\ln\sigma(\lambda)\rangle + \sum_{p=1,n} a_p^L f_p^L(\lambda), \qquad (2)$$

(3) parametrization by Lumpe *et al.* [7] (hereafter, the Lumpe parametrization), usually regarded as one of the most exact modes of parametrization:

$$\ln\sigma(\lambda) = \mu_0 + \mu_1\ln\lambda + \mu_2(\ln\lambda)^2. \qquad (3)$$

In expressions (1)–(3), λ is the wavelength; $\sigma(\lambda)$ is the aerosol extinction coefficient; a_p, a_p^L, and μ are the parametrization coefficients; $f_p(\lambda)$ and $f_p^L(\lambda)$ are the eigenvectors of the spectral covariance matrix for the aerosol extinction coefficient and for its logarithm, respectively; and the angular brackets denote averaging. In optimal parametrizations (1) and (2), the number of the terms in the expansion in the orthogonal basis was varied.

Inverse Problem Solution

To solve the problem, a two-step algorithm is used. At the first step, the vertical profile of the total coefficient of atmospheric extinction is retrieved for each wavelength (a spectral measurement channel). A random noise with a level of 0.03%, which approximately corresponds to the noise level characteristic of the SAGE-III satellite spectrometer, is added to the atmospheric transmittance values. At the second step, the atmospheric gas compositions and the parameters of aerosol extinction are retrieved from each spectrum of the total extinction coefficient taken at an individual height level. At the two steps, the algorithm based on the well-known method of statistical regularization is used [15]. At the first step, the prior information includes the model covariance matrices and the mean profiles of the total extinction coefficient computed on the basis of the set of profiles under testing. At the second step, the climatically mean gas concentrations, mean coefficients, and covariance matrices of the coefficients in the aerosol extinction parametrization computed over the entire ensemble of random realizations are used for each height. The cross covariances of various atmospheric parameters are not taken into account. In order to determine the ultimate retrieval errors associated only with the aerosol-extinction parametrization, exact values of the total extinction coefficient rather than its retrieved values are used as the input data at the second step of the algorithm. However, at the second step of the algorithm of solving the inverse problem, the weights of the measurements performed in different spectral channels are determined by the errors of total extinction coefficient retrieval at the first step. This procedure allows us to take into account those spectral channels that give information during measurements at each tangent height and to exclude (through small weights) opaque and totally transparent measurement channels. Such an approach allows the determination of the minimum errors in the solution of the inverse problem, i.e., allows the determination of the ultimate accuracy of retrieving different atmospheric parameters.

In the numerical experiments, the spectral measuring scheme corresponding to the SAGE-III satellite instrumentation with one channel operating at 1500 nm and 80 channels operating within the spectral range from 290 to 1030 nm is taken.

Mean errors in the ozone and nitrogen dioxide retrieval for specified height ranges on the basis of different parametrizations of the aerosol extinction spectral behavior

Parametrization	O_3, 12–75 km			NO_2, 20–45 km		
	absolute error, cm^{-3}	mixing ratio, g/g	relative error, %	absolute error, cm^{-3}	mixing ratio, g/g	relative error, %
Linear optimal, 4 parameters	0.62×10^{10}	0.61×10^{-8}	0.65	0.16×10^{7}	0.94×10^{-11}	1.34
Linear optimal, 5 parameters	0.57×10^{10}	0.35×10^{-8}	0.42	0.10×10^{7}	0.33×10^{-11}	0.38
Logarithmic optimal, 4 parameters	0.97×10^{10}	0.40×10^{-8}	0.27	0.21×10^{7}	0.30×10^{-11}	0.30
Lumpe	0.20×10^{11}	0.14×10^{-7}	0.75	0.24×10^{8}	0.66×10^{-10}	4.6

Statistical Analysis of the Results

To analyze the results of numerical simulation, including 500 sets of the retrieved profiles for each of the three aerosol parametrizations, the vertical profiles of the mean errors for each of the atmospheric parameters, height-mean errors for each random realization, and total mean errors over all realizations are computed. These characteristics are computed for the concentrations and mixing ratios of gases and also for the relative errors. For aerosol, the absolute and relative mean errors are computed. In addition, the following characteristics are computed for aerosol: the spectral behavior of the errors for each atmospheric state and for each tangent height and also the spectral behavior of the errors over all realizations for each tangent height and over all tangent heights for each realization. For each gaseous component, a specific height range is used to compute the mean errors. A height step of 1 km is used in the computations.

RESULTS OF NUMERICAL EXPERIMENTS

Mean Errors in Ozone and Nitrogen Dioxide Retrieval

In the table, absolute and relative errors in the retrieved concentrations and mixing ratios of ozone and nitrogen dioxide are averaged over the height range and realization set. These data are computed for different parametrizations of the spectral behavior of aerosol extinction.

An analysis of the data listed in the table leads to the following conclusions.

(1) The ultimate accuracy of ozone retrieval is very high for each parametrization. The mean relative error ranges between 0.27 and 0.75% for the height range from 12 to 75 km. We note that the error of ozone retrieval for lower atmospheric layers increases dramatically independent of the parametrization. This effect is associated with a low transmittance of the troposphere in the absorption bands of ozone. For the height layer from 45 to 50 km, the error of retrieval has a local maximum, because the measuring scheme of the SAGE-III instrument contains no optimal spectral channels for these heights.

(2) The ultimate accuracy of nitrogen dioxide retrieval for the height range from 25 to 45 km is also very high and is equal to 0.30–4.6%, depending on the parametrization. However, the errors increase dramatically beyond the height range between 20 and 35 km because of a significant depletion of nitrogen dioxide and the resulting decrease of the NO_2 contribution to the total absorption of solar radiation. We note that, although NO_2 contributes to radiation absorption much less than O_3, the errors in the ozone and nitrogen dioxide concentrations are close to each other. This closeness is due to the fact that the 20–45-km layer is chosen to analyze NO_2 retrieval and by a high accuracy of determining the aerosol extinction in the range of NO_2 absorption (in the vicinity of 440 nm) with the use of the optimal parametrizations [14].

(3) The Lumpe parametrization always leads to greater (in comparison with the optimal parametrizations) errors: two to three times for O_3 and about ten times for NO_2. For the height range under consideration, the relative errors of ozone retrieval are equal to 0.42% for the optimal linear (five parameters) parametrization and 0.27% for the optimal logarithmic (four parameters) parametrization. These errors are significantly smaller than the error characteristic of the Lumpe parametrization (0.75%). For nitrogen dioxide, the differences are still more significant, because NO_2 contributes to the solar radiation extinction less than O_3 does and solar radiation extinction by NO_2 in the vicinity of 440 nm is comparable with the mean aerosol extinction. As a consequence, NO_2 retrieval is dramatically influenced by the accuracy of the aerosol extinction parametrization in the NO_2 absorption band. The mean relative errors in NO_2 retrieval with the linear (five parameters) and logarithmic (four parameters) optimal parametrizations are equal to 0.38 and 0.30%, respectively, while the error of the results obtained with the Lumbe parametrization is much higher and is equal to 4.6%.

Variability of Errors

The height-mean errors of O_3 and NO_2 retrieval are not the same for different random realizations. For the

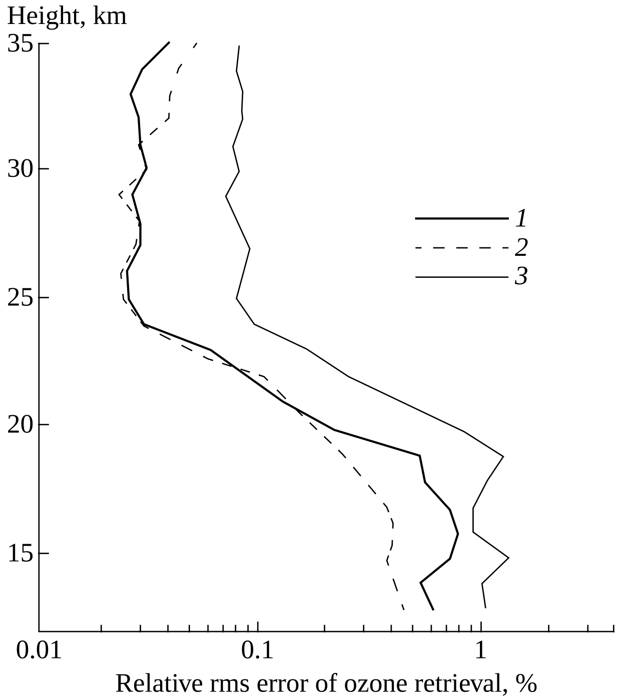

Fig. 1. Vertical profiles of the mean relative error of ozone retrieval: (*1*) the logarithmic optimal parametrization with four parameters, (*2*) the linear optimal parametrization with five parameters, and (*3*) the Lumpe parametrization of the aerosol extinction spectral dependence.

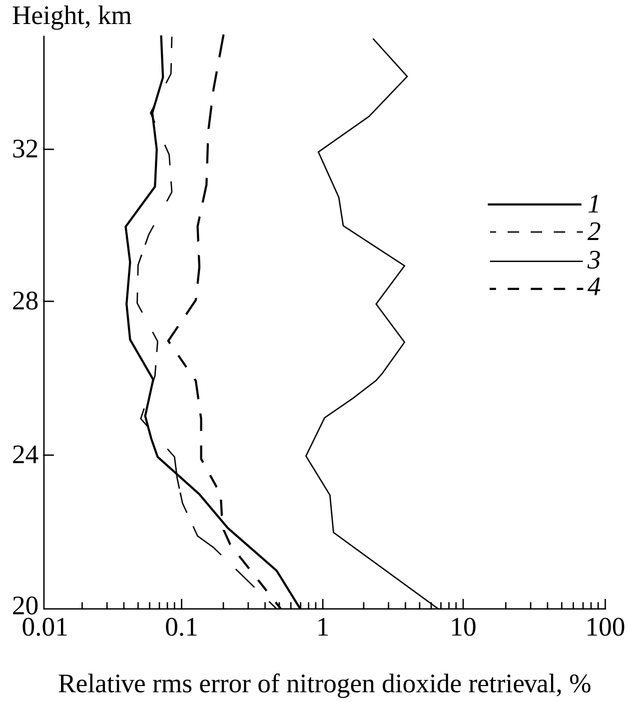

Fig. 2. Vertical profiles of the mean relative error of nitrogen dioxide retrieval: (*1*) the logarithmic optimal parametrization with four parameters, (*2*) the linear optimal parametrization with five parameters, (*3*) the Lumpe parametrization, and (*4*) the linear optimal parametrization with four parameters.

majority of the realizations, the mean errors of ozone retrieval with the optimal parametrizations of aerosol extinction for the height range from 12 to 35 km is equal to 0.1–1.0%. For individual realizations constituting about 10% of the total number of the realizations, these errors reach 2–4%. As a rule, high errors are observed for the same realizations when different parametrizations are applied to the atmospheric layer between 12 and 35 km, where the effect of aerosol extinction is maximum. For these realizations, the errors in aerosol-extinction retrieval are maximal for the spectral range corresponding to those of the measuring channels that are characterized by a significant ozone absorption. Thus, the difficulties in the retrieval of the vertical ozone profiles for the height range between 12 and 35 km are primarily caused by the behavior of aerosol extinction and by the accuracy of its determination in solving the inverse problem. The use of the Lumpe parametrization extends the retrieval-error range, and the number of realizations with errors exceeding 1% increases by a factor of about three.

Analogously, the height-mean errors of NO_2 retrieval are different for different realizations. All examples of NO_2 retrieval demonstrate the advantage of the linear optimal parametrization. This conclusion can be explained by the ability of this parametrization to closely approximate the aerosol extinction behavior in the 440-nm spectral range characteristic of radiation absorption by nitrogen dioxide. On the other hand, high errors in the NO_2 concentration retrieved on the basis of the Lumpe parametrization are caused by the errors in retrieving the aerosol extinction behavior in the NO_2 absorption band.

Vertical Profiles of the Mean Errors of Retrieval

Figures 1 and 2 present the vertical profiles of the relative errors in the O_3 and NO_2 concentrations retrieved on the basis of different parametrizations of the aerosol extinction spectral behavior and averaged over 500 realizations for the stratospheric region characterized by a significant aerosol effect on the extinction of solar radiation.

Figure 1 shows that the ultimate accuracy of ozone retrieval for the atmospheric layer 12–35 km is very high and reaches 0.03–0.8% for the optimal parametrizations. The Lumpe parametrization allows ozone retrieval with an error of 0.1–1.3%. For heights below 20 km, the linear parametrization with five parameters gives the highest accuracy. For heights above 20 km, the logarithmic parametrization with four parameters and the linear parametrization give virtually the same retrieval accuracies.

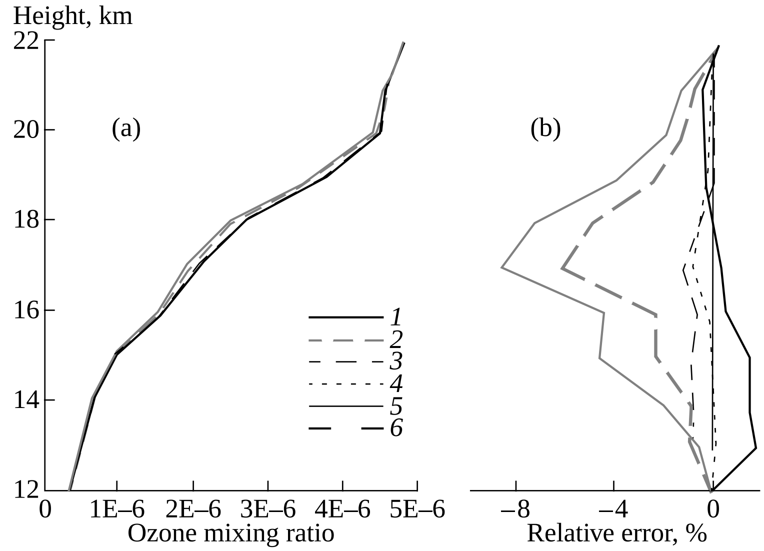

Fig. 3. Vertical profiles of (a) the retrieved ozone mixing ratio and (b) the relative retrieval error: (*1*) the logarithmic optimal parametrization with four parameters; (*2*), (*3*), and (*4*) the linear optimal parametrizations with three, four, and five parameters, respectively; (*5*) the Lumpe parametrization; and (*6*) the original profile.

An analysis of the relative errors in NO_2 (Fig. 2) distinguishes the following main features.

(1) The optimal parametrizations offer a significant advantage over the Lumpe parametrization, namely, for heights of 20 to 35 km, the errors for the former and latter vary between 0.05 and 0.7% and between 1 and 7%, respectively.

(2) For different heights, different optimal parametrization are preferable, namely, the logarithmic one is preferable for heights above 24 km and the linear one with five parameters is preferable for heights below 24 km.

Examples of Retrieval of the O_3 and NO_2 Concentrations

To gain a better understanding of the listed peculiarities of height variations in the errors of the O_3 and NO_2 concentration retrieval, several examples of retrieval performed for individual realizations are considered below. Figure 3 presents an example of retrieval of the ozone concentration profile and gives the profiles of errors of retrieval performed on the basis of different parametrizations of aerosol extinction. The errors of retrieval performed on the basis of the Lumpe parametrization reach 8%. The linear optimal parametrizations decrease the error to 1% as the number of parameters increases from three to five. The maximum error of retrieval on the basis of the logarithmic optimal parametrization with four parameters is equal to 2%. The example presented in Fig. 3 corresponds to an atmosphere heavily turbidized by aerosol and exhibits a strongly pronounced effect of the aerosol-extinction parametrization, thus demonstrating the results of retrieval with the use of different parametrizations.

An analysis of the errors in the aerosol extinction spectral behavior retrieved on the basis of different parametrizations for height layers under consideration shows that the peculiarities described above are caused by a deficiency of the Lumpe parametrization for retrieval of the aerosol extinction in the 600-nm range characteristic of radiation absorption by ozone [14].

Figure 4 presents an example of the effect of the aerosol extinction parametrization on retrieval of the NO_2 concentration vertical profile. The error of retrieval performed on the basis of the Lumpe parametrization reaches 6%, while the logarithmic optimal parametrization with four parameters and the linear optimal parametrization with five parameters allow retrieval with an accuracy better than 1%.

PRINCIPAL CONCLUSIONS

In this paper, the framework and peculiarities of numerical experiments focused on the retrieval of the vertical profiles of the ozone and nitrogen dioxide concentrations and the aerosol extinction coefficient are described in detail. These experiments were aimed at clarifying the limiting possibilities of the SAGE-III instrumentation installed aboard the Russian satellite Meteor-3M. The numerical experiments lead to the following conclusions.

(1) The ultimate accuracy of ozone concentration retrieval for the height range from 12 to 75 km on the basis of the SAGE-III instrumentation is very high. The mean retrieval error ranges between 0.27 and 0.75%, depending on the aerosol-extinction parametrization. The use of different optimal parametrizations proposed in [12] for description of the aerosol extinction spectral

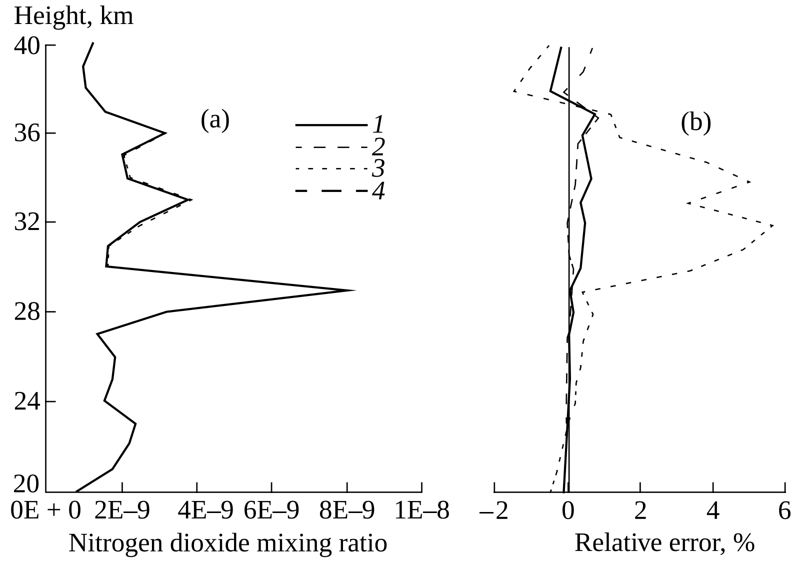

Fig. 4. Vertical profiles of (a) the retrieved nitrogen dioxide mixing ratio and (b) the relative retrieval error: (*1*) the logarithmic optimal parametrization with four parameters, (*2*) the linear optimal parametrization with five parameters, (*3*) the Lumpe parametrization, and (*4*) the original profile.

behavior and based on the expansion of the spectral coefficient of aerosol extinction into four or five vectors of the empirical orthogonal basis makes it possible to raise the accuracy usually by a factor of 2 to 3 as compared to the accuracy attained with the traditional Lumpe parametrization.

(2) The ultimate accuracy of nitrogen dioxide retrieval in the height range from 20 to 45 km is equal to 0.3–4.6%, depending on the parametrization, and the optimal parametrizations of the aerosol extinction spectral behavior are preferable. The error of retrieval on the basis of the Lumpe parametrization, which is now accepted as one of the most exact parametrizations, can exceed the error of retrieval on the basis of the optimal parametrizations by a factor ranging between three and ten.

(3) The above features of retrieval of gas concentrations are due to the dependence of the ozone and nitrogen dioxide retrieval errors on the errors in the description of the aerosol extinction spectral behavior. When the errors in the aerosol extinction retrieval performed on the basis of the Lumpe parametrization are significant, i.e., in the spectral ranges of radiation absorption by ozone and nitrogen dioxide, the errors of retrieval of the concentrations of these gases increase.

(4) The linear optimal parametrization is most promising for the interpretation of transmittance measurements with the SAGE-III instrumentation. We note that, owing to its simple linear form, this parametrization presents no difficulties in solving the complex inverse problem—the simultaneous retrieval of the profiles of ozone, nitrogen dioxide, and the spectral aerosol extinction coefficient. The logarithmic parametrization sometimes provides a high accuracy of retrieval; however, it takes a significantly longer time to solve a nonlinear inverse problem because of a slow convergence of the algorithm. In addition, the procedure based on the logarithmic parametrization gives no possibility for elimination of the solutions corresponding to local rather than global minima of the minimized functional. Such a solution may prove to be indefinitely far from the true solution. The last remark relates also to the Lumpe parametrization, because this parametrization also uses the operation of taking the logarithm and thus leads to the necessity of solving a nonlinear inverse problem.

The above analysis of the ultimate accuracy of ozone and nitrogen dioxide retrieval allows us to establish the limit of retrieval errors that should be approached in designing a more sophisticated algorithm for processing data of real satellite measurements.

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