

INFLUENCE OF ERRORS IN THE PARAMETERIZATION AND SPECTROSCOPIC INFORMATION ON THE ACCURACY OF CALCULATING THE OUTGOING THERMAL RADIATION RECEIVED IN HIRS RADIOMETER CHANNELS

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We propose a new method to parameterize the transfer equation, when calculating outgoing thermal radiation, that allows one to minimize the errors introduced when taking into account the molecular absorption. We have analyzed the errors in data on the intensity and halfwidths of the spectral lines of six gases, namely of H₂O, CO₂, O₃, N₂O, CH₄, and CO, compiled in the HITRAN-96 database. It is shown in this paper that the errors in the integral intensities of the absorption bands of the gases under study are within 3–10% while typical errors in the halfwidths of individual strong lines are about 10%. The majority of these estimates are the summed errors in the intensities of individual lines, thus being the upper estimates. In a number of spectral intervals, we have revealed systematic deviations in the integral intensities of the absorption bands. The computer modeling conducted has shown that the main contribution into the error in the intensity of outgoing radiation, detected with a HIRS radiometer, is due to systematic components of the errors in the integral intensity of the bands and line halfwidths.

At present the satellite data can not provide reliable short-term and medium-term weather predictions, because of low accuracy of the temperature estimations. Thus, for instance, measurements with HIRS radiometers provide only about 2.5 K accuracy in a 2-km thick layer, while making reliable predictions requires¹ the accuracy on the order of 1K. Low spectral resolution of the space-based radiometers is the main cause of that low accuracy. However, it is worth noting, that removing this drawback does not yet guarantee a success.

Omitting numerous problems concerning the uncertainties in the atmospheric aerosol composition and effects of clouds, let us point out only two factors which are of principle importance thus essentially influencing the accuracy of solving the inverse problem on reconstruction of the atmospheric parameters. Those are the errors in parameterization of the molecular absorption, and the errors in the spectroscopic information used.

In this paper a new method of the transfer equation parameterization is proposed, that provides for the accuracy of calculating the outgoing thermal radiation that compares with that of the direct line-by-line method. Actually, the method is brought to the level of a technique, and can be easily reproduced

for any spectral device with an arbitrary instrumental function and spectral resolution. The methodology is described, and analysis is done of the influence of the accuracy with which the parameters of spectral lines are given in the HITRAN-96 database on the errors of calculating the outgoing radiation.

1. PARAMETERIZATION OF THE RADIATION TRANSFER EQUATION FOR THE CASE OF A CLOUDLESS EARTH'S ATMOSPHERE

A solution to the transfer equation for a monochromatic long-wave radiation in a clear and non-scattering atmosphere has the form²²:

$$\begin{aligned} \hat{I}^{\uparrow}(v, z, \mu) = & \delta_v B_v(\theta_0) \exp \{-\mu \tau_v(z_0, z)\} + \\ & + \int_0^z B_v(\theta(z')) \frac{d [\exp \{-\mu \tau_v(z', z)\}]}{dz'} dz' + \\ & + 2(1 - \delta_v) \exp \{-\mu \tau_v(z_0, z)\} \times \\ & \times \int_0^z B_v(\theta(z')) \frac{dE_3(\tau_v(z', z_0))}{dz'} dz', \end{aligned} \quad (1)$$

where $B_v(\theta(z))$ is the Plank function, $\theta(z)$ is the temperature at the height z ; δ_v is the surface emission

coefficient; $\tau_v(z', z)$ is the optical thickness of the layer $z' - z$ at the frequency ν ; $\mu = \sec(\vartheta)$; ϑ is the zenith angle of the path;

$$E_3(\tau) = \int_1^\infty \exp(-\mu\tau) \mu^{-3} d\mu. \quad (2)$$

The space-based radiometer records the intensity of the upward going radiation in the spectral interval determined by the transmission band of an interference filter used:

$$I_v^\uparrow(z, \mu) = \int G(\nu') I^\uparrow(\nu', z, \mu) d\nu'. \quad (3)$$

Formula (1) is valid only at small zenith angles of the viewing paths. At large angles the curvature of the Earth's atmosphere must be taken into account³ in the first two terms of the expression (1). The matter is that in this case the quantity μ varies along the viewing path and one have to use the following expression to calculate the optical thickness:

$$\tau(z, z') = \int_z^{z'} \mu(h) \alpha(h) dh, \quad (4)$$

where $\alpha(h)$ is the absorption coefficient, while

$$\mu(h) = \frac{(R+h)}{\sqrt{(R+H)^2 \cos^2 \varphi - (H-h)(2R+H+h)}}; \quad (5)$$

R is the Earth's radius; H is the height of a satellite above the Earth surface; φ is the angle of sighting from the satellite. The refraction is not taken into account in Eq. (5), since its contribution is too small.

The brightness temperature T_J , that is the temperature of a black body that emits radiation $J_\nu(\mu)$, in units of $\text{mW}/(\text{m}^2 \cdot \text{sr} \cdot \text{cm}^{-1})$,

$$J_\nu = \frac{1.1910659 \cdot 10^{-5} \nu^3}{[\exp(1.438833\nu/T_J) - 1]}, \quad (6)$$

(from this expression it follows that

$$T_J = 1.43868 \nu / \ln [1.19057 \cdot 10^{-5} \nu^3 / J_\nu + 1],$$

where ν is the wave number in cm^{-1}) is usually introduced in each channel instead of the intensity of outgoing radiation, $J_\nu(\mu)$.

Calculating $I_v^\uparrow(z, \mu)$ by formulas (1) to (6) is quite a laborious process. The absorption coefficient is a function that oscillates very fast. The Voigt profile of a line shape that is often used to describe a shape of an isolated absorption line in the case of an inhomogeneous atmospheric path is a convolution of the Doppler and Lorentz contours and involves an improper integral. Besides, calculating the absorption coefficients assumes summing of a large number of spectral lines (in the ozone absorption bands one is forced to consider up to 10^3 lines). Regardless of many attempts to develop fast algorithms for

calculating the molecular absorption properties use of direct methods requires long computer time, thus being unacceptable for handling the satellite data.

Parameterization of the transmission functions is technique that is most widely used to improve the calculation efficiency. Two approaches are being used for this purpose. In case when the spectral width of the instrumental function is enough narrow, so that the Plank function may be considered constant, expressions (1) and (2) can be reduced to the following form:

$$\begin{aligned} I_v^\uparrow(z, \mu) = & \delta_\nu B_\nu(\theta_0) P_\nu(\mu, z, z_0) + \\ & + \int_0^z B_\nu(\theta(z')) \frac{d[P_\nu(\mu, z', z)]}{dz'} dz' + \\ & + 2(1 - \delta_\nu) P_\nu(\mu, z, z_0) \times \\ & \times \int_z^{z_\infty} B_\nu(\theta(z')) \frac{dE_3(\nu, z', z_0)}{dz'} dz'; \end{aligned} \quad (7)$$

$$E_3(\nu, z', z) = \int_1^\infty P_\nu(\mu, z', z) \mu^{-3} d\mu; \quad (8)$$

$$P_\nu(z', z) = \int_{\nu-\Delta\nu/2}^{\nu+\Delta\nu/2} G(\nu) \exp(-\mu \tau_\nu) d\nu, \quad (9)$$

where $\Delta\nu$ is the spectral width of the instrumental function.

Parameterization of the transmission functions in the form (9) is, as a rule, performed using methods of model representation of the absorption spectra, what can lead to considerable errors, especially in the cases with the carbon dioxide and ozone.⁴⁻⁶ To reduce these errors, one is forced to give up the standard Curtis-Godson method,⁷ what results in a more complicated dependence of the transmission function on the meteorological quantities. The parameterization efficiency in this case depends, to a large extent, on the skillfulness of a researcher. Thus, for instance, in Ref. 8 the scatter diagrams are presented for the transmission functions calculated by line-by-line method, and by different approximate methods. The largest scatter is observed for the bands method based on the fitting of parameters to standard calculations, while the least one corresponds to the method of k -distribution, which yields data most close to that obtained by the direct method of calculation.

It should be noted that the k -distribution method has so far been applied only to the cases with rectangular instrumental functions. Therefore the spectral interval in Ref. 8 was divided into the subintervals within which the instrumental function may be considered constant, so that the intensity of the outgoing radiation could be presented in the following form:

$$I = \sum_{i=1}^N G(v_i) I_i(0, \mu) \tag{10}$$

and the transmittance within each subinterval could be determined by the formula

$$P_i = \frac{1}{\Delta v_i} \int_{\Delta v} \exp(-\tau_v) dv. \tag{11}$$

It is seen from equation (11) that the calculation of transmission function in the *i*th interval is done for a rectangular instrumental function. This parameterization scheme, though provides as a rule for higher accuracy, leads, however, to an unjustifiably large number of the parameters needed, and, as a consequence, to a very long computer time.

It is shown below that such an approach is worthwhile only in the case when the width of the instrumental function is large, so that the Plank function may undergo noticeable changes within the interval in question. Otherwise, one may apply the approach described in Ref. 9 to the expression (9), that provides for a possibility of presenting the transmission function in the following form:

$$P = \int_0^1 \exp\{-\tau(g)\} dg. \tag{12}$$

The following expressions have been obtained¹⁰ for calculating the function $\tau(g)$:

$$g(\tau) = \int_{v_1}^{v_2} G(v) W(v) dv; \tag{13}$$

$$W(v) = \begin{cases} 1, & \tau(v) < \tau, \\ 0, & \tau(v) > \tau. \end{cases} \tag{14}$$

The technique for calculating $g(\tau)$ is reduced to summing intervals with the weights $G(v)$, for which the condition $\tau(v) < \tau$ holds. As a result, one obtains the function $g(\tau)$ that monotonically grows and its inversion readily yields the function $\tau(g)$.

Expressions (12)–(14) allow one to replace the rapidly oscillating function $\tau(v)$ by a monotonic function $\tau(g)$, and nothing more. The parameterization problem is still to be solved, since under variations of thermodynamic parameters of the atmosphere it is necessary to perform new calculations of $\tau(v)$ using the line-by-line method, and then to calculate $\tau(g)$ function. In this case, there is no gain as compared with conventional line-by-line method, since the computer time is mainly spent on calculating $\tau(v)$ rather than on frequency integration. In Refs. 11 and 12 the method of *c-k* correlation has been used for parameterization of $\tau(g)$.

The latter method provides for a high accuracy and allows one to approximate the optical thickness by the following expression:

$$\tau(g, z, z') = \mu \int_z^{z'} K(g, p(h), T(h)) \rho(h) dh, \tag{15}$$

where $K(g, p(h), T(h))$ is the absorption coefficient at the frequency g , and at the height h ; $\mu = 1/\cos \vartheta$, ϑ is the zenith angle. A qualitative interpretation of the *c-k* correlation may be found in Ref. 12, while the numerical estimations of the *c-k* correlation applicability in Refs. 11 and 12. The error of the transmission function calculations did not exceed, as a rule, 1%. Exceptions are only the cases when large temperature gradients occur (for example, in flames).

Since the integrand in equation (12) is a smooth function (typical dependences of the absorption coefficients on height and temperature are presented in Figs. 1 and 2) the Gaussian quadratures were used to calculate the integral. As practice has shown the consideration of 10 series terms provides for obtaining the error that does not exceed 1%:

$$P_v(z, z') = \sum_{i=1}^n C_i \exp \left\{ -\mu \int_z^{z'} K(g_i, p(h), T(h)) \rho(h) dh \right\}. \tag{16}$$

For calculating the absorption coefficients at the altitudes from 0 to 100 km, we have isolated 36 pressure levels (from 10^4 and down to 10^{-3} mbar), and 18 temperature levels within the range from 330 K and down to 160 K.

The overlapping of the absorption bands has been taken into account by the most simple and conventional approach by taking a product of the relevant transmission functions. According to our estimations,¹³ the error of such an approximation is usually about 1%, and may increase up to 3% only in cases when the width of the instrumental function is small, while contributions due to selective absorption by different gases are close in value. Our analysis has shown that no such situations occur in measurements with HIRS-radiometers.

Calculation of the molecular absorption coefficients for each spectral channel of a HIRS-14 device has been performed by the direct line-by-line method, discussed in detail in Refs. 14–16, based on the data from the spectral line database HITRAN-96.^{17,18} Absorption by the main atmospheric gases like H₂O, CO₂, O₃, N₂O, CO, and CH₄ was taken into account along with the continuous absorption by H₂O, according to data from Ref. 19, continuous absorption beyond the edge of the 4.3- μ m CO₂ band,²⁰ and the pressure induced absorption by N₂ according to Ref. 21.

The accuracy of numerical solution of the transfer equation depends on the quadratures used, and on the number height nodes. As the modeling performed has shown, the error in calculated radiation temperature may be 0.1 K as low, if the absorption coefficient is calculated using a linear interpolation of the coefficients $K(g_i, p_j, T_k)$ calculated beforehand. Then calculations of

the optical thickness are to be done by integrating those coefficients using trapezoidal technique. Integrals over the height in the equation (6) have been calculated by rectangles method using the technique proposed in Ref. 12, according to which the Plank function is assumed to vary linearly with height within a single layer. The atmosphere was divided into layers according to the standard AFGL model.²² The temperature, pressure, and concentration of the absorbing gases have been set at the boundaries of each layer, while being continuously varying inside the layer. To verify the accuracy of integrating over the height, we made use of a standard trick when additional layers are being introduced, and calculations are repeated. As a result we have shown that the standard grid of heights provides for a sufficiently good accuracy (the error in the calculated radiation temperature did not exceed 0.2 K).

2. INFLUENCE OF ERRORS IN THE SPECTRAL LINE PARAMETERS ON THE ACCURACY OF CALCULATING THE EARTH'S LONG-WAVE RADIATION

The comparisons, that have been made in a large number, among the absorption spectra of atmospheric gases measured experimentally and those calculated using the line-by-line technique show that noticeable discrepancies can occur in some spectral regions, if, especially, the measurements have been carried out using lasers. It is worth noting that even for the well understood water vapor absorption spectra the discrepancies among the experimental data obtained by different authors, as well as among the calculated data, may amount to tens of percent, see for example Refs. 23–27.

The main sources of errors in the calculated transmission functions can be the uncertainties in the thermodynamic parameters (temperature, pressure, and concentration of a gas), as well as inaccurate line shapes, errors in line parameters (line centers, line shifts, intensity, halfwidth, and energy of the lower level).

In our opinion, the initial spectroscopic information available from recent databases^{17,18} is the main source of errors, while the first two factors are of a minor importance. The first reason to think so is that modern experimental instrumentation provides quite high accuracy of acquiring data on the thermodynamic parameters. This is especially true with the laboratory experiments. Secondly, the HIRS radiometers are low-resolution instruments, that means that we are dealing with broad-band transmission functions. In that case it is important, when calculating these functions, to account for the main regularities in the line shape within its wing, because the deviations from the dispersion contour near the line center like those due to Dicke effect, interference of lines, and negligence of the line shift are of minor importance. The databases presented in Refs. 17 and 18 are a sort of compilations,

that means that those contain information about spectral line parameters both calculated and retrieved from the experiment by different authors. As a result, this information is of different quality, and there are parameters obtained with low accuracy along with recent highly accurate data.

No papers have been published so far that would deal with analysis of how the uncertainties in line parameters can influence the accuracy of calculating the broad-band transmission functions. Only a few publications are known^{28,29} that consider separate aspects of the problem in question. Most logical, that is, the statistical approach to the problem has been formulated in Ref. 30 though having been applied only to CH₄ molecule. The difficulty in solving this problem is connected with the lack of data on errors in the spectroscopic information, as well as with the absence of such data at all, in some cases. For example, among the gases which were of interest for us, most complete information is available in the HITRAN–96 database only about CO₂, CO, and CH₄ (the rms errors in the line-center positions, intensities, and halfwidths), while for O₃ molecule such data are available only for some transitions, while being absent for H₂O and N₂O molecules. It has been shown in Ref. 30 that the main contribution into the error of calculating the molecular absorption characteristics is introduced by the systematic errors in line intensities and halfwidths, therefore, the main efforts in the spectroscopic information analysis were concentrated on the estimation of errors in the integral intensity for the bands that determine the absorption in each channel of a HIRS radiometer.

2.1. Analysis of the spectroscopic information available in the HITRAN–96 database

Analysis has been done by comparing the intensity values and the errors in these values available from the HITRAN database, with the literature data both experimental and calculated. Unfortunately, the existing methods of calculations are insensitive to the systematic errors in the line intensities. Therefore, only in some spectral regions the systematic errors in the intensities of lines have been revealed for H₂O, CO₂, and O₃ molecules, where it was possible to compare the data from HITRAN with the experimental values. For other spectral regions the errors in the intensity of lines have been determined by summing the errors for individual lines. Therefore, thus obtained estimations are mostly the upper-boundary values.

Water vapor and carbon dioxide absorb, practically, in all spectral channels of the radiometer, therefore the main attention was paid to H₂O molecule. In the 1st to 7th channels (from 667 to 757 cm⁻¹) of the radiometer the absorption is due to pure rotational transitions of the H₂O molecule in the ground vibrational state. The data from the HITRAN–96 atlas on the line intensities in this region repeat the compilation completed in 1986 that involves

the calculated values.¹⁷ There are no new data available on the intensities in this region. The accuracy of calculations of the pure rotational transitions is usually high enough, and can be estimated to be about 10%.

In the 8th to 20th channels of the radiometer the absorption is mainly due to the transitions within the ν_2 absorption band of H_2O .^{31,32} The transition intensities of the ν_2 band as taken from the database can deviate from the experimental data^{31,32} by 2–20%. Comparison of data from Refs. 31 and 32 with the results of recent theoretical study by Coudert³³ has shown quite good agreement, with the discrepancies between the line intensities within the ν_2 band being evidently random. It was found that for hot bands, $2\nu_2 - \nu_2$, (see Ref. 34) and $\nu_1 - \nu_2$, $\nu_3 - \nu_2$ the HITRAN-96 database provide only old data that can deviate from the experimental values by 20 to 45% (see Ref. 35). Intensities of the $\nu_1 - \nu_2$ band are presented in the HITRAN-96 with a distinct systematic overestimation up to 45% and for the ν_3 band the intensities are overestimated by 10 to 20%. Under these conditions a conclusion about possible systematic bias has been drawn for channels where the absorption by hot bands exceeded 75% of the integral absorption. Those are the 15th to 20th channels. According to our estimations the average systematic error may comprise 8 to 10%.

For CO_2 molecule the information on the errors in spectral lines intensities presented in the HITRAN database is available for all channels of interest. In this case the error code is, as a rule, "6B" that means a 2 to 5% error, and, more rarely, it is "5B" that means 5 to 10% error. For carbon dioxide the calculated data obtained by the Direct Numerical Diagonalization (DND) method³⁶ have extensively been used in the HITRAN database. This method provides quite a good agreement with the experiment, as well as good predictions for the low lying vibrational bands, though the DND calculations may give rise to errors of tens percent for highly excited vibrational states, especially in the case of strong resonance interactions. It was shown in Ref. 37 that deviations of the results calculated by the DND from experiment, for a number of bands in 544–791 cm^{-1} region, may amount up to 7%. To check up the data compiled in HITRAN-96 database, the experimental data from papers 38 to 46 have been used, the accuracy of the latter being from 2 to 10%. On the whole, the data from the HITRAN atlas deviate from the experimental values by 0 to 2% for strong bands (1st to 4th, and the 18th channels), and up to 10% for weak bands. In some cases the deviations from the experimental data are of a systematic character.

Comparison of the HITRAN-96 and GEISA-96 databases has shown that the line intensities for H_2O and CO_2 are practically the same in both databases.

Information on the parameters of O_3 spectral lines from the 9.4- μm band in the HITRAN database was practically entirely taken from the "Atlas of ozone spectral parameters from microwave to medium infrared, B 1990 (see Ref. 47). These are the computational results, and the authors of Ref. 47 define their accuracy for the basic bands to be comparable with the corresponding experimental errors (4–10%). Vibrational bands ν_3 centered at 1042.08398, and ν_1 at 1103.13728 cm^{-1} analyzed in Ref. 48 are the main contributors into the absorption in the 10th channel. The dipole moment parameters for both bands were retrieved by applying the fitting to 350 absorption lines, that provide for reproducing the initial data with the average accuracy of 6%. Actually, as in the case with ν_2 and $2\nu_2 - \nu_1$ bands, the measured values are relative intensities, which have then been normalized, in a certain way, to retrieve the absolute values. The authors of Ref. 48 warn that changing the normalization conditions requires all the intensities to be corrected. If allowing for possible systematic bias, the accuracy of the absolute intensity determination, in the region of interest, is obviously poorer or equal to 10%, that agrees with the estimations made in Ref. 49.

There are no any estimations of possible errors in the intensity of lines for N_2O molecule available from the HITRAN database (all the error codes are equal to zero). Comparison of line intensities from the HITRAN-96 database with data from Ref. 50 to 53 has shown their quite a satisfactory agreement, that is, within 1 to 2% for strong lines, and 5 to 10% for the weak ones. The comparison has been done optionally only for the strong lines since the complete array of data on N_2O lines compiled in the HITRAN-96 database contains about 20000 lines.

Estimations of errors in the intensities of CO and CH_4 lines have been obtained using the HITRAN-96 database by summing errors in the intensities of individual lines.

Estimations of the random and systematic errors in the integral absorption in the HIRS channels obtained from the analysis made are presented in Tables I and II for all the six gases under consideration.

Analysis of errors in the halfwidths has been done only for H_2O molecule, since the situation with the halfwidths is typical for all molecules. It is worth noting here, that only a limited bulk of experimental data on the halfwidths is available, being mostly used to test theoretical models and for optimizing calculation procedures. Therefore, the HITRAN-96 database contains only calculated data on the halfwidths obtained using the QFT⁵⁴ method. This method provides for a good agreement with the experimental data, the calculation error is, on the average, about 10%.

TABLE I. Estimations of errors in the integral absorption within the HIRS channels.

Number of channel	v _{min} , cm ⁻¹	v _{max} , cm ⁻¹	Errors in the integral intensity, %									
			H ₂ O		CO ₂			O ₃	N ₂ O	CO	CH ₄	
			Σ	Σ _s	Σ _H	Σ	Σ _s	Σ	Σ	Σ _H	Σ _H	
1	667.40	670.40	10		3.5	5	-2					
2	674.80	684.80	10		3.5	5	2					
3	684.10	696.10	10		3.5	3						
4	695.20	711.20	10		3.5	5	-2					
5	707.80	723.80	10		3.5	6						
6	725.10	741.10	10		3.5	7	-4					
7	741.10	757.10	10		3.5	10	-7					
8	788.80	804.80	12		3.6	10	-7					
9	882.60	917.60	15		3.7	11			6			
10	1017.40	1042.40	27		3.6	11		10	10			
11	1195.50	1255.50	8		3.5	10		10	6			3.5
12	1344.30	1384.30	6		3.5	10			10			2.7
13	1448.10	1528.10	5		0							7.9
14	2176.70	2199.70	9		7.0	14	4		4	3.5		
15	2200.90	2223.90	13	8 - 10	6.4	9			4			
16	2230.60	2253.60	15	8 - 10	4.3	10			4			
17	2261.20	2284.20	16	8 - 10	3.7	13	-10		6			
18	2347.00	2370.00	17	8 - 10	3.5	4	+1					8.5
19	2407.30	2435.30	18	8 - 10	3.5	10						7.7
20	2482.50	2517.50	17	8 - 10	3.5	10						7.9
21	2609.60	2709.60	2		3.5	10						

Note: Σ is the expert estimation of the error in the integral intensity calculated as a sum of errors for individual lines; Σ_s is the systematic error in the integral intensity; Σ_H is the error in the integral intensity calculated using the HITRAN-96 data as a sum of errors for individual lines.

TABLE II. Typical errors in the intensities of spectral lines in the methane absorption bands.

Intensity, cm ⁻¹ /(mol cm ⁻²)	<10 ⁻²⁵	10 ⁻²³	10 ⁻²⁰	10 ⁻²⁰
Relative error in the intensity	≥20%	5 - 10%	2 - 5%	1 - 2%

However, a number of fine effects seem to be neglected. For example, the vibrational dependence of the line-shift coefficients is usually believed to be rather weak, thus being neglected in the HITRAN database. Nevertheless, it may be essential for some transitions, when the bending vibration is excited due to strong centrifugal distortion effect. For narrow lines corresponding to transitions between rotational states with large values of the angular momentum it is necessary to take into account the influence of the short-range part of the potential, as well as bending of the trajectory due to collisions. Calculations performed by Robert-Bonamy method⁵⁵ have shown that the contribution of these effects may be quite considerable - up to 50%.

Nevertheless, for the majority of strong lines the results of different calculations agree quite satisfactorily not only with each other, but also with the experimental data, that normally are about 10% accurate (the best ones being accurate to 5%). This very value, most likely, must be used as an error in

calculation of the line halfwidths presented in the HITRAN database. Note, that authors of Ref. 56 have arrived at an analogous conclusion.

2.2. Influence of random and systematic errors in the line parameters on the accuracy of calculating the molecular absorption characteristics

This study has been carried out assuming that the errors in line intensities and halfwidths are uncorrelated random values described by the normal distribution, and their average value is unbiased.

The absorption coefficient α(v, z) is presented in the form

$$\alpha(v, z) = \bar{\alpha}(v, z) + \sum_i \frac{\partial \alpha(v, z)}{\partial S_i} \Delta S_i + \sum_i \frac{\partial \alpha(v, z)}{\partial \gamma_i} \Delta \gamma_i, \tag{17}$$

where ΔS_i, Δγ_j are the errors in the line intensity and halfwidth, respectively; $\bar{\alpha}(v, z)$ is the absorption coefficient at the average halfwidth and intensity of a line. The summing in formula (17) is performed over all lines contributing into the absorption coefficient at the frequency v. Since S and γ are non-correlating random values, the rms deviation can be easily calculated:

$$\sigma_{\alpha}^2(v, z) = \sum_i \left(\frac{\partial \alpha(v, z)}{\partial S_i} \right)^2 \sigma_S^2 + \sum_i \left(\frac{\partial \alpha(v, z)}{\partial \gamma_i} \right)^2 \sigma_{\gamma}^2. \quad (18)$$

The absorption coefficient and the optical thickness are related by the following linear relationship:

$$\tau(v) = \alpha(v, z) L, \quad (19)$$

where L is the path length.

Since the halfwidths and intensities are described by normal distributions, one can obtain the expression for the first two moments of the spectral transmittance:

$$\bar{P}(v) = \exp \left\{ -\bar{\tau}(v) + \frac{1}{2} \sigma_{\tau}^2 \right\};$$

$$\sigma_P^2 = \bar{P}(v) [\exp \{ \sigma_{\tau}^2 \} - 1], \quad (20)$$

where $\sigma_{\tau} = \sigma_{\alpha} L$.

Similar parameters have been obtained for the broad-band transmission function:

$$\bar{P}_{\Delta v} = \frac{1}{\Delta v} \int_{v_0 - \Delta v / 2}^{v_0 + \Delta v / 2} \bar{P}(v') dv'; \quad (21)$$

$$\sigma_P^2 = \frac{1}{(\Delta v)^2} \iint_{\Delta v} [\overline{P(v') P(v'')} - \bar{P}(v') \bar{P}(v'')] dv' dv'' =$$

$$= \frac{1}{(\Delta v)^2} \iint_{\Delta v} \bar{P}(v') \bar{P}(v'') \times$$

$$\times \{ (\exp [2 R_{\tau\tau}(v', v'')] - 1) \} dv' dv''; \quad (22)$$

$$R_{\tau\tau}(v', v'') = R_{\alpha\alpha}(v', v'') L^2; \quad (23)$$

$$R_{\alpha\alpha}(v', v'') = \sum_i \frac{\partial \alpha(v', z)}{\partial S_i} \frac{\partial \alpha(v'', z)}{\partial S_i} \sigma_S^2 +$$

$$+ \sum_i \frac{\partial \alpha(v', z)}{\partial \gamma_i} \frac{\partial \alpha(v'', z)}{\partial \gamma_i} \sigma_{\gamma}^2, \quad (24)$$

where $R_{\tau\tau}(v', v'')$ may be interpreted as the covariance coefficient between $\tau(v')$ and $\tau(v'')$. It follows from expression (22) that the σ_T value essentially depends on the behavior of the coefficient $R_{\tau\tau}(v', v'')$.

The expressions obtained are too complicated for analysis, therefore a model case has been considered for an isolated line with the Lorentz shape. In this case the first and second moments of the absorption coefficient distributions take the form:

$$\bar{\alpha}(v) = \frac{\bar{S}}{\pi} \frac{\bar{\gamma}}{(v - v_0)^2 + \bar{\gamma}^2};$$

$$\sigma_{\alpha}^2(v) = \bar{\alpha}^2(v) \left[\frac{\sigma_S^2}{S^2} + \frac{\sigma_{\gamma}^2}{\gamma^2} F^2(v) \right]; \quad (25)$$

$$R_{\alpha}(v, v') = \bar{\alpha}(v) \bar{\alpha}(v') \left[\frac{\sigma_S^2}{S^2} + \frac{\sigma_{\gamma}^2}{\gamma^2} F(v) F(v') \right],$$

$$F(v) = \frac{(v - v_0)^2 - \gamma^2}{(v - v_0)^2 + \gamma^2}. \quad (26)$$

The function $F(v) = -1$ in the vicinity of the line center ($v = v_0$); while $F(v) = 1$ in the line wing, while $F(v) = 0$ at $(v - v_0) = \gamma$. Let us consider the case when $\sigma_S/S = \sigma_{\gamma}/\gamma = \delta$. Then the correlation coefficient $r_{\alpha}(v, v') = R_{\alpha}(v, v')/\sigma_{\alpha}(v) \sigma_{\alpha}(v')$ and the rms deviation is described in the following way:

$$r_{\alpha}(0, v) = \frac{1 - F(v)}{\sqrt{2(1 + F^2(v))}};$$

$$\sigma_{\alpha}^2(v) = \bar{\alpha}^2(v) \frac{\sigma_S^2}{S^2} [1 + F^2(v)]. \quad (27)$$

It follows from the latter relationships, that the correlation coefficient equals to 1 in the vicinity of the line center; at $(v - v_0) = \gamma$ it equals to $(1/\sqrt{2})$, and it rapidly vanishes as the frequency detuning increases. Behavior of the variance of the absorption coefficient values has a more complicated character because $F^2(v)$ has a minimum at $(v - v_0) = \gamma$. Typical behavior of the covariance coefficient and the rms deviation of the absorption coefficient is presented in Fig. 1.

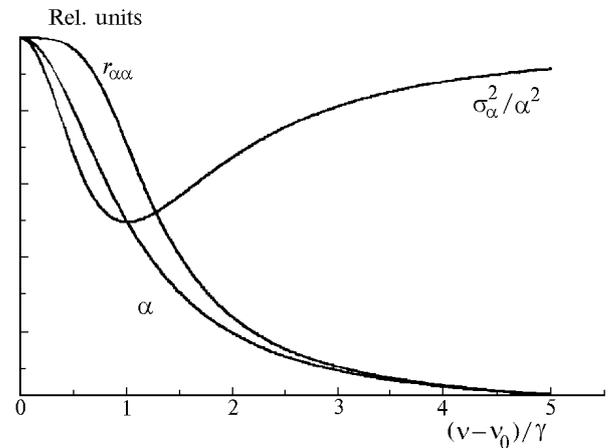


FIG. 1. Spectral dependence of the absorption coefficient, the rms deviation, and the correlation coefficient in case of an isolated line.

It follows from the qualitative consideration that the error in transmission function determined by the relationship (22) will essentially depend on the spectral interval width Δv (the error in the transmission function should decrease as Δv increases).

To verify the conclusions drawn, and to estimate actual error values, we have achieved a numerical modeling for the methane absorption band in the 1000–1400 cm^{-1} region since in that case the HITRAN-96 database provides most complete information about line intensities and halfwidths.

Typical errors in the line intensities are presented in Table II.

It is seen from Figs. 1 and 2 that the errors in calculated absorption and monochromatic transmission coefficients may be quite considerable and reach tens percent. Numerical simulations have shown that the maximum error in the transmission function calculated using a 5 cm^{-1} -wide rectangular instrumental function (the spectral interval was the same as in Fig. 2, $\nu_0 = 1302.5\text{ cm}^{-1}$) does not exceed 1%. Thus, even at the spectral resolution of 5 cm^{-1} , random errors in the spectral parameters of lines may be neglected.

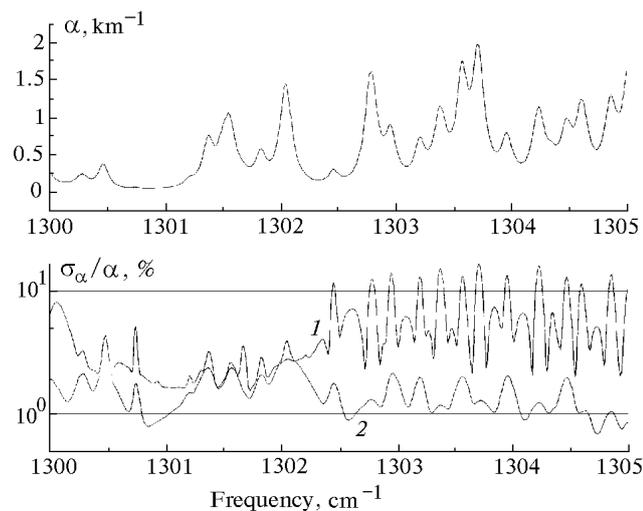


FIG. 2. CH_4 spectral dependence of the absorption coefficient and error in it: both the error in the intensity and in the halfwidth are taken into account (1); only errors in the line intensity are taken into account (2).

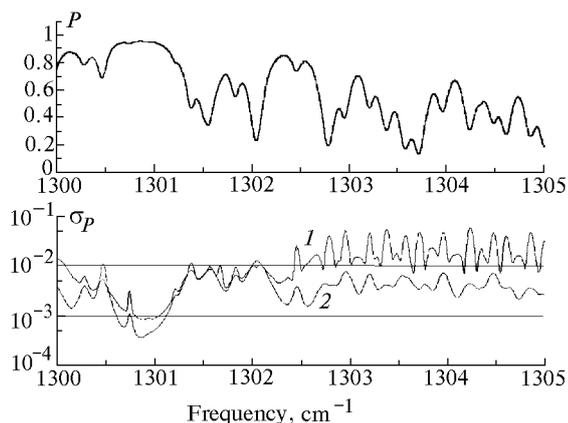


FIG. 3. CH_4 spectral dependence of the transmittance and error in it: both the error in the intensity and in the halfwidth are taken into account (1); only errors in the line intensity are taken into account (2).

It is worth noting that the error in transmission function rapidly vanishes as $\Delta\nu$ grows owing to two factors. First, the correlation coefficients between

absorption coefficients rapidly vanish at large frequency detuning and the value within the curly brackets in equation (22) also becomes small. In fact, only narrow spectral interval contributes into the integral in expression (22). Second, in the spectral regions where the absorption coefficients are small, (see Figs. 2 and 3), the spectral transmittance is close to 1 and even large uncertainties in the line parameters cause no noticeable errors in the transmittance.

Quite different situation we have in the case when there are systematic errors in the spectral line parameters. Molecular absorption coefficients of CO_2 and errors in the calculated, using the HITRAN-96 database, values for the spectral region $700\text{--}800\text{ cm}^{-1}$ are presented in Figs. 4 and 5. The k -functions method provides a possibility of illustratively representing the spectral dependence of these coefficients and errors in their values in the space of cumulative frequencies. The systematic errors have been calculated as the difference between the absorption coefficient values calculated with and without the account for errors in the line parameters. Errors in the lines parameters were taken into account by increasing the intensity and halfwidth of each line by the value corresponding to error code in the database.

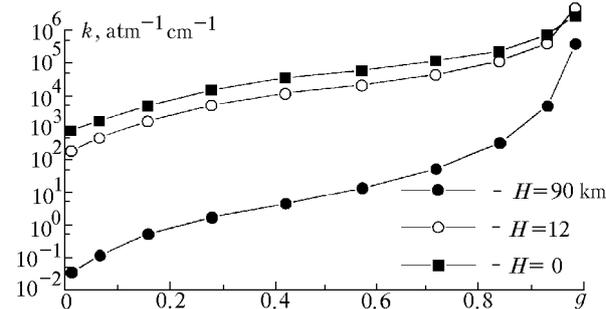


FIG. 4. The CO_2 absorption coefficient behavior in the $700\text{--}800\text{ cm}^{-1}$ spectral region.

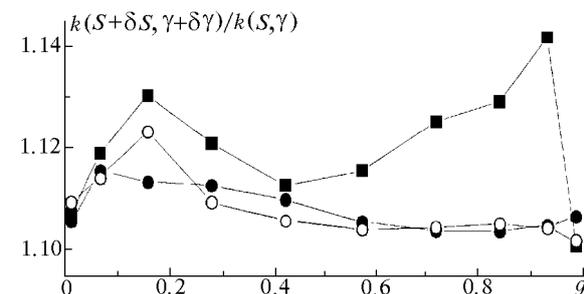


FIG. 5. The error in the CO_2 absorption coefficient.

It is seen from Fig. 5 that the spectral and height dependences of the errors in absorption coefficient are weak, that means that the errors in calculating the outgoing radiation intensity caused by the inaccuracy of spectral information can be

accounted for quite simply by introducing a constant factor for the absorption coefficient which is determined by the value of a systematic error in the integral intensity and halfwidth.

Estimations of possible errors in the outgoing radiation intensity were made using this approach for 19 channels of a HIRS-14 radiometer (Tables III and IV).

TABLE III. Error in the intensity of outgoing radiation caused by the uncertainties in the spectroscopic data. Winter at polar latitudes.

Number of channel	Center, cm ⁻¹	Radiation temperature, K	Error in radiation temperature, K	Intensity, mW/(m ² · sr · cm ⁻¹)	Error in the intensity, mW/(m ² · sr · cm ⁻¹)
1	668.90	222.75	0.21	48.032	0.197
2	679.36	217.30	0.04	42.035	0.038
3	689.63	217.26	0.01	41.018	0.013
4	703.56	223.71	0.46	45.443	0.430
5	714.50	231.49	0.65	51.819	0.648
6	732.28	241.15	0.63	59.998	0.693
7	749.64	248.93	0.39	66.768	0.463
8	898.67	257.16	0.00	57.016	0.004
9	1028.31	238.90	0.82	26.515	0.561
10	796.04	256.33	0.07	69.704	0.083
11	1360.95	245.85	0.48	10.434	0.160
12	1481.00	233.76	0.50	4.251	0.083
13	2191.32	249.15	0.48	0.400	0.010
14	2207.36	242.80	0.79	0.267	0.011
15	2236.39	235.69	0.89	0.157	0.008
16	2268.12	221.75	0.36	0.056	0.001
17	2420.24	254.13	0.24	0.189	0.002
18	2512.21	257.12	0.01	0.148	0.000
19	2647.91	257.09	0.01	0.081	0.000

TABLE IV. Error of outgoing radiation intensity caused by the uncertainties of the spectroscopic data. Summer at midlatitudes.

Number of channel	Center, cm ⁻¹	Radiation temperature, K	Error in radiation temperature, K	Intensity, mW/(m ² · sr · cm ⁻¹)	Error in the intensity, mW/(m ² · sr · cm ⁻¹)
1	668.90	238.74	0.39	64.436	0.429
2	679.36	228.04	0.33	52.090	0.324
3	689.63	226.59	0.13	49.613	0.128
4	703.56	235.25	0.64	56.896	0.676
5	714.50	246.74	0.91	68.444	1.066
6	732.28	261.24	1.06	84.388	1.401
7	749.64	272.71	0.83	98.028	1.201
8	898.67	291.98	0.18	104.420	0.289
9	1028.31	268.88	1.23	53.013	1.333
10	796.04	287.05	0.42	113.262	0.668
11	1360.95	258.98	0.74	15.627	0.337
12	1481.00	242.48	0.57	5.902	0.121
13	2191.32	278.54	0.88	1.520	0.053
14	2207.36	269.30	1.30	0.967	0.054
15	2236.39	257.38	1.37	0.495	0.032
16	2268.12	235.75	0.68	0.135	0.005
17	2420.24	287.77	0.47	0.937	0.018
18	2512.21	293.80	0.03	0.856	0.001
19	2647.91	292.81	0.10	0.494	0.002

According to data presented in Table I, the errors in the integral intensities of the bands fall within 5 to 10% interval. Since these estimations have been made by summing the errors in individual lines, those are

upper-limit estimations. The error in the spectral line halfwidths of 10% value is the upper-limit estimation as well. In view of the aforesaid, the modeling performed has assumed the same total error of 10% in the

spectroscopic data for H₂O, O₃, and N₂O molecules within all channels of the radiometer, while for CO₂ the error is taken to be 8%. For water vapor continuum the error has been taken to be 5% .

The calculations have shown that in the channels where the absorption in the atmosphere is weak (for example, the 19th channel), the errors caused by the uncertainties in the spectroscopic data are small as well. In the channels where absorption is strong, the error is larger. However, the maximum error is observed for the channels where the contribution coming from the continuum is essential enough. The results obtained are in a qualitative agreement with the data from Ref. 57.

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