Remote sensing of temperature and gas composition of the atmosphere using ground-based Fourier transform infrared spectrometers

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We have developed a methodology and a software package for implementation of the technology of ground-based remote sensing of the atmosphere using Fourier transform spectrometers (FTS) with the spectral resolution from 0.1 to 1 cm^{-1} (of the FTIR-2 type). This technology makes it possible to measure the altitude profiles of temperature and moisture content, as well as the content of some trace gases in the atmosphere (ozone, methane, etc.) based on the spectra of thermal IR radiation measured with FTS. The software package developed has been tested using an array of experimental data acquired with an OASIS FTS. We present examples of interpretation of the spectra of downwelling thermal IR radiation, as well as analyze the reconstruction of atmospheric parameters by comparing thus obtained results with the data of independent measurements. This comparison demonstrated that practically for all measurements coordinated in time the temperature profiles obtained with radiosondes and from data of interferometric measurements for the atmospheric boundary layer coincide accurate to 1–1.5 K. Discrepancy between the column density of water vapor obtained from radiation measurements and from radiosonde data does not exceed 5%. The discrepancy between interferometric measurements of the total ozone content and data acquired with TOMS satellite does not exceed 3–7%.

Introduction

The remote sensing methods (satellite, ground-based, airborne, etc.) provide a considerable body of information on the state of the atmosphere useful in solving many scientific and applied problems in meteorology, atmospheric physics, climatology, oceanology, etc.[1–3] It is worthy to note that special attention has been recently paid to the problem of increasing the accuracy and vertical resolution of remote measurements. This is primarily caused by that the current technologies not always meet the requirements to remote measurements formulated by various international working groups. For instance, until so far the measurement accuracy of 1 K has not yet been achieved in operative temperature sensing in the troposphere at the vertical resolution of 1 km. There are also problems in achieving the required accuracy in determination of vertical profiles of water vapor and ozone content in the atmosphere.

At present, Keldysh Center Federal State Unitary Enterprise, Moscow, develops a ground-based prototype of a spaceborne infrared (IR) Fourier Transform Spectrometer (FTS) FTIR-2 to be installed onboard a Meteor-3M No. 2 (Ref. 4) new-generation Russian polar-orbiting meteorological satellite. Together with the microwave sounder, the FTIR-2 instrument should become the main satellite facility of the operative monitoring of the atmosphere. The increased information content of FTIR-2-based measurements under clear sky conditions in the atmosphere (with little or no clouds) are to be used for creation of the technology of remote sensing of the fields of temperature, humidity, and concentration of the most important minor gaseous constituents (MGCs) of the atmosphere (O_3, CH_4, and N_2O) with improved (compared with the existing technologies of satellite monitoring) accuracy. This, in turn, should considerably improve the quality of numerical weather prediction on different timescales and stimulate modern studies of climate change on our planet.

Preliminary development and implementation of a ground-based analog of the considered method is important for a detailed validation of the measurement technique and interpretation of atmospheric sensing data acquired with satellites. Moreover, the ground-based measurement technique can be used both for validation of satellite measurements and determination of their actual accuracy and, independently, for studying the variations of different atmospheric parameters with high time resolution. The ground-based method is especially important for study of the tropospheric parameters because of the well-known low information content of satellite methods for this height region of the atmosphere.[3]

1. The technique for interpreting the spectra

Physical-mathematical model of ground-based remote measurements of the atmospheric parameters measurements of the IR spectra of downwelling thermal radiation has been considered in detail in

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Refs. 5 and 6. This model is based on the integral form of radiative transfer equation.

The downwelling thermal radiation and its variational derivatives are calculated with use of the specially written program[7] based on the direct method of calculation and modern data on parameters of the fine structure of absorption bands and continuum absorption by the atmospheric gases. The radiation model used both for modeling of the spectra in the region 700–1350 cm^{-1} and for solution of the inverse problem, was described in Ref. 7. Remind that it takes into account the selective and continuum molecular absorption by CO_2, H_2O, O_3, CH_4, N_2O, CFC-11, and CFC-12.

In solving the inverse problem, we combine the profiles of temperature, pressure, and content of the atmospheric gases into a single vector $\mathbf{x}$ of the atmospheric parameters sought. Then, the inverse problem can be formulated as the problem on seeking a solution to the equation, which takes into account the dependence of the vector of radiation $\mathbf{y}$ on the vector of atmospheric parameters $\mathbf{x}$:

$$\mathbf{y} = \mathbf{F}(\mathbf{x}_i) + \boldsymbol{\varepsilon}. \tag{1}$$

Here $\mathbf{F}(\mathbf{x})$ is, in the general case, a nonlinear operator of the direct problem, $\boldsymbol{\varepsilon}$ is the measurement error caused by the noises of different origin, as well as by the method of absolute calibration of the emission spectra.

The solution of nonlinear equation (1) can be interpreted as a limit of the sequence of linear problems, each being solved by the method of statistical regularization.[8] In so doing, *a priori* information on solution and measurement errors remains the same, while the linear approach to the operator $\mathbf{F}(\mathbf{x})$ is successively refined in the neighborhood of the solution.[9] The iteration process of determination of the most probable estimate $\hat{\mathbf{x}}$ is described by the following formula:

$$\mathbf{x}_{i+1} = \mathbf{x}_i + (\mathbf{S}_\mathrm{a}^{-1} + \mathbf{K}_i^\mathbf{T}\mathbf{S}_\varepsilon^{-1}\mathbf{K}_i + \mathbf{L}^{-1})^{-1} \times$$
$$\times\{\mathbf{K}_i^\mathbf{T}\mathbf{S}_\varepsilon^{-1}\left[\mathbf{y} - \mathbf{F}(\mathbf{x}_i)\right] - \mathbf{S}_\mathrm{a}^{-1}(\mathbf{x}_i - \mathbf{x}_\mathrm{a})\}. \tag{2}$$

Here $\mathbf{K}$ is the matrix of the variational derivatives of the radiation with respect to the atmospheric parameters, $\mathbf{S}_\varepsilon$ is the covariance matrix of the measurement errors, $\mathbf{x}_\mathrm{a}$ and $\mathbf{S}_\mathrm{a}$ are the *a priori* set average vector and covariance matrix of the atmospheric parameters sought, $\mathbf{L}$ is a certain positive-definite matrix introduced for stabilization of the solution and restricting variations of the solution at each step of the iteration process.

As the experience of interpretation of ground-based measurements of the spectra of thermal radiation shows, practically all experimental data, to a certain degree, contain errors of the absolute calibration. In addition, we presently do not know with a required accuracy the parameters of continuum absorption of different atmospheric gases. Also, we cannot correctly take into account the influence of aerosol component in calculating the radiation because of the absence of required information on aerosol during the measurements. To compensate for these errors and uncertainties, modelers introduce a correcting linear term I_corr (Ref. 5):

$$I_\mathrm{corr} = c_1\frac{\nu_2 - \nu}{\nu_2 - \nu_1} + c_2\frac{\nu - \nu_1}{\nu_2 - \nu_1}. \tag{3}$$

Here c_1 and c_2 are the calibration coefficients assumed to be constant in a certain region of the spectrum bounded by the wave numbers ν_1 and ν_2. These coefficients represent biases of the intensity from its actual values at the boundaries of this region. It should be noted that the coefficients c_1 and c_2, determined together with the sought atmospheric parameters, are constant only in narrow spectral intervals (~50 cm^{-1}), i.e., in each (part of) the absorption band of one or another gas they differ.

2. Potential accuracy of the method

To conduct numerical experiments, we created a bank of *a priori* information on thermodynamic state and gas composition of the atmosphere. Random profiles of the atmospheric parameters were modeled based on the specified mean profile, root-mean-square variations, and exponential correlation matrix with the use of a specially developed algorithm and a program of random number generation. In calculations, we used, as the initial data for statistical modeling, the profiles of temperature, pressure, and content of the atmospheric gases from the AFGL-86 model.[10] The statistical characteristics of modeled ensembles (means and variability) correspond to variability of ensembles of field measurements (see, e.g., Refs. 11–13). The constructed ensembles were used in closed numerical experiments while modeling the FTS-measured radiation and also as *a priori* information in solving the inverse problem on determination of the atmospheric parameters [see formula (2)].

The numerical experiments conducted using an ensemble of 200 realizations showed that the error in the temperature profile reconstructed is 1–2 K up to the heights of 5 to 8 km and less than 1 K in the atmospheric boundary layer (0–2 km). Using the measurement scheme taking into account also the spectral channels within the ozone absorption band, it is possible to improve the estimates of temperature profile in the stratosphere as well. For the atmospheric boundary layer, the error of determination of the profile of moisture content is less than 5%.

Moreover, the ground-based interferometric FTS measurements have high information content on the column density of water vapor. For the *a priori* specified uncertainty of 30–45%, the error of determination of the column density of water vapor is less than 1–2%. Study of the accuracy of the considered remote method in case of sounding other gases showed that column densities of such MGCs as O_3, CH_4, and N_2O, as well as the ozone content in the troposphere are measured with the error of 2 to 9%, depending on the atmospheric model and scheme of measurements.

Estimates of the potential accuracy of determination of the column densities of atmospheric gases are demonstrated in the Table. The third column of the table gives the estimates of potential error in MGC column density determination for the ground-based prototype of FTIR-2 instrument assuming the random noise of radiation measurements to be equal to $\sigma = 0.1$ mW/($m^2 \cdot sr \cdot cm^{-1}$). This value of the random noise is recommended for calculations by designers of the FTIR-2 instrument.[4] The second column of the table gives the values of natural variations of the considered parameters, specified *a priori*.

Table. Estimates of the potential accuracy of measurements of the column densities of atmospheric gases by Fourier transform spectrometers: FTIR-2 and OASIS

MGC	*A priori* uncertainty, %	Retrieval error, %	
		FTIR-2 ($\sigma_I = 0.1$)	OASIS ($\sigma_I = 0.5$)
H_2O	40	1–2	2–5
O_3	10	3–5	4–7
O_3 (troposphere)	30	6–10	8–12
N_2O	10	~3	4–6
CH_4	10	~2.5	2.5–3

For a comparison, the fourth column gives the errors of MGC measurements obtained for OASIS, another FTS to be considered in section 3 in a more detail. Note that for a FTIR-2 instrument, increase of the error of radiation measurement by a factor of 10 (from 0.1 to 1.0 mW/($m^2 \cdot sr \cdot cm^{-1}$)) may result in an increase of the uncertainty of determination of the atmospheric parameters by several times.

3. Experimental data

For validation of the technology of interpretation of ground-based FTIR-2 measurements, we used the measurement data from Ocean and Atmospheric Sounding Interferometer System (OASIS) FTS operated by Max Plank Institute for Meteorology in Hamburg, Germany.[6,14] Note that OASIS has characteristics identical to those declared for the FTIR-2 prototype.

We had the spectra of downwelling thermal IR radiation, recorded by OASIS instrument during the measurement campaigns in Baltic Sea in April and June 2000, as well as in June 2001. Note that the interferometric measurements were supported by observations with radiosonde, launched 4 times daily that provided information on temperature, humidity, and wind velocity profiles.

In the first stage of analysis of the spectra, we selected the cases of the clear sky atmospheric conditions, overall about 500. The selection was performed through analysis of the spectral behavior of intensity of radiation in the regions of atmospheric transmission window 800–900 cm^{-1}, as well as in the shortwave wing of the carbon dioxide absorption band at 4.3 μm wavelength.

For analysis of information content and measurement error of the selected spectra we have calculated, for each measurement campaign, the covariance matrices of the measured spectra and studied the sensitivity of the intensity of radiation to variations of different atmospheric parameters. Analysis of eigenvalues and eigenvectors of the covariance matrices has shown that in the campaign I (April 2000), strong variability of the temperature profile occurred, while in the campaigns II and III (June 2000 and 2001) high variability was characteristic of profiles of moisture content. In addition, in year 2000 there were also strong variations of ozone content in the atmosphere.

The pattern of the decrease of the eigenvalues of covariance matrices of the measured spectra has allowed us to determine the random measurement error, found to be 0.6–0.9 mW/($m^2 \cdot sr \cdot cm^{-1}$) for all the campaigns. In solving the inverse problem, these noise values were taken only for one of the criteria of the termination (according to the root-mean-square discrepancy in the measured and calculated radiation) of the iteration process.[5]

4. Interpretation of the measured spectra

In interpretation of the spectra, measured by OASIS instrument, the scheme of solution of inverse problem, used by ourselves, included the spectral channels from the region 700–725 cm^{-1} (for determination of temperature profile), from region 730–830 cm^{-1} (for determination of moisture content), as well as from the region of ozone absorption band 995–1070 cm^{-1}. Thus, from the interferometric measurements we reconstructed the temperature profile, as well as the water vapor and ozone contents in the atmosphere.

As was already noted above, during the interferometric measurements, regular radiosonde launches were performed. Thus, the moisture content and temperature were measured by two independent methods. Comparison of the two methods makes it possible to judge on the actual accuracy of the developed technology of remote sensing of the atmosphere with the use of the ground-based Fourier transform spectrometers.

Analysis of comparison performed has shown that practically in all cases the temperature profiles, reconstructed from radiosonde data and OASIS interferometric data coincide, in the atmospheric boundary layer, accurate to 1–1.5 K. Figure 1 presents two examples of the temperature profiles reconstructed from the radiosonde data and from the data of interferometric measurements.

For the profiles obtained from interferometric measurements, Figure 1 also presents the estimate of the potential uncertainty of the method. One can clearly see in Fig. 1 good coincidence between the data obtained by both methods. In particular, the interferometric measurements reveal with high accuracy the near-ground inversion of the temperature profile.

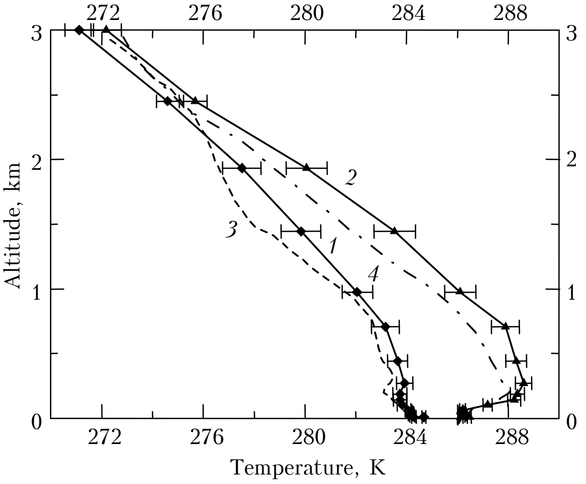

Fig. 1. An example of determination of temperature profile from data of measurements of Fourier transform spectrometer OASIS on June 6, 2001 at 05:15 LT (curve *1*) and on June 16, 2001 at 17:41 LT (curve *2*) and from the radio sensing measurements on June 14, 2001 at 05:17 LT (curve *3*) and on June 16, 2001 at 17:31 LT (curve *4*).

Figure 2 presents an example of time behavior of the column density of water vapor observed in the measurement campaign III (June 2001). For interferometric measurements, Fig. 2 also indicates the estimates of the potential measurement error.

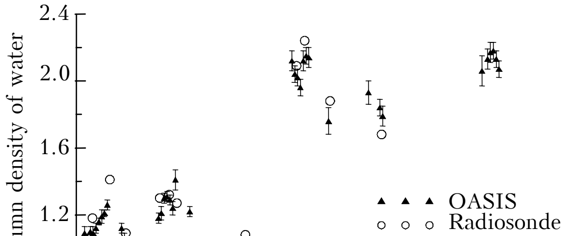

Fig. 2. Total moisture content, obtained from data of measurements by Fourier transform spectrometer OASIS and data of radio sensing during the measurement campaign in Baltic Sea.

As seen from Fig. 2, column water vapor density for period from June 13 to 19, 2001, varied by almost a factor of 3 (from 0.8 to 2.3 cm). At the same time, in most cases there is a good agreement between the moisture content retrieved from spectrophotometric data and those obtained with radiosondes. The measurement error for radiosonde data is not presented, but it is known that the radiosondes measure the profile of moisture content in the troposphere with the error on the order of 5 to 10%. Thus, we can conclude that the results obtained by two independent methods of measurements of moisture content coincide accurate within the uncertainties of both methods.

Figure 3 presents an example of time behavior of the total ozone content in the atmosphere (measurement series in June 2000).

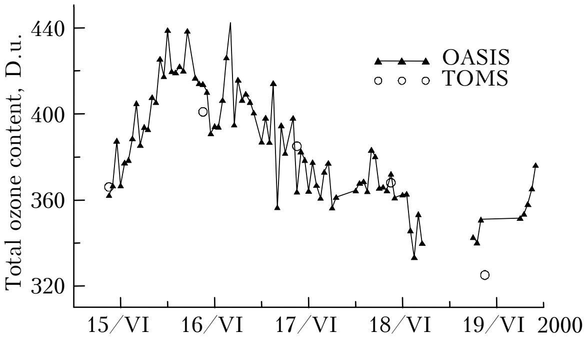

Fig. 3. Total ozone content obtained from data measured with a Fourier transform spectrometer OASIS and from TOMS satellite data during measurement campaign in Baltic Sea.

Triangles denote the results obtained from the spectra of downwelling thermal IR radiation, measured with the OASIS instrument and circles show the data acquired with the Total Ozone Mapping Spectrometer (TOMS).[15] The TOMS data on the total ozone have been taken at a free site ftp://toms.gsfc.nasa.gov/pub/omi/data/Level3e/ozone/.

From Fig. 3 one can see considerable variations of the total ozone over short period between June 15 and 19, 2000 (from 320 to 440 D.u.), which have been traced by the ground-based Fourier transform spectrometer with a high time resolution. It is shown that the data of TOMS satellite instrument, which measured once a day the total ozone over the location of interferometric measurements, well agree with the data of OASIS measurements. The data from other two measurement campaigns also agree with TOMS data within 4 to 7% accuracy limits, i.e., within the estimated error of the total ozone measurements with a Fourier transform spectrometer.

In addition to the total ozone, we also obtained data on ozone content in the thick atmospheric layers: in the troposphere (0–8.5 km) with the error 3–7%, in the region of tropopause (8.5–11.5 км) with the error 10–40%, and in the stratosphere (11.5–50 km) with the error 8–15%. The random error of reconstructing the atmospheric parameters depends on the number of averaged emission spectra. Ozone varies slower than the temperature and humidity; therefore, for solution of the problem of determination of the total ozone it is possible to average the measured spectra over an hour-long time interval. Ozone variations in the layers make it possible to judge on which layer and, correspondingly, which mechanism is responsible for the total ozone variations.

5. Main results and conclusions

For implementation of the technology of remote atmospheric sensing with the use of Fourier transform spectrometers (with the spectral resolution better than 1 cm^{-1}) by measuring the thermal IR radiation in the spectral region 4–16 μm, we have created methods and programs for determination of the altitude profiles of temperature and humidity, as well as of the total content of a number of MGCs.

The developed methodology and the software package were tested using the spectra measured with an OASIS FTS, having characteristics similar to those of the FTIR-2 prototype.

Comparison of the obtained results with the data of independent measurements showed that:

– practically for all measurements coordinated in time the temperature profiles obtained from radiosonde data and from data of interferometric measurements in the atmospheric boundary layer coincide accurate to 1–1.5 K;

– discrepancy between the results, obtained from the radiation measurements, and the data of radiosonde measurements of the moisture content does not exceed 5%;

– discrepancy between the interferometric measurements and TOMS satellite measurements of the total ozone content does not exceed 3–7%.

The results obtained by interpretation of the spectra of downwelling thermal IR radiation have demonstrated an important advantage of the method that demonstrates the possibility of studying in detail time variations of the atmospheric parameters in the troposphere.

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