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REMOTE SENSING OF ATMOSPHERE, HYDROSPHERE, AND UNDERLYING SURFACE

Multiparameter Technique for Interpreting Ground-Based Microwave Spectral Measurements in the Problem of Ozone Vertical Profile Retrieval

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Abstract—The algorithm for interpreting ground-based measurements of the brightness temperature of downwelling microwave radiation in absorption lines traditionally used for to retrieve ozone vertical profiles is described. The inverse problem is formulated as a multiparameter with respect to ozone vertical profile (target parameter), as well as vertical profiles of the temperature, pressure, water vapor content, and cloud liquid water (controlled parameters). This approach allows one to use independent measurements of atmospheric parameters in different altitude ranges (if available) in any combinations and accounting for physical relationships between the parameters (e.g., the hydrostatic equation for temperature and pressure). Error estimates for retrieving the mean ozone concentration in the 22–30-, 30–40-, 40–50-, and 50–60-km layers are presented for summer and winter conditions (for different tropospheric total water content) and different scenarios of interpreting the downwelling microwave radiation measurements in the 110-GHz ozone absorption line.

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INTRODUCTION

Remote sensing of the ozonosphere at millimeter waves (microwave sensing) from the Earth's surface enables the long-term monitoring of the ozone vertical profile in the stratosphere and mesosphere (at altitudes of about 20–70 km) at a preset geographical point with a high temporal resolution almost independently of the weather conditions [1–4]. At present, these microwave measurements are carried out at some stations of the Network for the Detection of Atmospheric Composition Change (NDACC) International Network [5]. In Russia, ozone microwave monitoring has been carried out for a long time at the Physical Institute of the Russian Academy of Sciences and Institute of Applied Physics of Russian Academy of Sciences (IAP RAS, Nizhny Novgorod) [6, 7].

A widely used technique for processing the microwave spectra for the purpose of ozone profile retrieval consists of estimating the so-called tropospheric absorption and distinguishing the stratospheric component of the radiation, which contains information on the vertical ozone distribution in the stratosphere and mesosphere [1, 2]. In this approach, the optical depth, which is caused by the only ozone absorption, often acts like a measured parameter.

The need for data on the temperature and pressure in the stratosphere and mesosphere and microwave radiation attenuation in the atmosphere is one of the key problems in ground-based microwave ozone sensing. The tropospheric absorption is usually estimated from measurements in the so-called reference spectral channels, which are characterized by high-frequency tuning out of the center of the line (of several hundreds of megahertz), in order to neglect the radiation formed in the stratomesosphere.

In this work, we describe and analyze a new multiparameter approach to solving the problem of microwave ozone sensing. The tropospheric attenuation is considered implicitly and simultaneously with the retrieval of the vertical ozone distribution. As a consequence, there are reduced requirements for measurements in the reference channels. In this case, the suggested approach allows the use of all available data on the distribution of atmospheric parameters at various altitudes in any combination, e.g., radiosonde and satellite, and accounting for the correlations between the atmospheric parameters, e.g., the hydrostatic equation for the temperature and pressure.

The algorithm was developed for interpreting spectra in the ozone absorption lines 110.836 and 142.176 GHz recorded by the corresponding instrumentation that was designed at IAP RAS and operates at the Physical Department of St. Petersburg State University [8], as well as by the GROMOS instrumentation operating at Bern University, Switzerland [9]. The results presented in this work have been obtained for the first of the above microwave instrumentation.

INSTUMENTATION AND EXPERIMENT

The microwave ozonometer in operation at the Physical Department of St. Petersburg State University is a heterodyne radiometric detector of the millimeter wavelength range and a multichannel spectral analyzer. The device records a spectrum of the downwelling thermal radio radiation (in terms of the brightness temperature) in the 110.836-GHz ozone absorption line. The total analyzing band of the signal under study is 240 MHz with the 1–10-MHz spectral resolution at a total of 31 spectral channels. The device is calibrated by measurements of radiation of two black bodies, i.e., a heated one with the temperature of the ambient air and a cold one with the boiling temperature of liquid nitrogen. The line-of-sight zenith angle is 70°.

The device operates in the automated quasi-continuous mode. A spectrum is recorded and based every 100 s. The preliminary stage of data processing includes the quality check of the spectra (on the basis of numerical criteria), data averaging over the specified time intervals, and the estimation of random errors of averaged values of the brightness temperature. The main stage of data processing includes the preparation of the results of independent (radiosonde and satellite) measurements of atmospheric parameters for use in algorithm for solving the inverse problem, as well as the direct solution of the inverse problem of ozone profile retrieval.

PROBLEM STATEMENT AND ANLYSIS OF WEIGHT FUNCTIONS

The initial relationship for the considered inverse problem is the integral form of the microwave radiation transfer equation in the Rayleigh–Jeans approximation for the brightness temperature recorded by the device:

$$T_b(\nu) = \int_0^{s_0} T(s)\alpha(\nu, s)\exp\left[-\int_0^{s}\alpha(\nu, s')ds'\right]ds + T_0\exp\left[-\int_0^{s_0}\alpha(\nu, s)ds\right], \tag{1}$$

where $T_b(\nu)$ is the brightness temperature of downwelling radiation at the frequency ν, s is the coordinate along an optical path, s_0 is the conventional upper boundary of the atmosphere, T is the air temperature, α is the absorption coefficient, and T_0 is the brightness temperature of the cosmic background radiation (2.7 K). The radiation absorption by oxygen, water vapor, warm clouds, and ozone is taken into account. The linearized form of the transfer equation can be written as follows:

$$\delta T_b(\nu) = \sum_{i=1}^{N}\int_0^{s_0} F_i(\nu, s)\delta x_i(s)ds, \tag{2}$$

where δ is the variation (summing over the number of unknown profiles of different atmospheric parameters, designated as x_i) and F_i indicates the kernels of the linearized equation (weight functions), which corresponds to variations in different atmospheric parameters. In the considered case, the total number of unknown parameters is equal to five and include the temperature, pressure, water vapor content, cloud liquid water, and ozone content profiles. Sometimes, it is easier to analyze the weight functions that correspond to relative variations in parameters, but not absolute. In this case, the linearized equation can be written as

$$\delta T_b(\nu) = \sum_{i=1}^{N}\int_0^{s_0} F_i'(\nu, s)\frac{\delta x_i(s)}{x_m(s)}ds, \tag{3}$$

where the subscript m denotes the mean value of a parameter and F' is the weight function corresponding to relative variations in parameters ($F'(\nu, s) = F(\nu, s)x_m(s)$). The difference weight functions defined as the difference in weight functions (3) at neighboring measurement frequencies are the most illustrative. The analysis of the weight functions allows estimation of the altitude range for parameter measurement, the attainable vertical resolution, and the information content of measurements relative to the values of the target parameter at different altitudes.

The difference weight functions of the profiles of three parameter, i.e., the ozone number density, temperature, and pressure, are shown in Fig. 1, from which it is evident that the data on ozone content can be obtained for altitudes of about 20–65 km.

The halfwidth of the weight functions, which correspond to frequencies near the center of the line, is 15–20 km and is about 10 km at frequencies in the line wing. Thus, preliminary estimates of the vertical resolution yield values of about 10 km in the stratosphere and 15–20 km in the mesosphere. Let us note that the weight functions are monotonic in the troposphere and close in value for different channels of the microwave detector; they are not shown in Fig. 1. These values differ significantly in different channels at stratosphere–mesosphere altitudes. The weight functions for the profile of relative variation in the ozone number density are opposite in sign; however, they are close in absolute value and shape.

The weight functions for the profile of relative variation in the temperature have clearly pronounced local peculiarities in both negative and positive regions of their values. These local peculiarities are displaced upward to several kilometers in comparison with altitudes of the maxima of weight functions for other parameters (ozone content, pressure). The absolute values of the weight functions for the profiles of relative variations in the temperature and pressure are comparable to those for the profile of the relative variation in the ozone number density in the order of magnitude. This implies that, e.g., a 5% uncertainty in the temperature or pressure values deteriorates the relative accuracy of the ozone concentration retrieval by about 5%; hence, high requirements should be imposed on the accuracy of assigning the temperature and pressure values.

To change to the vector-matrix representation of equations, let us introduce the following cumulative vector of variations in target parameters:

$$\begin{aligned}\delta\mathbf{x}^{+} = {} & (\delta T(z_1), \delta T(z_2), \ldots, \delta T(z_L),\\ & \delta p(z_1), \delta p(z_2), \ldots, \delta p(z_L),\\ & \delta q(z_1), \delta q(z_2), \ldots, \delta q(z_L),\\ & \delta w(z_1), \delta w(z_2), \ldots, \delta w(z_L),\\ & \delta n(z_1), \delta n(z_2), \ldots, \delta n(z_L)),\end{aligned} \tag{4}$$

where z are the altitude levels enumerated from 1 to L, T is the temperature, p is the pressure, q is the water vapor content, w is the cloud liquid water, n is the ozone concentration, and + indicates transposition.

All available data on the atmosphere parameters (a priori statistical, measurement results corresponding to the time and site of a specific event of microwave sensing, in their presence) and correlations between the parameters should be included in the algorithm for solving the inverse problem. These data (extra conditions) can be formally represented as a set of independent, generalized measurements. Thus, the inverse problem is formulated as the set of vector-matrix equations

$$\begin{cases}\delta\mathbf{y} = \mathbf{A}\delta\mathbf{x},\\ \delta\mathbf{r}_1 = \mathbf{C}_1\delta\mathbf{x},\\ \ldots\ldots\ldots\\ \delta\mathbf{r}_\mathbf{M} = \mathbf{C}_\mathbf{M}\delta\mathbf{x}.\end{cases} \tag{5}$$

Here, the first equation is the vector-matrix analog of the linearized radiation transfer equation (2), and the following M vector-matrix equations describe the complementary measurements of atmospheric parameters or extra conditions imposed on them in linearized form. The vector $\delta\mathbf{y}$ is the vector of variations in the brightness temperature relative to the mean values calculated based on the mean profiles of the atmospheric parameter, $\mathbf{A}$ is the linearized integral operator of the direct problem formed from the values of weight functions with corresponding quadrature coefficient, $\delta\mathbf{r}$ is the vector of variations in the results of generalized measurements relative to their mean

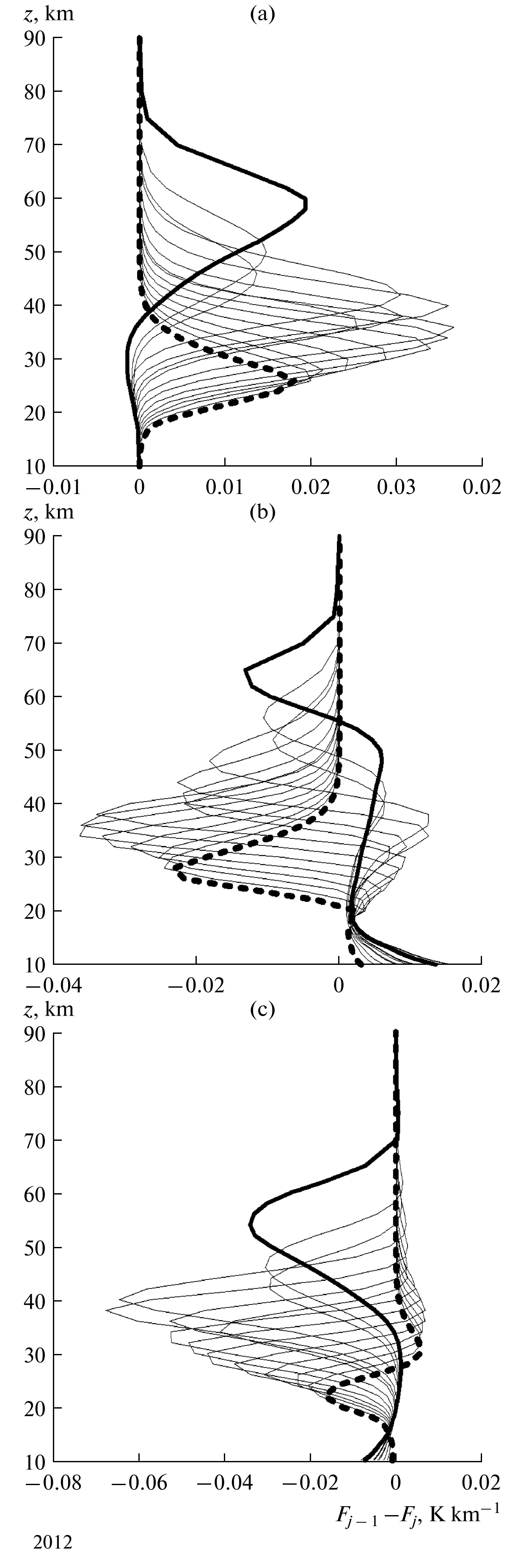

Fig. 1. Difference weight functions $F_{j+1} - F_j$ (j is the number of spectral channel) for the profile of relative variation in the (a) ozone number density, (b) temperature, and (c) pressure. The AFGL86 model of the atmosphere, midlatitudes, summer. Heavy dashed curve corresponds to the values in the line wing, the heavy curve corresponds to the center of the ozone absorption line, and thin curves correspond to intermediate frequencies.

Table 1. Scenarios for calculating error matrix

Description of the scenario	Season	
	Summer	Winter
Standard: radiosonde measurements of pressure, temperature, and humidity; satellite measurements of temperature; hydrostatic equilibrium approximation	S1	W1
Standard without radiosonde measurements	S2	W2
Standard without satellite measurements	S3	W3
Standard without accounting for the hydrostatic equilibrium	S4	W4
Standard without all additional conditions	S5	W5

Table 2. Measurement errors of mean ozone concentration (in percentage of a priori values) in layers of 8–10 km in depths and total ozone content in 22–60-km altitude range. Averaging of microwave measurements of brightness temperature during 1 h (36 individual spectra). σ_a is the a priori uncertainty of the mean ozone concentration in percentage of the a priori values

Layer, km	Scenario					σ_a
	W1/S1	W2/S2	W3/S3	W4/S4	W5/S5	
22–30	7.0/13.8	7.7/14.2	8.0/13.9	9.7/14.3	15.2/22.0	42
30–40	5.3/7.3	9.1/10.4	6.0/7.9	12.9/9.7	16.3/21.1	41
40–50	13.1/16.1	14.8/17.8	14.5/16.4	22.8/23.7	23.4/27.9	41
50–60	22.7/27.2	23.0/27.6	23.2/27.5	27.0/29.7	27.4/31.6	41
60–70	26.4/33.6	26.5/33.6	26.7/33.6	29.3/34.4	29.7/35.3	42
22–60	3.5/7.7	5.6/8.9	4.8/8.0	3.5/7.8	9.4/16.7	33

values, and **C** is the linearized operator that describes the generalized measurements.

This approach to solving the inverse problem (complex, with the use of different types of extra conditions in the form of generalized measurements) was successively used in the interpretation of satellite measurements of outgoing radiation in experiments with the CRISTA instrumentation and was described in [10], where the equation for iteration solution was given. In particular, it should be noted that one of the extra conditions considers the a priori covariance matrix of parameters, which corresponds to the standard method of statistical regularization.

ANALYSIS OF ERRORS OF THE INVERSE PROBLEM SOLUTION

The main factors that influence the error of ozone profile retrieval are as follows:

(1) spectral measurement errors;

(2) errors of assignment of the controlled atmospheric parameters that influence the radiation transfer;

(3) tropospheric absorption (attenuates a useful signal that is formed in the stratosphere and carries information on the ozone profile).

To study the degree of influence of the second and third factors, we have calculated the error matrix for processing several scenarios spectra in the 110.836-GHz line for two typical examples in summer and winter measurements using microwave instruments at the Physical Department of St. Petersburg State University. The spectra recorded on January 26, 2009 (winter, clear air) and July 25, 2009 (summer, strato-cumulus) were taken as source data along with radio and satellite sensing data for these dates and the St. Petersburg region. The scenarios presented in Table 1 differ in the volume of supplementary information.

The scenarios S1 and W1 use the maximum data volume, i.e., radiosonde measurements of pressure, temperature, humidity; satellite measurements of temperature; and the hydrostatic equilibrium approximation. The other considered processing scenarios of ground-based microwave measurements use individual complementary measurements and extra conditions, or no ones (scenarios W5 and S5). The following values of errors of radisonde measurements were used in the calculations: the pressure was 0.5%, the temperature was 2 K, the air humidity was 7%, and data from the Voeikovo radiosensing station (50 km from the ground-based measurement site) [11].

Data from the atmospheric infrared sounder (AIRS) were used as satellite measurements of the temperature data; they are freely accessible in the form of vertical profiles of daily average values on a coordinate grid with a step of 1° [12]. The error of the satellite temperature data was taken equal to 2 K. The altitude ranges of radio and satellite sensing were equal to 0–24 and 0–44 km, respectively, on January 26, 2011 and 0–30 and 0–50 km on July 25, 2009.

Table 2 presents the calculation errors of the mean ozone concentration in layers of 8–10 km in depth and the total content in the 22–60 km altitude range, calculated based on the error matrix for different scenarios. An analysis of the data from Table 2 allows the following conclusion to be drawn:

1. The ozone content is measured most accurately in a cloudless atmosphere during winter in the two lower air layers under consideration (22–30 and 30–40 km when using the maximum volume of complementary measurements and the hydrostatic equilibrium approximation; in this case, the errors are equal to 7.0 and 5.3%, i.e., they are quite small in comparison with the a priori uncertainty, which is equal to about ~40% (the last column in Table 2).

2. The errors increase with the layer altitude and equal about 26–34% in both summer and winter conditions at altitudes of 60–70 km, even using the maximum data volume. A comparison of these values with the a priori uncertainty in the ozone content shows the relatively low information content of the device for altitudes of 60–70 km.

3. An increase in the moisture content of the troposphere during the summer results in a noticeable increase in the error of ozone content calculation, especially in the two lower stratospheric layers. The errors increase in these layers from 5–7 to 7–14%. This increase is insignificant in layers with lower information content because the errors are quite high at altitudes of 50–70 km.

4. The errors in the ozone content calculation increase with a decrease in the volume of supplementary information. This increase can be small (1–2%) when individual measurements that duplicate measurements of another type, e.g., satellite measurements of temperature relative to the radiosonde measurements, are excluded to a certain extent. However, the increase in the errors can be very high when no supplementary information is used. In particular, in this last case, the errors of ozone content calculation increase by two to three times in the two lower atmospheric layers (compare the errors for W1/S1 and W5/S5 scenarios in the 22–30 and 30–40 km layers). This increase is relatively insignificant in the upper stratosphere and lower mesosphere, since at these altitudes, the errors are significant, even for the W1/S1 scenarios, and reach 22–33%.

5. We can note that the exclusion of radiosonde measurements negatively affects the quality of ozone sensing more strongly than the exclusion of satellite measurements. This is connected with the fact that only satellite data on the temperature were used in this study, but not on the water vapor content in the troposphere.

6. Accounting for the condition of hydrostatic equilibrium is important up to an altitude of about 60 km. If neglecting this condition, the errors of ozone content calculations can increase from 5.3 to 12.9% in the 30–40-km layer and from 13.1 to 22.8% in the 40–50-km layer during the winter.

7. The ozone column density in the 22–60-km layer can be measured with an error of about 3.5% during winter and 8% during summer when accounting for all of the available supplementary data. If no complementary measurements or extra conditions are used, then the measurement errors of the ozone column density increase significantly up to 9.4 and 16.7%, respectively, in the 22–60-km layer.

Let us compare the estimated errors of the vertical ozone profiles measured with other ground-based techniques and instruments. Work [4] estimates the errors and vertical distribution when retrieving the ozone profiles from microwave measurements in the 110-Hz line with the instrument designed for the NDSC (former NDACC) network. The value of the vertical resolution was set equal to 8–10 km below 3 mbar (about 40 km) with an increase to 17 km at a level of 0.2 mbar (about 60 km), which completely agrees with our results; i.e., about 10 km in the stratosphere and 15–20 km in the mesosphere. The values of total random and total systematic errors obtained in [4] are equal to 4–6 and 6–10%, respectively. They are lower than the values given in this work, which can be explained by the different number of spectral channels and differences in the specifications of instruments. For an instrument close in specifications to that used at the Physical Department of St. Petersburg University, independent estimates yield errors of ozone profile retrieval in the 20–60 km altitude range as “no worse than 20%” [7], which corresponds to our estimates.

To monitor the gas composition from the Earth’s surface, IR measurements of the atmospheric transparency with high-resolution Fourier spectrometers operated by direct solar radiation are widely used. Therefore, it is interesting to compare the errors of microwave and IR techniques for ozone vertical profile retrieval. The IR technique is studied in detail in [14], where the altitude range of ozone profile retrieval is determined to be 0–40 km, and the vertical resolution is determined to be 5 and 10 km at altitudes of 10–20 and 20–30 km, respectively. The random errors of ozone profile retrieval are estimated to be 4, 13.4, and 1.6% in the 0–10-, 12.5–17-, and 20–30.5-km layers, respectively. Thus, the comparison of the microwave and IR methods allows the following two main conclusions to be drawn: (1) altitudes ranges of the ozone profile retrieval by microwave and IR techniques are shifted relative to each other (20–60 and 0–40 km, respectively); (2) the IR technique is characterized by significantly lower errors then the IR one in the altitude range of 20–40 km. Nevertheless, we should

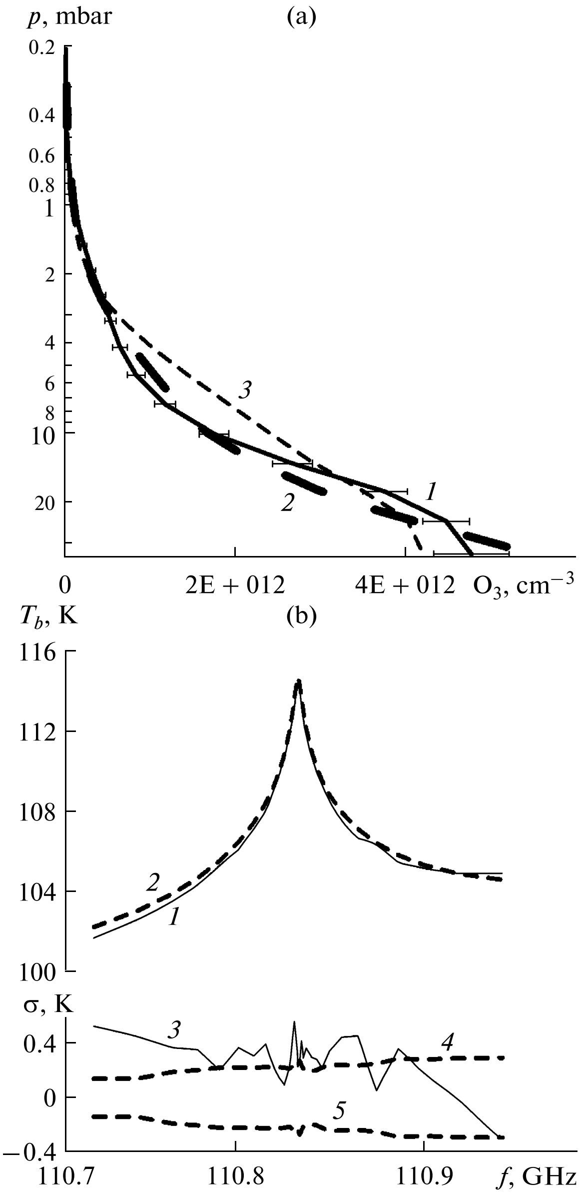

Fig. 2. Ozone content near St. Petersburg on January 26, 2011 (a) according to microwave (*1*) and MLS satellite (*2*) measurements. Curve *3* shows the a priori ozone profile; (b), top: the initial spectrum (*1*) and the spectrum calculated from the retrieved ozone profile (*2*); bottom: the spectral discrepancy (*3*) and the range of measurement errors (*4* and *5*).

emphasize that the microwave technique has an advantage; i.e., it allows around-the-clock measurements (independently on weather conditions) and mesospheric sensing.

The operation of the multiparameter technique is exemplified in Fig. 2, where the profile of the ozone concentration retrieved from microwave measurements taken on January 26, 2011 is shown in comparison with the ozone concentration profile retrieved from the data of the MLS satellite microwave sensor [13]. These two profiles agree within the limits of total errors of satellite and ground-based methods. In addition, the spectra of the brightness temperature recorded and calculated from the retrieved profiles of atmospheric parameters are shown. The shift of the spectral discrepancy relative to the middle of the range of random errors of spectral measurements is evidence of the correlation between the errors in different spectral channels of the instrument.

CONCLUSIONS

A new multiparameter technique for interpreting ground-based measurements of downwelling microwave radiation in the ozone absorption lines has been developed with the aim to receive information on ozone vertical profiles. The technique is based on statistical regularization and the use of complementary (available) measurements (radiosonde and satellite) of different atmospheric parameters. The technique has the following advantages: (1) capabilities of accounting for different types of information on atmospheric parameters in the algorithm for solving the inverse problem and (2) the absence of rigorous requirements for the presence and quality of measurements in the channels used in the common approach to estimation of the tropospheric attenuation.

The dependences of the errors of ozone content measurements in different atmospheric layers on the volume of supplementary information during winter and summer for the instrument produced at IAP RAS and used at St. Petersburg State University have been studied. It has been shown that the maximum ozone sensing accuracy can be attained with the simultaneous use of radiosonde measurements of the vertical profiles of temperature, pressure, and humidity up to 25–30 km, satellite measurements of temperature up to 44–50 km, and account for the hydrostatic equilibrium condition. In this case, the errors of ozone content measurements in the stratosphere can be equal to 5–7% during winter and 7–14% during summer. In the lower mesosphere, the errors can reach ~22–26% during winter and 27–33% during summer. The ozone column density in the 22–600-km layer can be measured with errors of ~3.5% during winter and ~8% during summer taking into account all available supplementary information.

The profiles of ozone number density retrieved by the described technique from microwave measurements at St. Petersburg State University are in a good agreement with the independent results of satellite measurements (MLS device). The technique was successfully validated using the data of the microwave radiometer of Bern University (Switzerland) that operates in the 142-GHz line; however, a detailed description of the corresponding results are beyond the scope of this work.

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