Retrieval of temperature and humidity profiles from the Earth's IR spectra based on singular decomposition of covariance matrices

K.G. Gribanov, V.I. Zakharov, and A.Yu. Toptygin

Sverdlovsk Affiliate of the Scientific Research and Design Institute for Power Engineering
A.M. Gorky Ural State University, Ekaterinburg

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An economic algorithm for retrieval of atmospheric temperature and humidity profiles from high-resolution Earth's IR spectra obtained from space is developed. It is based on representation of the solution sought by a series expansion in terms of eigenvectors of the covariance matrix constructed on a set of probe measurement data. The coefficients of this series expansion are determined in the process of solution of inverse IR radiative transfer equation. Approximation of the solution by several first terms of the series decreases the dimension of the inverse problem and, consequently, the time of computation without loss in accuracy. Test retrievals showed that the method is resistant to measurement noise with the level reported for ADEOS/IMG, and errors in temperature and water vapor concentration retrievals in the lower troposphere are no greater than 1K and 10%, respectively.

Introduction

The technology of atmospheric sensing for monitoring of weather parameters and pollution has been developed for already more than three decades,[1–3] with the particular attention paid to creation of an efficient spaceborne system for monitoring of atmospheric constituents. Such a spaceborne monitoring system includes instrumentation of different kind, which can be classified by the sensing geometry. This paper is devoted exclusively to nadir thermal sensing, since only this geometry allows us to conduct sensing at any time of a day and has the widest vertical range, including the lower troposphere.

The use of high-resolution IR spectra allows high-accuracy retrieval of atmospheric parameters with high vertical resolution, but this causes the increasing volume of data to be processed, which, in its turn, imposes high requirement on the computer resources. The FIRE-ARMS software[4] was developed for high-accuracy calculations of radiative transfer in the atmosphere and retrieval of temperature and concentration profiles. The inverse problem in this software is solved by the Fletcher-Reeves method[5] with the temperature and gas concentrations on a vertical grid as parameters. Thus, the number of unknowns is multiple to the number of grid nodes.

The technique described in this paper is based on the use of *a priori* information about atmospheric parameters. Construction of the covariance matrix of the profiles of atmospheric parameters and its singular decomposition allow us to represent the inverse retrieval problem in different coordinates: unknowns are the coefficients in the series expansion of a profile in terms of eigenvectors of the covariance matrix. Truncating the series at several first terms, we can decrease the dimension of the problem and, thus, speed up the solution of the inverse problem. This paper is devoted to further development of the idea put forward in Ref. 6, which describes application of singular decomposition of the covariance matrix of the profiles for solution of the inverse problem with the use of the linearized direct model for GOES-8/9 multichannel spectroradiometers. In this paper, we use a more rigorous nonlinear model of radiative transfer in the atmosphere and spectra of higher resolution, which allow us to expect a higher accuracy in the profile retrieval. The technique proposed was tested with ADEOS/IMG spectra.[7]

Eigenvalues and eigenvectors of the covariance matrix of the profiles

The state of the atmosphere is described by the vector $\mathbf{P} = (T_s, T_1, ..., T_N, q_1, ..., q_N)$, which includes the surface temperature, the vertical profile of the air temperature, and the vertical profile of the water vapor concentration. Let $\mathbf{P}^1 ... \mathbf{P}^M$ be the set of vectors of atmospheric parameters obtained from sensing or from other direct measurements. The covariance matrix for this set is calculated by the equation:

$$\Sigma_{kl} = \frac{\sum_{i=1}^{M} (P_k^i - P_k^0)(P_l^i - P_l^0)}{M-1}, \qquad (1)$$

where $\mathbf{P}^0$ is the vector, with respect to which covariance is calculated; the subscripts k and l range from 1 to $2N + 1$, where N is the number of nodes in the vertical grid $\{h_1, ..., h_N\}$ of a profile; M is the number of vectors in the set. As $\mathbf{P}^0$ we can take a

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vector averaged over the set $\mathbf{P}^1 \ldots \mathbf{P}^M$, then the element Σ_{kl} is the correlation of parameters between the kth and lth components of the state vector, and elements of Σ_{kl} describe the corresponding variance.

Singular decomposition of the matrix is

$$\Sigma = \mathbf{USV}', \tag{2}$$

where $\mathbf{S}$ is the diagonal matrix of eigenvalues; $\mathbf{U}$ and $\mathbf{V}$ are orthogonal matrices, whose columns contain left and right eigenvectors of Σ. The standard methods of singular decomposition assume decreasing order of eigenvalues in the matrix $\mathbf{S}$. Using Eq. (2), we can represent any N-dimensional vector $\mathbf{P}$ in the form

$$\mathbf{P} = \mathbf{P}^0 + \sum_{i=1}^{N} C_i \mathbf{u}_i , \tag{3}$$

where $\mathbf{u}_i$ are eigenvectors of Σ. In accordance with the vector $\mathbf{P}$ splitting, every eigenvector can be represented as $\mathbf{u}_i = (u_i^s, u_{i1}^T, \ldots, u_{iN}^T, u_{i1}^q, \ldots, u_{iN}^q)$, where the superscripts s, T, and q denote the surface temperature, temperature profile, and humidity profile, respectively. If we take the number of terms in the sum (3) equal to $n \le N$, then we can obtain some approximation of the vector $\mathbf{P}$. To construct the matrix (1), we use the TIGR database of atmospheric parameters.[8] Figure 1 depicts a typical temperature profile and its approximate expansions for $n = 10$ and 20 at $N = 34$. The mean vertical error was 1.8 and 0.5 K, respectively, for these values of n, while the maximum one was 5.6 and 2.7 K. Thus, restricting the number of terms in Eq. (3), we can decrease the dimension of the inverse problem in retrieval of the profile of T and, consequently, diminish the number of iterations in the algorithm of goal function minimization used at realization of the least-squares method.

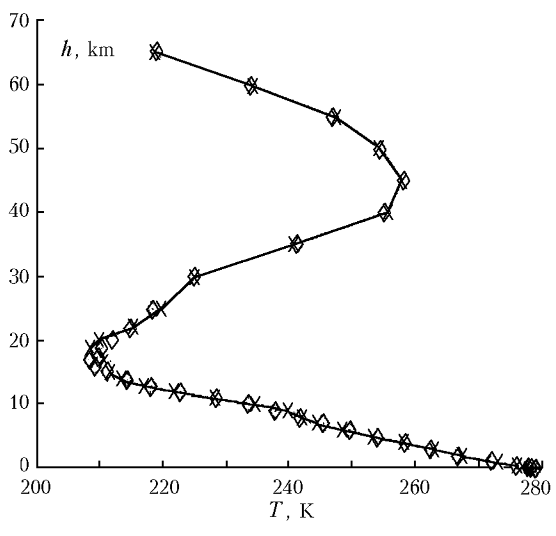

Fig. 1. Vertical temperature profile and its expansions (3) with the number of terms equal to 10 (rhombs) and 20 (crosses).

Method for retrieval of temperature and humidity profiles using singular decomposition

The spectrum of cloudless atmosphere radiation in the case of nadir observations is determined by the following equation[1]:

$$\begin{aligned} W_\nu &= \varepsilon(\nu) B_\nu(T_s) \exp\left(-\int_0^H K_\nu \mathrm{d}h \right) + \\ &+ \int_0^H K_\nu B_\nu(T) \exp\left(-\int_h^H K_\nu \mathrm{d}h' \right) \mathrm{d}h, \end{aligned} \tag{4}$$

where $B_\nu(T)$ is the black-body brightness; $\varepsilon(\nu)$ is the surface emissivity; H is the atmospheric top boundary; K_ν is the atmospheric absorption coefficient. The absorption coefficient is calculated assuming local thermodynamic equation and no scattering by the line-by-line method using parameters from the HITRAN-96 database.[9]

In this paper we use the following goal function:

$$F = \frac{1}{2} \sum_{i=1}^{M} \left[\frac{W_i^{\text{obs}}}{W_i^{\text{calc}}} - \frac{W_i^{\text{calc}}}{W_i^{\text{obs}}} \right]^2 \tag{5}$$

where W_i^{obs} and W_i^{calc} are the observed and model spectra at the ith frequency. The function (5) is minimized with the least-squares method by the Fletcher–Reeves conjugate gradient algorithm. The variable parameters are the coefficients C_i in the expansion of an atmospheric parameter profile (3). The Fletcher–Reeves method is an extension of the conjugate directions method to the case of arbitrary functions. The methods of conjugate directions are characterized by the fact that in the rate of convergence they excel the gradient methods[10] and approach the Newton method, but, unlike the Newton method, they do not require calculation of the second derivatives of the function (5). Calculation of the second derivatives of Eq. (5) would lead to calculation of the second derivatives of Eq. (4), whose computer realization is quite laborious. The Fletcher–Reeves method can be represented as the following sequence of steps:

(a) step 0: C^0 is the initial state (coefficients corresponding to expansion of the model atmospheric profile); $d^0 = -\nabla F(C^0)$ is the direction of the first step;

(b) step k: λ^k is determined from solution of the problem of one-dimensional minimization for the function $g(\lambda) = F(C^k + \lambda d^k)$, then it is assumed that:

$$C^{k+1} = C^k + \lambda^k d^k; \; \beta^k = \left\| \nabla F(C^{k+1}) \right\|^2 / \left\| \nabla F(C^k) \right\|^2 ;$$

$$\mathbf{d}^{k+1} = -\nabla F(C^{k+1}) + \beta^k \mathbf{d}^k ; \tag{6}$$

(c) the procedure continues until the needed accuracy is achieved.

Calculation of ∇F assumes calculation of the derivatives like $\partial F/\partial C_k$, where $k = 1, ..., L$ is the number of coefficients in the expansion (3), and this, in its turn, leads to calculation of the derivatives like

$$\frac{\partial W_i^{\text{calc}}}{\partial C_k} = \varepsilon_i \frac{\partial B_i(T_s)}{\partial T_s} u_k^s \exp\left(-\int_0^H K_i \mathrm{d}h\right) -$$
$$-\varepsilon_i B_i(T_s)\left[\int_0^H \frac{\partial K_i}{\partial T} u_k^T(h)\mathrm{d}h\right] \exp\left(-\int_0^H K_i \mathrm{d}h\right) -$$
$$-\varepsilon_i B_i(T_s)\left[\int_0^H \frac{\partial K_i}{\partial q} u_k^q(h)\mathrm{d}h\right] \exp\left(-\int_0^H K_i \mathrm{d}h\right) +$$
$$+\int_0^H \frac{\partial K_i}{\partial T} u_k^T(h) B_i \exp\left(-\int_h^H K_i \mathrm{d}h'\right)\mathrm{d}h +$$
$$+\int_0^H \frac{\partial K_i}{\partial q} u_k^q(h) B_i \exp\left(-\int_h^H K_i \mathrm{d}h'\right)\mathrm{d}h +$$
$$+\int_0^H K_i \frac{\partial B_i}{\partial T} u_k^T(h) \exp\left(-\int_h^H K_i \mathrm{d}h'\right)\mathrm{d}h -$$
$$-\int_0^H K_i B_i \left(\int_h^H \frac{\partial K_i}{\partial T} u_k^T(h')\mathrm{d}h'\right) \exp\left(-\int_h^H K_i \mathrm{d}h'\right)\mathrm{d}h -$$
$$-\int_0^H K_i B_i \left(\int_h^H \frac{\partial K_i}{\partial q} u_k^q(h')\mathrm{d}h'\right) \exp\left(-\int_h^H K_i \mathrm{d}h'\right)\mathrm{d}h, \quad (7)$$

it is taken into account here that

$$\frac{\partial K_\nu[P(h)]}{\partial C_k} = \frac{\partial K_\nu[P(h)]}{\partial P(h)} \frac{\partial P(h)}{\partial C_k} = \frac{\partial K_\nu}{\partial P} u_k(h),$$

which follows from Eq. (3); $u_k(h)$ can be found through linear approximation between the grid nodes $h \in [h_j, h_{j+1}]$.

The algorithm for retrieving the profiles of atmospheric parameters based on the singular decomposition (3) using the method (6) and Eq. (7) was implemented through modification of the open FIRE-ARMS source code.

Results and discussion

The technique described above was used to conduct a series of numerical experiments on retrieval of the temperature and water vapor concentration profiles.

The model experiment was conducted by the following scheme:

1. The surface temperature T_s, temperature $\mathbf{T}_0$ and humidity $\mathbf{q}_0$ profiles are selected from the TIGR database of profiles and the brightness spectrum of the atmosphere–surface system is simulated in the spectral ranges of 675–825, 1200–1220, and 1550–1620 cm^{-1} for the state of the atmosphere chosen. A random signal distributed uniformly over the range $[-r_N, r_N]$ is added to the model spectra; here $r_N = 0.0002$ W/(m$^2 \cdot$ cm$^{-1} \cdot$ sr) is the equivalent noise brightness reported in Ref. 11 for the IMG interferometer.

2. The surface temperature (819–821 cm^{-1}), the vertical profiles of temperature (680–685, 714–715, 749–751, and 760–761 cm^{-1}) and humidity (1210–1213 and 1560–1610 cm^{-1}) are reconstructed from model spectra in the chosen narrow spectral ranges. One of the standard atmospheric models[12] is used as the initial approximation $\mathbf{P}^0$, and the spectral intervals are chosen based on the analysis of the weighting functions of Eq. (4) [Ref. 1].

3. Then the preset and reconstructed profiles are compared.

Figure 2 exemplifies comparison of the initial and retrieved temperature profiles; similar example for the water vapor profile is depicted in Fig. 3. Figures 4 and 5 demonstrate fitting of the spectra simulated based on the initial and retrieved states of the atmosphere.

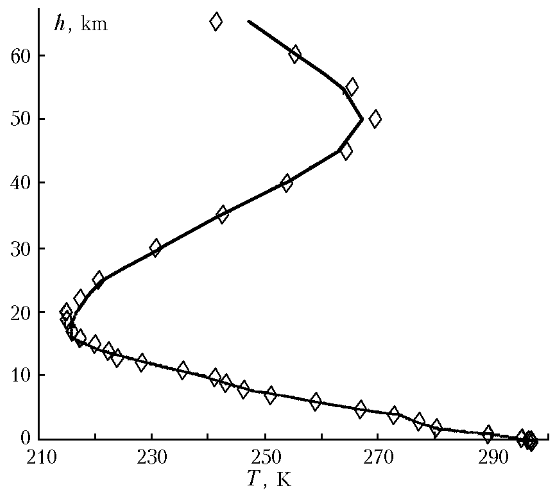

Fig. 2. Initial (solid line) and retrieved (rhombs) vertical temperature profiles.

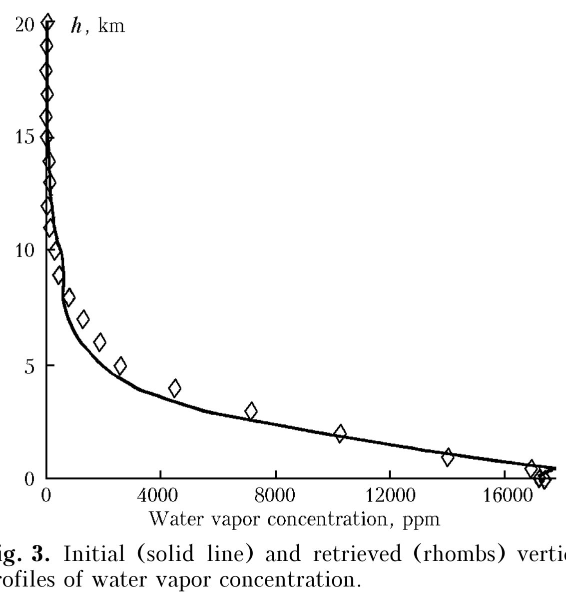

Fig. 3. Initial (solid line) and retrieved (rhombs) vertical profiles of water vapor concentration.

Based on a large number of model experiments, we have drawn the root-mean-square (rms) error of retrieval from model both with addition of a noise signal and without it. The results are depicted in Figs. 6 and 7 for temperature and humidity, respectively.

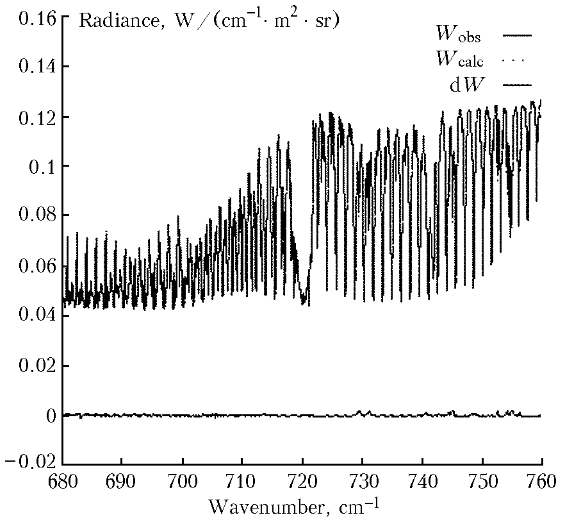

Fig. 4. Fitting of the initial model spectrum and spectrum simulated based on the retrieved temperature profile (see Fig. 2).

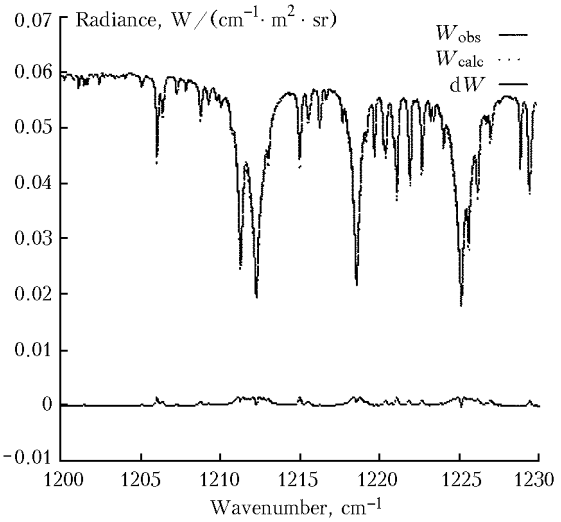

Fig. 5. Fitting of the initial model spectrum and spectrum simulated based on the retrieved profile of water vapor concentration (see Fig. 3).

The model vertical grid in the experiment included 34 nodes, and the dimension of the covariance matrix was 69 × 69 (2 · 34 + 1 = 69), which meant 69 terms in the sum in Eq. (3). However, the experiments have shown that, to retrieve the temperature and humidity profiles with the acceptable accuracy, it is sufficient to use 15–20 first terms of the series (3), which means more than triple decrease in the dimension of the problem and the corresponding decrease of the time for its solution.

The method developed was tested using real spectra of the IMG sensor installed onboard an ADEOS satellite. Figures 8 and 9 depict the retrieved

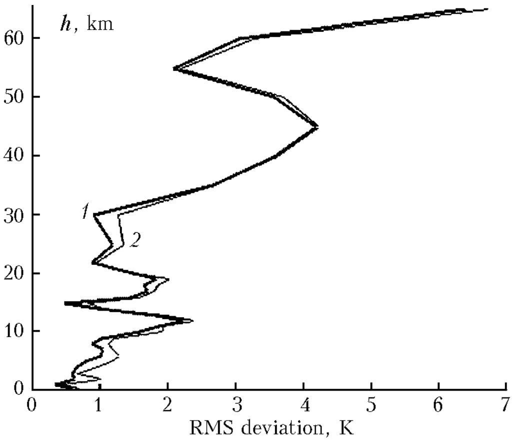

Fig. 6. RMS error of retrieval of the vertical temperature profile from model spectra neglecting noise (curve *1*) and with the ADEOS /IMG noise level (curve *2*).

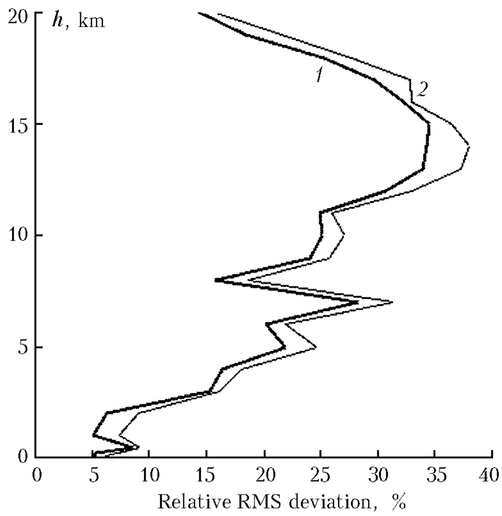

Fig. 7. RMS error of retrieval of the vertical profile of water vapor concentration from model spectra neglecting noise (curve *1*) and with the ADEOS /IMG noise level (curve *2*).

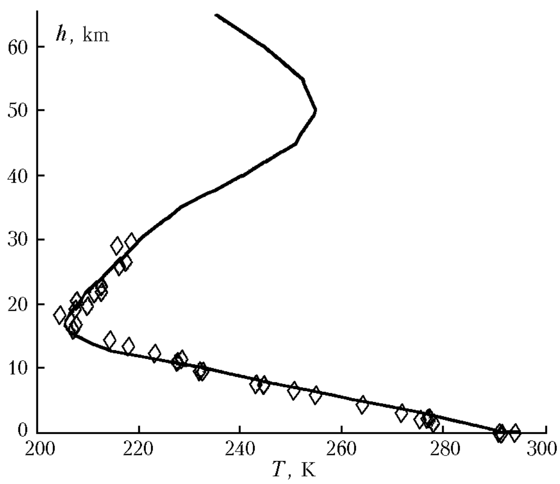

Fig. 8. Temperature profile retrieved from IMG spectrum (solid line) along with the radiosonde profile (rhombs) shown for a comparison.

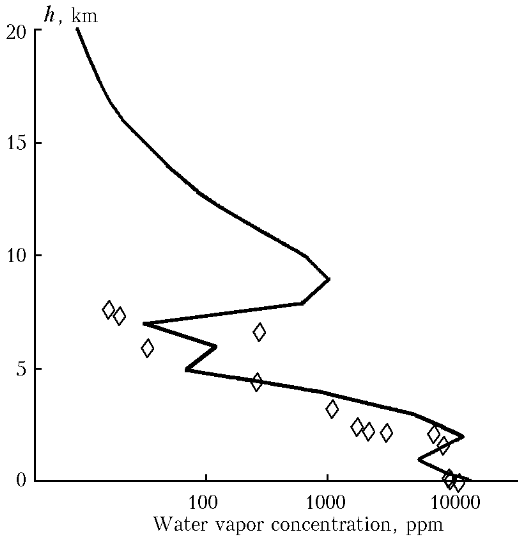

Fig. 9. Water vapor concentration profile retrieved from the IMG spectrum (solid line) along with the probe profile (rhombs) shown for comparison.

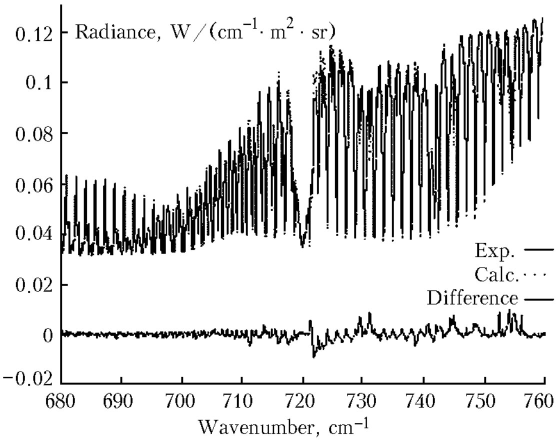

Fig. 10. Fitting of the IMG spectrum and spectrum simulated based on the retrieved temperature profile (see Fig. 8).

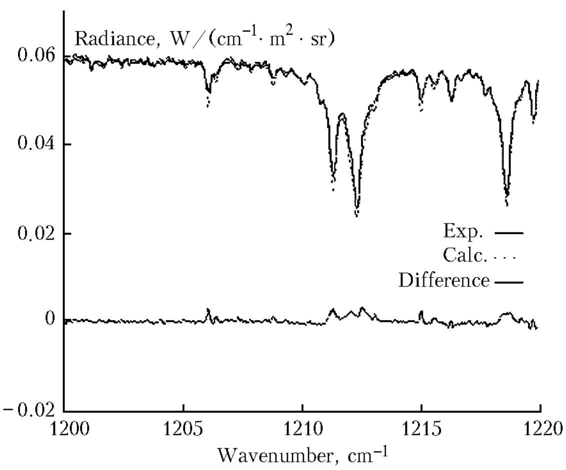

Fig. 11. Fitting of the IMG spectrum and spectrum simulated based on the retrieved water vapor concentration profile (see Fig. 9).

temperature and humidity profiles, along with the results of radiosonde measurements close to them in time and coordinates. Both measurements were conducted over the Pacific Ocean on April 22 of 1997 at the points with the coordinates of 25.175°S, 151.675°W (IMG) and 29.04°S, 177.92°W (radiosonde). Figures 10 and 11 depict the recorded and calculated spectra in the bands used for determination of the temperature and humidity profiles.

Conclusion

We have developed an efficient method for retrieval of the vertical temperature and humidity profiles based on singular decomposition of the covariance matrix of probe measurements. The effect of noise with the level characteristic of the ADEOS/IMG sensor on the error in retrieval of the temperature and humidity profiles has been studied. The model experiment has shown that the effect of the noise component of the brightness spectrum on the error of retrieval by the proposed method from IMG spectra is low. The method is primarily aimed at retrieval of atmospheric parameters from high-resolution spectra recorded with new-generation orbiting Fourier transform spectrometers. It combines efficiency and sufficient accuracy, which makes it promising for processing the data from such future sensors as IASI,[14] TES,[15] EarthCARE FTS,[16] etc. The method has been implemented on a computer as a Fortran code and is accessible through the Internet at *atmosphere.ur.ru*.

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