OPTIMAL PLANNING OF THE EXPERIMENTS ON SOUNDING THE UPPER LAYERS OF THE EARTH'S ATMOSPHERE IN THE 15-μm BAND OF CO_2. TEMPERATURE, KINETICS, COMPOSITION

A.I. Dem'yanikov

The results of the solution of the problem on choosing a set of spectral measuring channels which minimize the error in reconstructing the temperature with remote sounding of the upper layers of the Earth's atmosphere based on the nonequilibrium emission in the 15μm- band of CO_2 are presented. The approach used for solving the inverse problem gives, in addition to the temperature, information about the vertical profile of the CO_2 mixture ratio and the photon survival probability on scattering.

It is shown that the temperature can be determined with an accuracy of up to 1 K at altitudes up to 100 km using modern cooled radiation detectors.

INTRODUCTION

Preparations are now being made for performing a complex experiment on sounding the atmosphere from space shuttles.[1] The main item on the scientific program of future flights will be measurements of the IR radiation of the Earth's atmosphere in the range from 1.4 to 16.5 μm,[2] encompassing the absorption bands of important atmospheric components such as CO_2, O_3, NO, H_2O, NO_2, HNO_3, and OH. Angular scanning with a radiometer yields information about the thermal structure of the atmosphere and its chemical composition from 0 to 250 km.

The transfer of IR radiation for most (if not all) of the components listed above in the indicated range of altitudes, generally speaking, cannot be studied without taking into account the breakdown of local thermodynamic equilibrium (LTE). The region of breakdown of LTE in the atmosphere depends on the specific spectral band. Thus for the 15-μm band of CO_2 it lies above 70 km.[3]

The possibility of reconstructing the temperature distribution $T(z)$ in this region of the atmosphere from remote measurements on oblique paths was first studied correctly in Ref. 4. The method of inversion proposed there is a direct extension of the method described in Ref. 5 and is based on the assumption of LTE. The method of Ref. 4 has the drawback that the vertical profile of the photon survival probability on scattering $\Lambda(z)$, whose value depends on the content of atomic oxygen in the atmosphere, must be given a priori.[6]

It is shown in Ref. 7 that $T(z)$ and $\Lambda(z)$ can be determined simultaneously from measurements in the 15-μm band only if two spectral channels each of which combines sections of the band in which the transmission function has the same dependence, but different in each channel, on the temperature of the atmosphere.

In all works mentioned above it was assumed that the CO_2 content in the atmosphere is known. At the same time direct measurements of the CO_2 mixture ratio, $q_{CO_2}(z)$, showed that above the turbopause (~ 100 km) it could differ from the widely employed model profiles by a factor of five and in some cases by a factor of ten.[8]

In this work a method of remote determination of $T(z)$ in the region of breakdown which does not require *a priori* data on $\Lambda(z)$ and $q_{CO_2}(z)$ is presented. The method Is based on solving exactly the problem of making an optimal choice of the three spectral channels, which give information about $\Lambda(z)$ and $q_{CO_2}(z)$, in addition to $T(z)$, in the analysis of the experimental data. An improved, as compared with Ref. 7, variant of the two spectral channels for solving the problem of simultaneous reconstruction of $T(z)$ and $\Lambda(z)$ when $q_{CO_2}(z)$ is known Is also presented here.

MATHEMATICAL FORMULATION OF THE PROBLEM

We shall start from the following expression for the Intensity of outgoing radiation owing to the fundamental transition of the main Isotope of CO_2:

$$I_{\Delta\nu}(h) = \int_h^{z_{max}} R^{LTE}_{\Delta\nu}(h,z) S_{10}(z) dz, \quad (1)$$

where

$$R^{LTE}_{\Delta\nu}(h,z) = \sum_m \frac{\partial P_m(h,z)}{\partial z} E_m(z) \quad (2)$$

is the kernel of the Integral equation for finding the temperature under the conditions of LTE[S];

$$P_m(h,z) = \int_0^\infty d\nu P_{m,\nu}(h,z) \quad (3)$$

is the transmission function for atmospheric radiation from the altitude z to the top boundary of the atmosphere with tangential height h determined by the absorption In the m-th spectral band; $S_{10}(z)$ is the source function for the frequency of the vibrational transition 1 → 0; and, the function

$$E_m(z) = \left(\frac{\nu_{10}}{\nu_m}\right)^3 \exp\left[-\frac{\delta E_{10,m}}{KT(z)}\right] \quad (4)$$

which takes Into account the spectral dependence of the source function within the vibrational band under study.

It Is well known[3] that S_{10} satisfies the integral equation

$$S_{10}(z) = \frac{\Lambda_{10}(z)}{2} \int_0^{z_{max}} K_{10}(z,z')S_{10}(z')dz' + [1-\Lambda_{10}(z)]B_{10}(z), \quad (5)$$

which takes into account, by means of the kernel $K_{10}(z, z')$, the contribution of scattered photons arriving from all levels of the atmosphere to $S_{10}(z)$. In dense layers where $\Lambda_{10}(z) = 0$ the solution of this equation is identical to the Planck function B_{10} — LTE is realized. In the general case the solution of Eq. (5) can be written In terms of Green's function[9]

$$S_{10}(z) = \int_0^{z_{max}} G_{10}(z,z')B_{10}(z')dz'[1-\Lambda_{10}(z')]. \quad (6)$$

Varying (1) with respect to $T(z')$, $\Lambda_{10}(z')$, and $q_{CO_2}(z')$ at an arbitrary level z' we obtain

$$\delta I_{\Delta\nu}(h) = \int_h^{z_{max}} \left\{\left[R_{\Delta\nu}(h,z')[1-\Lambda_{10}(z)]\frac{\delta B_{10}(z')}{\delta T(z')} + M_{\Delta\nu}(h.z')\right]\delta T(z') + R_{\Delta\nu}(h.z')\frac{S_{10}(z')-B_{10}(z')}{\Lambda_{10}(z')}\delta\Lambda(z') + Q_{\Delta\nu}(h,z')\delta q_{CO_2}(z')\right\}dz, \quad (7)$$

where the component

$$R_{\Delta\nu}(h,z') = \int_h^{z_{max}} R^{LTE}_{\Delta\nu}(h,z)G_{10}(z,z')dz \quad (8)$$

takes into account the variation of radiation owing to the temperature dependence of the source function; $\eta_{10}(z') \equiv (S_{10}(z') - B_{10}(z'))/\Lambda_{10}(z')$ was derived in Ref. 6; the component

$$M_{\Delta\nu}(h,z') = \int_h^{z_{max}} \Big[\underbrace{\sum_m \frac{\partial^2 P_m(h,z)}{\partial z \delta T(z')} E_m(z) S_{10}(z)}_{I} + \underbrace{\frac{\partial P_m(h,z)}{\partial z} S_{10}(z) \frac{\delta E_m(z)}{\delta T(z')}}_{II}\Big] dz \quad (9)$$

takes into account the temperature dependence of the transmission function and the frequency dependence of the source function within the band under study; and, the component

$$Q_{\Delta\nu}(h,z') = \int_h^{z_{max}} \sum_m \frac{\partial^2 P_m(h,z)}{\partial z \delta q_{CO_2}(z')} E_m(z) S_{10}(z) dz \quad (10)$$

takes into account the dependence of the transmission function on the CO_2 content along the path.

Choosing arbitrarily three spectral channels, writing Eq. (7) for each channel, transforming to the finite subspace of the corrections sought, and eliminating $\delta\vec{\Lambda}_{10}$ and $\delta\vec{q}_{CO_2}$ from the algebraic systems obtained we obtain

$$K_{T;1,2,3}\delta\vec{T} = \delta\vec{I}_{1,2,3}, \quad (11)$$

where

$$K_{T;i,j,k} = \delta Q^{-1}_{ij}\delta M_{ij} - \delta Q^{-1}_{jk}\delta M_{ik}; \quad (12)$$

$$\delta M_{ij} = (R^{LTE}_i)^{-1}M_i - (R^{LTE}_j)^{-1}M_j; \quad (13)$$

$$\delta Q_{ij} = (R^{LTE}_i)^{-1}Q_i - (R^{LTE}_j)^{-1}Q_j; \quad (14)$$

$$\delta I_{ijk} = \delta Q^{-1}_{ij}\delta I_{ij} - \delta Q^{-1}_{jk}\delta I_{jk}; \quad (15)$$

$$\delta I_{ij} = (R^{LTE}_i)^{-1}\delta I_i - (R^{LTE}_j)^{-1}\delta I_j. \quad (16)$$

Here the indices enumerate the spectral measuring channels.

One can see from Eqs. (11)—(16) that when $\Lambda_{10}(z)$ and $q_{CO_2}(z)$ are unknown the kinetic temperature of the upper layers of the Earth's atmosphere can be determined only if the temperature dependence of the transmission function and the frequency dependence of the source function within the absorption band under study are taken into account. An analogous conclusion was drawn in Ref. 7 for the problem of determining $T(z)$ and $\Lambda_{10}(z)$ at the same time; in Ref. 7 the contributions I and II of the term in Ref. 9 were compared and it was concluded that the contribution of the term I was larger than that of II.

We note that all inverse problems of determining the temperature from the radiation in the 15-μm absorption band of CO_2 under conditions of LTE were based on the temperature dependence of the source function[10] while the temperature dependence of the transmission function was taken into account only in the iterative refinement of the function. Thus the basic distinguishing feature of inverse problems under conditions of breakdown of LTE is that the temperature dependence of the atmospheric transmission is employed.

The temperature dependence of the transmission function along the path is complicated. The temperature dependence of the line intensities,[11] the mass of the absorbing matter,[5] and finally the contour of the spectral absorption line enter here. The first two factors are the main factors. For the average temperature of the atmosphere $T = 200$ K the derivative of the volume absorption coefficient with respect to the temperature, taking into account the main factors in the temperature dependence of the transmission, changes sign at frequencies of spectral lines with rotational quantum numbers $j \sim 30$. This is the basis for the choice of the optimal measuring channels.

The a posteriori temperature covariation matrix can be derived assuming that the errors in separate measuring channels are uncorrelated with one smother and in altitude:

$$V_T = K^{-1}_{T;1,2,3}\Big\{\delta Q^{-1}_{1,2}\sum_{l=1}^{2}[(R_l^{LTE})^{+}(R_l^{LTE})]^{-1}(\delta Q^{+}_{1,2})^{-1} + \delta Q^{-1}_{2,3}\sum_{l=2}^{3}[(R_l^{LTE})^{+}(R_l^{LTE})]^{-1}(\delta Q^{+}_{2,3})^{-1} + \delta Q^{-1}_{1,2}[(R_2^{LTE})^{+}(R_2^{LTE})]^{-1}(\delta Q^{+}_{2,3})^{-1} + \delta Q^{-1}_{2,3}[(R_2^{LTE})^{+}(R_2^{LTE})]^{-1}(\delta Q^{+}_{1,2})^{-1}\Big\}(K^{+}_{T;1,2,3})^{-1}, \quad (17)$$

the diagonal elements of this matrix are the variance $\sigma_T^2(z)$ of the errors in the reconstruction of the temperature.

We shall regard the spectral measuring channels as optimal for determining the temperature if they give a minimum of the quantity

$$D = \mathrm{Sp}\left(\frac{V_T}{\sigma_T^2}\right). \quad (18)$$

The problem of finding the minimum of expression (18) was solved with the help of the approach developed In Ref. 12. The vibrational band under study in the interval from 620 to 720 cm^{-1} was divided into N spectral sections. Each of the quantities determined by relations (2) and (9)–(10) was represented as a sum of contributions from all spectral sections with weight α_L. For example,

$$R_i^{LTE}(h,z') = \sum_{l=1}^{N} R_l^{LTE}(h,z')\alpha_{l+(i-1)\cdot N}; \quad i=1,2,3, \quad (19)$$

where all α_l can assume values in the interval $0 \le \alpha_l \le 1$. This leads to the problem of finding the minimum of a function that depends on $3N$ variables with simple bilateral constraints

Analogous problems of finding optimal measuring channels for determining Λ_{10} and q_{CO_2} can be easily formulated by replacing in Eq. (18) V_T by the matrices V_λ or V_q corresponding to the problem at hand.

NUMERICAL RESULTS

The problem of finding the minimum of expression (18) was solved by the conjugate gradient method.[13]

At the first stage separate isolated lines were studied instead of spectral intervals. The large dimension of the function obtained in the process makes it difficult to solve the problem. The rigid rotator approximation, which permits representing in an explicit form the dependence of the intensity of the spectral lines on the rotational quantum number, and substituting $R_1^{LTE}(h, z')$, $M_1(h, z)$, and $Q_1(h, z')$ for $R_1^{LTE}(h, h)\delta(z' - h)$, $M_1(h, h)\delta(z' - h)$, and $Q_1(h, h)\delta(z' - h)$, which makes it unnecessary to invert a large matrix, were employed. This substitution can be Justified by the fact that the outgoing radiation in the region of the atmosphere near $z' = h$ makes the main contribution.[5] The collection of lines selected from the approximate solution of the problem was employed to divide the band into spectral intervals which now include groups of lines. There turned out to be 12 such intervals.

At the second stage the approximations described above were no longer employed and the Intensities of the spectral lines corresponded to Ref. 11. The main difference in the positions of the channels obtained at the first and second stages is associated with the R branch of the fundamental band where lines with different rotational quantum numbers are mixed while in the P and Q branches the boundaries of the channels differ by not more than the distance between the neighboring spectral lines.

TABLE I.

Limits of the spectral sections of the measuring channels, cm^{-1}

two-channel system		three-channel system		
1st channel	2nd channel	1st channel	2nd channel	3^{d} channel
648-668 671-677 —	620-647 668-671 688-720	620-638 669-677 688-720	639-668 677-682 —	659-667.4 668-671 668-720

Table I gives the results of the solution of the problems of selecting two and three optimal measuring channels for determining $T(z)$ when $\Lambda_{10}(z)$ is unknown and $T(z)$ when $\Lambda_{10}(z)$ and $q_{CO_2}(z)$ are unknown, respectively.

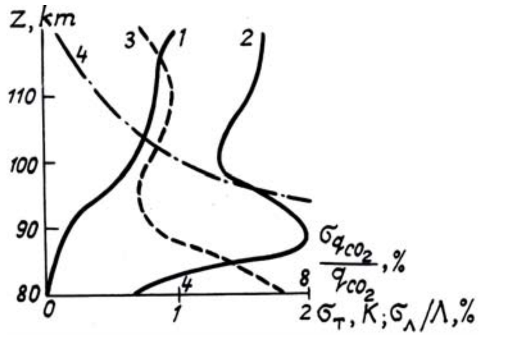

FIG. 1. Theoretical vertical profiles of the reconstruction errors: curve 1 — $\sigma_T(z)$ with known composition (two-channel measuring system); curve 2 — $\sigma_T(z)$ with unknown composition (three-channel measuring system); curve 3 — $\sigma_\Lambda/\Lambda_{10}$ with unknown composition; curve 4 — σ_{CO_2}/q_{CO_2}.

Figure 1 shows the vertical profiles of the theoretical evaluation of the errors in reconstructing the temperature and the relative error in $\Lambda_{10}(z)$ and $q_{CO_2}(z)$ .using the three-channel measuring system as well as the errors in reconstructing the temperature using the improved variant of the two-channel, system.

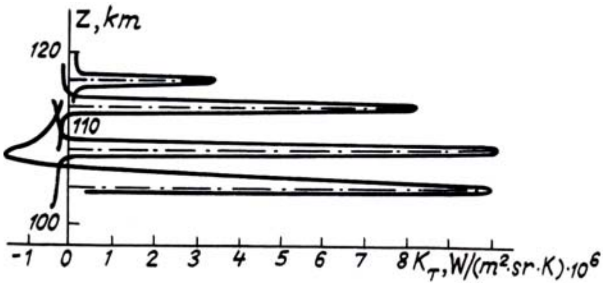

FIG. 2. The weighting function of the three-channel method for reconstructing the temperature, $K_{T,1,2,3}(h, z')$. The dot-dashed lines mark the tangential sounding heights.

Comparing the data presented in Fig. 1 with the analogous data in Ref. 7 shows that using the exact approach to optimize the choice of measuring channels can improve the accuracy of the method by a factor of 5–6.

Figure 2 shows the weighting function given by relations (11)—(14} for the three-channel method. As in the case of the two-channel measuring system its form is close to that of a δ-function. This shows that the proposed method is highly stable.

In conclusion I thank V.V. Rozanov for useful suggestions made in the course of this work and A.A. Kutepov for the opportunity of using the program for calculating the source functions when LTE breaks down.

REFERENCES

1. A.S. Zachor and R.D. Sharma, J. Geoph. Res., No. A1, 467 (1985).
2. A.T. Stair, R.D. Sharma et al., J. Geoph. Res., No. A10, 9763 (1985).
3. A.A. Kutepov and G.M. Shved, Izvestiya Akad, Nauk SSSR, Ser. Fiz. Atmos, i Okeana, **1**, 28 (1978).
4. A.I. Dem'yanikov and A.A. Kutepov, Izvestiya Akad. Nauk SSSR, Ser. Fiz. Atmos. i Okeana, **23**, 5, 510 (1987).
5. Y.C. Gille and F.B. House, J. Atmos. Sci. **28,** No. 11, 1427 (1971).
6. A.I. Dem'yanikov and A.A. Kutepov. Izvestiya Akad. Nauk SSSR, Ser. Fiz. Atmos, i Okeana, **24**, No. 4, 387 (1987).
7. A.I. Dem'yanikov, *Two-channel Method of Thermal Sounding of the Upper Atmosphere Using Tangent Light Paths in the 15-μm CO_2 Band at Broken Local Thermodynamic Equilibrium,* VINITI Akad. Nauk SSSR, No. 1398-B, 15 (1988).
8. D. Afferman, V. Friedrich et al, Planetary and Space Science, **29**, No. 7, 747 (1981).
9. V.V. Ivanov, *Radiation Transfer and Spectra of Celestial Bodies* (Moscow, Nauka, 1969).
10. K.Ya. Kondrat'ev and Yu.M. Timofeev, *The Meteorological Sounding of the Atmosphere from Space*, (Gidrometeolzdat, Leningrad, 1978).
11. R.A. McClatchey, W.C. Benedict, S.A. Clough, et al., *AFGRL Atmospheric Absorption Line Parameters Compilamion*, Rep. AFGRL-TR-73-0096, Cambridge, Mass.: Air Force Cambridge Res. Lab. (1973).
12. V.P. Kozlov, *Abel's Inversion and its GeneralIzlngs*, 68 (Novosibirsk, 1978).
13. F. Gill, U. Myrrey and M. Right, *The Practical Optimization* [Russian translation] (Mir, Moscow, 1985).