Calculation of transmission functions at small pressures

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Analytical expressions for the expansion coefficients in the series of exponents $s(g)$ are derived in the case of an individual line with the Lorentzian, Doppler, and Voigt contours. The method of estimation of the absorption function at small pressures is suggested based on the asymptotic value of the corresponding integral, written with the use of a series of exponents for the individual line and for the arbitrary number of lines. It is shown numerically that asymptotic estimations may be used in a wide range of pressures and are simple in applications. Qualitative evaluations of their areas of applicability are given. The availability is given of bending points on the curve $s(g)$ in places corresponding to the line maxima, and their possible influence on the calculation accuracy at small pressures is noted.

1. Introduction

Climatic models impose heavy demands on calculations of radiation propagation in the atmosphere.

Line-by-line calculations of the absorption by atmospheric gases with regular contour of spectral lines are suitable in the accuracy, however, are unacceptable in the radiation blocks of climatic models, because they consume plenty of time.

The solution of the problem of exact calculation turned out to be possible when using the expansions of radiation values in the series of exponential functions. This method, known as the k-distribution method, is now the most widespread in considering the radiation characteristics of the atmosphere. As a rule, the ways of finding the coefficients of such expansions are reduced to different methods of minimization, i.e., to a purely calculational procedure. The algorithms, which use the series of exponential functions in large models, run into problems when there is a need to make the calculations at small pressures in the high atmospheric layers. This is associated with the fact that because of specific behavior of the ordered absorption coefficients $s(g)$ at small pressures we must consider a great number of terms in a series of exponential functions for obtaining the necessary accuracy.

This problem has been detailed in the paper by Chon et al.[1] Hence, when calculating the transmission function for water vapor, it was shown that the contribution to the rate of cooling at pressures less than 1 mbar took place from very small part (< 0.005) of spectrum close to centers of absorption bands where the absorption coefficients varied by 4 orders of magnitude. This requires at least 100 terms in the k-distribution to calculate exactly the cooling rate.

In one of the most developed models of radiation transfer[2] the IR-range (10–3000 cm^{-1}) is divided into 16 bands. Each spectral band is divided, in its turn, into 16 intervals in g-space, in which 7 intervals are placed between $g = 0.98$ and $g = 1.0$, that is made to determine exactly the cooling rate under conditions when the main contribution is made by the line centers in the band, in other words, the part of k-distribution with the values of g about 1. It turns out that the calculation efforts become the greater, the lesser is the absorption coefficient and, consequently, the lesser is its contribution to the transmission function. Such a situation casts some doubt upon the rationality of the situation, when for calculating small values more time is required than for large values.

The typical form of the absorption coefficient is given in Fig. 1 for a part of the CO_2 spectrum at large and small pressures. At small pressures, evidently, the absorption is determined by narrow spectral regions close to strong lines. This is reflected in the difference of the behavior of $s(g)$ (see Fig. 2) for the same spectral range.

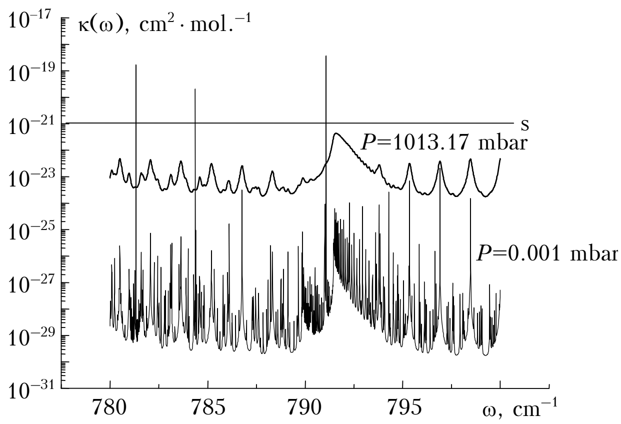

Fig. 1. CO_2 spectrum. $T = 296$ K, Lorentz contour up to 10 cm^{-1}, the interval equals 0.001 cm^{-1}, 780–800 cm^{-1}.

With the pressure decrease (see Figs. 1 and 2) the curves $s(g)$ (which remain monotonous) increase

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sharply in the vicinity of $g = 1$, as indicated above, and are determined by the peaks of the strongest lines in the range under study.

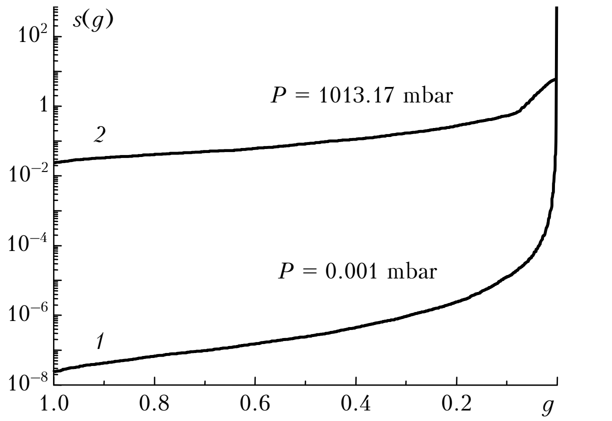

Fig. 2. Function $s(g)$ for CO_2. $T = 296$ K, Lorentz contour up to 10 cm^{-1}, the interval equals 0.001 cm^{-1}, 780–800 cm^{-1}.

It should be noted that, in contrast to the formula, commonly used to determine $s(g)$ minimization, there exist exact formulae for coefficients of expansion of radiation values in series of exponents,[3] expressed in terms of the absorption coefficients, which enable us to simplify considerably the necessary calculations. Moreover, the approach developed in Ref. 3 affords a new way to consider the problem associated with the situation of small pressures in the middle and upper atmosphere.

Chapter 1 describes the obtained analytical expressions for $s(g)$ for the Lorentzian, Doppler, and Voigt contours in the case of one line. In Chapter 2 an asymptotic estimation is given for the transmission function of one line with the use of $s(g)$ obtained in Chapter 1.

In chapter 3 the proposed asymptotic method is generalized for the case of the presence of an arbitrary number of lines in the considered interval.

2. Values of $S(g)$ for an isolated line

Now we present the general formulae for the expansion coefficients of radiation values in the series of exponents expressing them through the absorption coefficients (see, for example, Refs. 3–5).

The transmission function $P(\omega)$ in the frequency range $\Delta\omega = \omega'' - \omega'$ is of the form

$$P(z) = \frac{1}{\Delta\omega}\int\limits_{\omega'}^{\omega''} e^{-z\kappa(\omega)} d\omega = \int\limits_0^\infty ds\, f(s)\, e^{-sz} =$$

$$= \int\limits_0^1 dg\, e^{-zs(g)} = \sum_\nu b_\nu e^{-zs(g_\nu)}; \qquad (1)$$

$$f(s) = \frac{1}{2\pi i}\int\limits_{c-i\infty}^{c+i\infty} dz\, P(z) e^{sz}; \qquad (2)$$

$$g(s) = \int\limits_0^s f(s) ds = \frac{1}{2\pi i}\int\limits_{c-i\infty}^{c+i\infty} \frac{P(z)}{z} e^{sz} dz =$$

$$= \frac{1}{\Delta\omega}\int\limits_{\kappa(\omega)<s;\,\omega\in[\omega',\omega'']} d\omega = 1 - \frac{1}{\Delta\omega}\int\limits_{\kappa(\omega)>s;\,\omega\in[\omega',\omega'']} d\omega, \qquad (3)$$

where z is the optical depth, $\kappa(\omega)$ is the spectral absorption coefficient, $f(s)$ is the Laplace transform $P(z)$, $g(s)$ is the Laplace transform of the function $P(z)/z$, $s(g)$ is the function inverse to $g(s)$; and $s(g)$ denotes the ordered by magnitude values of $\kappa(\omega)$ for $\omega \in [\Delta\omega]$; b_ν, g_ν are ordinates and abscissas of the corresponding quadrature formula. The construction of the function $g(s)$ is shown in Fig. 3.

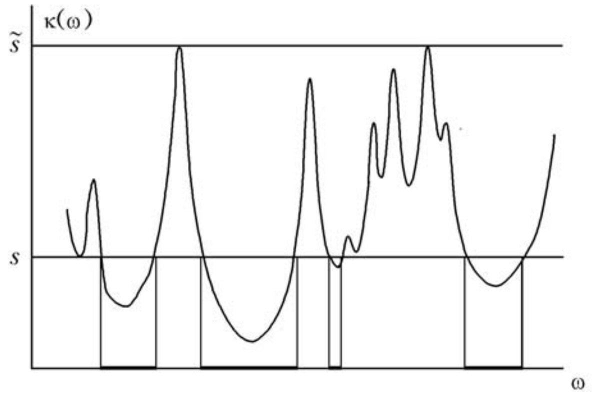

Fig. 3. Scheme of integration for $g(s)$. For a given S the value g is the sum of intervals, in which $\kappa(\omega) < s$.

Relation (3) enables us to derive the analytical expressions for $s(g)$ of one line in the case of the most usable contours: Lorentz, Doppler, and Voigt. Consider some methods of deriving $s(g)$. One of them is the use in relation (3) of definition g as a sum of frequency ranges, in which $\kappa(\omega) < s$.

Assume that we have the Lorentz contour (see Fig. 4), Q, a, ω_0 are the intensity, the collision half-width, and the spectral line centre, respectively, $\Delta\omega = \omega_2 - \omega_1$ is the spectral range, where the absorption is considered:

$$\kappa(\omega) = \frac{Q\alpha}{\pi}\frac{1}{(\omega-\omega_0)^2+\alpha^2}. \qquad (4)$$

For a certain value S of the absorption coefficient

$$s = \frac{Q\alpha}{\pi}\frac{1}{(\omega-\omega_0)^2+\alpha^2},$$

whence it follows that

$$(\omega-\omega_0) = \pm\sqrt{\frac{Q\alpha}{\pi s} - \alpha^2} \text{ and } \omega' - \omega'' = 2\alpha\sqrt{\frac{Q}{\pi s\alpha} - 1}.$$

The part of the range, in which $k > S$,

$$g(s) = \frac{\omega' - \omega''}{\Delta\omega} = \frac{2\alpha}{\Delta\omega}\sqrt{\frac{Q}{\pi s\alpha} - 1}. \qquad (5)$$

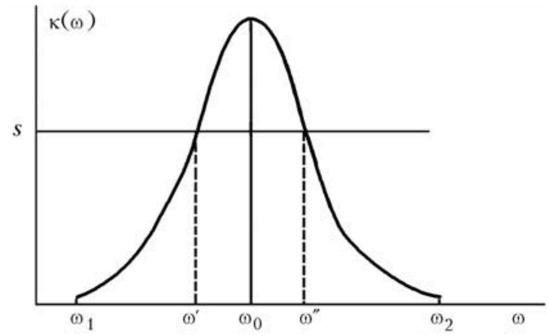

Fig. 4. To the calculation of $s(g)$ for Lorentz contour.

Hence, the exact formula for $s(g)$ in the case of one line with the Lorentz contour is

$$s(g) = \frac{Q}{\pi\alpha}\frac{1}{1+\left(\frac{\Delta\omega}{2\alpha}\right)^2(1-g)^2}. \quad (6)$$

For the Doppler line with the halfwidth $\Delta\omega_D$

$$I(\omega) = \frac{1}{\sqrt{\pi}\Delta\omega_D}\exp\left[-\left(\frac{\omega-\omega_0}{\Delta\omega_D}\right)^2\right] \quad (7)$$

we have

$$s = \frac{Q}{\sqrt{\pi}\Delta\omega_D}\exp\left[-\left(\frac{\omega-\omega_0}{\Delta\omega_D}\right)^2\right],$$

$$g = 1 - 2\frac{\Delta\omega_D}{\Delta\omega}\sqrt{\ln\left(\frac{Q}{s\sqrt{\pi}\Delta\omega_D}\right)},$$

$$s(g) = \frac{Q}{\sqrt{\pi}\Delta\omega_D}\exp\left[-\left(\frac{(1-g)^2\Delta\omega^2}{4\Delta\omega_D{}^2}\right)\right]. \quad (8)$$

Equation (6) can be also derived from Eq. (3), using the definition g as an integral of $P(z)/z$ through changing the variables

$$\omega - \omega_0 = \alpha\tan\varphi, \quad d\omega = \frac{\alpha}{\cos^2\varphi}d\varphi$$

and evaluating then the obtained contour integral. However, there is a simpler method of recording $s(g)$, used for any symmetric contour.

Let $s = \varphi(x)$ be the even function of the dimensionless variable x (see Fig. 5). It is evident that the interval value $[a, b] = 2x$ ($x = \varphi^{-1}(s)$ by definition of the inverse function).

Again, $[a, b] = 1 - g$ (by definition (3)), from where

$$\frac{1-g}{2} = \varphi^{-1}(s) \text{ or } s = \varphi\left(\frac{1-g}{2}\right).$$

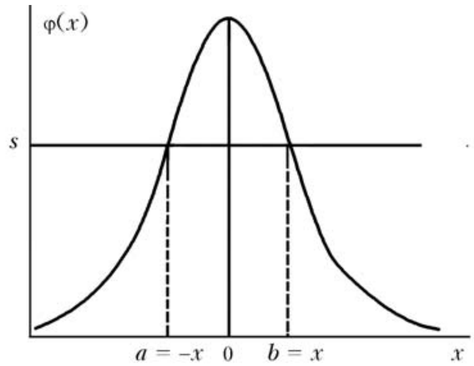

Fig. 5. To the construction of $s(g)$ for the arbitrary even function $\varphi(x)$.

If in the line contour $f(\omega - \omega_0)$ we go to the variable x

$$\omega - \omega_0 = ax, \text{ then } f(\omega - \omega_0) = f(ax) \equiv \varphi(x).$$

We can write $\frac{1-g}{2} = \frac{\Delta\omega}{a}$, where $\Delta\omega$ is the considered frequency range. Then

$$f(\omega-\omega_0) = f\left(\frac{(1-g)\Delta\omega}{2}\right), \quad s(g) = f\left(\frac{(1-g)\Delta\omega}{2}\right), \quad (9)$$

that is, the function $s(g)$ can be derived when substituting in the expression for the difference contour $\omega - \omega_0$ by $\frac{(1-g)\Delta\omega}{2}$. As is seen, the expressions for the Lorentz and Doppler contours confirm this rule. Now write the expression for $s(g)$ in the case of the Voigt contour.

The Voigt contour is of the form:

$$\kappa(\omega-\omega_0) = \frac{Q}{\omega_i}\left(\frac{mc^2}{2\pi kT}\right)^{1/2}\left(\frac{a}{\pi}\right)\int_{-\infty}^{\infty}\frac{e^{-y^2}}{a^2+(\xi-y)^2}dy =$$

$$= \frac{Q}{\beta}(\ln 2)^{1/2}\left(\frac{a}{\pi}\right)\int_{-\infty}^{\infty}\frac{e^{-y^2}}{a^2+(\xi-y)^2}dy; \quad (10)$$

$$a = \frac{\alpha}{\omega_0}\left(\frac{mc^2}{2\pi kT}\right)^{1/2} = \frac{\alpha}{\Delta\omega_D}(\ln 2)^{1/2},$$

where a and $\Delta\omega_D$ are the collision and Doppler halfwidths of a spectral line:

$$s(g) = \frac{Q}{\Delta\omega_D}(\ln 2)^{1/2}\left(\frac{a}{\pi}\right)\int_{-\infty}^{\infty}\frac{e^{-y^2}}{a^2+(\xi-y)^2}dy, \quad (11)$$

where

$$\xi = \frac{\omega-\omega_0}{\omega_0}\left(\frac{mc^2}{2\pi kT}\right)^{1/2} = \frac{\omega-\omega_0}{\Delta\omega_D}(\ln 2)^{1/2} =$$

$$= \frac{(1-g)\Delta\omega}{2\Delta\omega_D}(\ln 2)^{1/2}.$$

The values of $s(g)$ calculated by formulae derived here and immediately with the use of relations (3) through the absorption coefficient are in complete agreement, when the frequency range is considered, in which the line is located symmetrically in its centre.

3. Asymptotic estimation for the transmission function of one line

Characteristics of the $s(g)$ behavior at high and low pressures can be found in Fig. 2. In the case of one line these characteristics would remain as before, and the value of transmission at low pressures is determined by a small area close to $g = 1$.

For the considered in chapter 2 contours at $g = 1$

$$s'(1) = 0, \quad s''(1) < 0. \tag{12}$$

For the Lorentz contour (6) we have

$$s(1) = \frac{Q}{\pi\alpha}, \quad s''(1) = -\frac{Q\Delta\omega^2}{2\pi\alpha^3}.$$

For the Doppler contour (7)

$$s(1) = \frac{Q}{\sqrt{\pi}\Delta\omega_D}, \quad s''(1) = -\frac{Q\Delta\omega^2}{2\sqrt{\pi}\Delta\omega_D{}^3}.$$

In the case of the Voigt contour (10)

$$s(1) = \gamma_1 \int_{-\infty}^{\infty} \frac{e^{-y^2}}{a^2 + y^2} dy;$$

$$s''(1) = 2\gamma^2\gamma_1 \int_{-\infty}^{\infty} \frac{-e^{-y^2}\left[a^2 - 3y^2\right]}{\left(a^2 + y^2\right)^3} dy;$$

$$\gamma = \frac{\Delta\omega}{2\Delta\omega_D}(\ln 2)^{1/2}, \quad \gamma_1 = \frac{Q}{\Delta\omega_D}(\ln 2)^{1/2}\left(\frac{a}{\pi}\right).$$

The conditions (12) have made it possible to use the asymptotic estimation of the transmission function in the vicinity of $g = 1$ in case of low pressures. To follow the conditions of the use of the method of steepest descents, we consider the expression A connected with the unknown transmission functions in the form

$$A = \int_0^1 dg\, e^{\varphi(g)}, \quad \varphi(g) = \ln\left(1 - e^{-us(g)}\right). \tag{13}$$

This substitution is oriented to the problem physics, to low pressures in the upper atmospheric layers, i.e., it proposes the smallness of u. Further the standard procedure corresponding to the method of steepest descents[6] and the relation $P = 1 - A$ following from Eq. (13) give:

$$P_{as} = 1 - \sqrt{\frac{\pi}{2}}\left(1 - e^{-us(1)}\right)^{3/2} e^{\frac{1}{2}us(1)} \Big/ \sqrt{u\left|s''(1)\right|}. \tag{14}$$

At $u \to 0$ equation (14) results in $P_{as} = 1$.

Now we present an example of calculation of the absorption function using the asymptotic evaluation (14), see Fig. 6.

Selected conditions of the calculation refer to the standard atmosphere of mid-latitude summer. It is evident that the asymptotic estimation, which is independent of the precision in calculating the absorption coefficient, coincides with the *line-by-line* calculation at mean pressures and begins its deviation from it at low pressures and small distances. Note that the Doppler contour form was used in the asymptotic calculation.

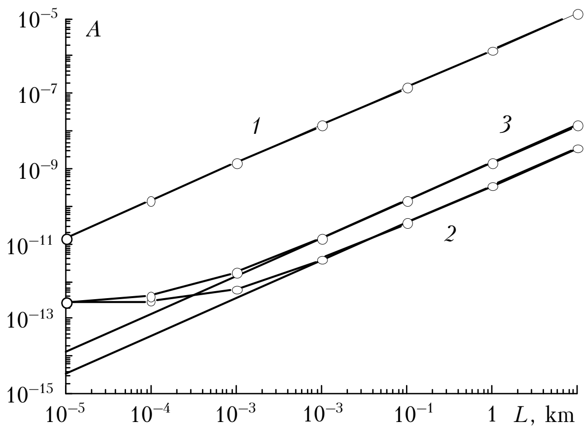

Fig. 6. The absorption function $A = 1 - P$ for one line, calculated using the asymptotic estimation (13) (curves) and the method *line-by-line* (points). (*1*) is the total pressure $p = 0.1$ mbar; $T = 230$ K; (*2*) is $p = 0.001$ mbar, $T = 190$ K; (*3*) is $p = 0.0001$ mbar, $T = 230$ K; a fraction of CO_2 is $3 \cdot 10^{-4}$.

At small pressures just the region of fast change of $s(g)$ makes the predominant contribution to the integral P. This region is the "influence zone" of Δg (in terms of asymptotic analysis), which is estimated by the standard way[7]:

$$\Delta g = O\left(\sqrt{\frac{2}{\varphi''(1)}}\right), \quad \varphi''(1) = \frac{e^{-us(1)}}{1 - e^{-us(1)}} u\left|s''(1)\right|. \tag{15}$$

For the case, considered in Fig. 6, $\sqrt{2/\varphi''(1)}$ equals 0.01 cm^{-1}.

This also gives the limitation for u, determining to some extent the applicability limits for Eq. (14):

$$\sqrt{\frac{\pi}{2}} \frac{e^{\frac{1}{2}us(1)}}{\sqrt{u\left|s''(1)\right|}} < 1. \tag{16}$$

Introduce the following designations:

$$f_1 = e^{\frac{1}{2}us(g)}, \quad f_2 = \sqrt{\frac{2}{\pi}}\sqrt{u|s''(g)|}.$$

The condition of the asymptotic form applicability is $f_1 > f_2$. As we can see from Fig. 7, for the spectral range 780.567–780.7, the applicability field of the asymptotic form is propagated from $L^*\kappa = 10^{-5}$ to the direction of the smaller $L^*\kappa$.

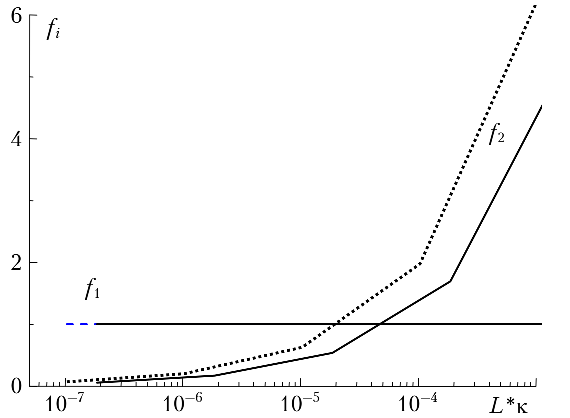

Fig. 7. Limitations imposed on the absorbing masses, following from (16). Dash lines f_1, f_2 correspond to a total pressure of 10 mbar, a CO_2 pressure of $3\cdot10^{-3}$ mbar, $T = 238$ K; solid curves f_1, f_2 correspond to a total pressure of 1 mbar, a CO_2 pressure of $3\cdot10^{-4}$ mbar, $T = 275$ K. Curves f_1, f_2 at lower pressures almost do not differ from those at 1 mbar.

4. Asymptotic estimation for the transmission function at an arbitrary number of lines in the range under study

At small pressure of the buffer gas the lines are not too far overlapped, because of their small halfwidths. Therefore, to point out some details, typical for such a situation, we consider the limiting case of non-overlapping lines (see Fig. 8). Here j is the line index.

In this case (direct consequence of Eq. (1))

$$P = \sum_j \frac{\Delta\omega_j}{\Delta\omega} P_j(z) = \sum_\nu b_\nu \sum_j \frac{\Delta\omega_j}{\Delta\omega} \exp[-zs_j(g_\nu)], \quad (17)$$

where $g(s)$ is constructed for each line and the transition to a series of exponents is performed for the P_j-function of transmission of an isolated line.

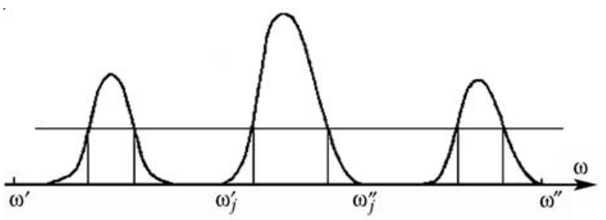

Fig. 8. Schematic spectrum from small pressures.

It is obvious that relation (17) increases the number of terms in the series. Further, the consequence of Eqs. (2) and (3) will be (for the spectrum in Fig. 8)

$$g(s) = \sum_j g_j(s). \quad (18)$$

However,

$$s(g) \neq \sum_j s_j(g). \quad (19)$$

Here $g(s)$ and $s(g)$ are constructed for a complete spectrum. Using the same designations the application of quadrature formulae gives

$$\sum_\nu b_\nu \sum_j \frac{\Delta\omega_j}{\Delta\omega} e^{-zs_j(g_\nu)} = \sum_\nu b_\nu \, e^{-zs(g_\nu)}. \quad (20)$$

However, equation (20) does not remove the inequality (19). In other words, even the asymptotic (Fig. 8) assumption about isolated lines does not remove the procedure of construction of $s(g)$ by reducing it to $s_j(g)$.

Thus, $s(g)$ for the range containing isolated lines, cannot be expressed through s_j for isolated lines. Although we can construct the expansions for isolated lines throughout the range Δw and use them in Eq. (20), but in this case the number of expansion terms increases considerably (in proportion to the number of lines). However, as we can see from Figs. 1 and 8, the transmission at small pressures is determined by the sum of the strongest lines,

$$P = \sum_j \frac{\Delta\omega_j}{\Delta\omega} P_j,$$

and in the case of asymptotic estimation we have

$$P_{as} = \sum_j \frac{\Delta\omega_j}{\Delta\omega} P_{j\,as}. \quad (21)$$

Figure 9 shows an example of calculation of the absorption function by Eq. (21) with successive taking account of the strongest lines in the range 780–790 cm^{-1} for several sets of conditions, corresponding to the mid-latitude summer atmosphere.

The calculation of *line-by-line* and the asymptotic estimation agree for intermediate distances and pressures (curves *2*, *3*). Deviations are observed at high pressures and long distances (curve *1*) and, on the contrary, for small pressures and distances (curves *1* and *2*). Asymptotic estimations conceptually are valid for small pressures and are preferable under these conditions than *line-by-line* results. It is hardly probable that the precise numerical criteria of their applicability can be indicated. In any case, they can be used, when the lines can be considered as Doppler ones, and, as is shown in Fig. 9, their coincidence with *line-by-line* calculation enables us to state that they are also valid for pressures, which are not very small. The calculation with the use of asymptotic estimations can be made, as we can see from the above formulae, simply and rapidly.

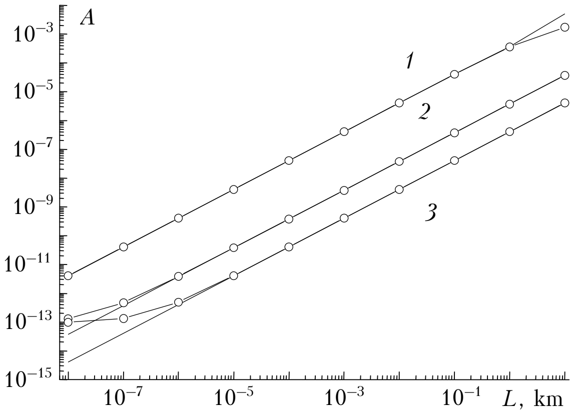

Fig. 9. The absorption function $A = 1 - P$ for the interval 780–790 cm^{-1}, calculated using the asymptotic estimations (13) (curves) and by the *line-by-line* method (points). (*1*) is the total pressure $p = 0.1$ mbar, $T = 230$ K, (*2*) is $p = 0.01$ mbar, $T = 170$ K; (*3*) is $p = 0.0001$ mbar, $T = 230$ K; a fraction of CO_2 is $3 \cdot 10^{-4}$.

The peculiarities of the behavior of $s(g)$ should be noted, which can be essential at small pressures. For the jth line

$$g_j(s) = 1 - f_j(s).$$

For several lines

$$g(s) = N - \sum_j f_j(s).$$

Let us find the derivative of $s(g)$ as the derivative of the inverse function

$$\frac{\partial s}{\partial g} = \frac{1}{\partial g / \partial s} = -\frac{1}{\left(\sum_j f_j(s)\right)'}.$$

$g = 1$ corresponds to the point $s = s_{j\max}$ for j-th line. At this point $g'_s = \infty$ and the corresponding term in the sum becomes zero, that is, $s'_g = 0$. The second derivative at this point $\frac{\partial^2 s}{\partial g^2} = -\frac{\partial^2 g / \partial s^2}{(\partial g / \partial s)^2}$ also becomes zero. Figure 10 shows this case. This implies that one the function $s(g)$ there appear the points of inflection. The case of two lines at frequencies 780.633483 and 780.756586 cm^{-1} in the range 780.6–780.8 cm^{-1} is given in Fig. 11.

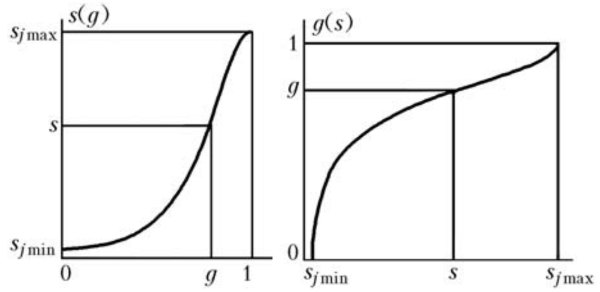

Fig. 10. To the construction of the inverse function for $s(g)$.

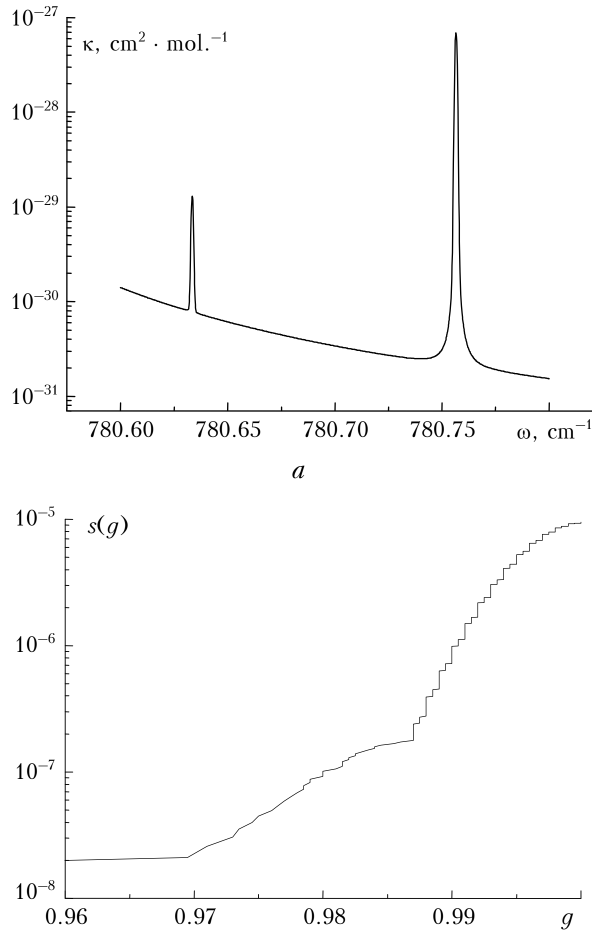

Fig. 11. Spectral lines in the range 780.6–780.8 cm^{-1} (*a*) and the corresponding function $s(g)$, having the inflection point (*b*).

The availability of such points of inflection on the curve $s(g)$ can be seen close to its maximum at any pressures (see Fig. 12).

For high pressures the availability of points of inflection is not of great importance in calculations because the contribution of great g is small. In case of low pressures these points may be important, because the transmission is determined just by the range g close to maximum.

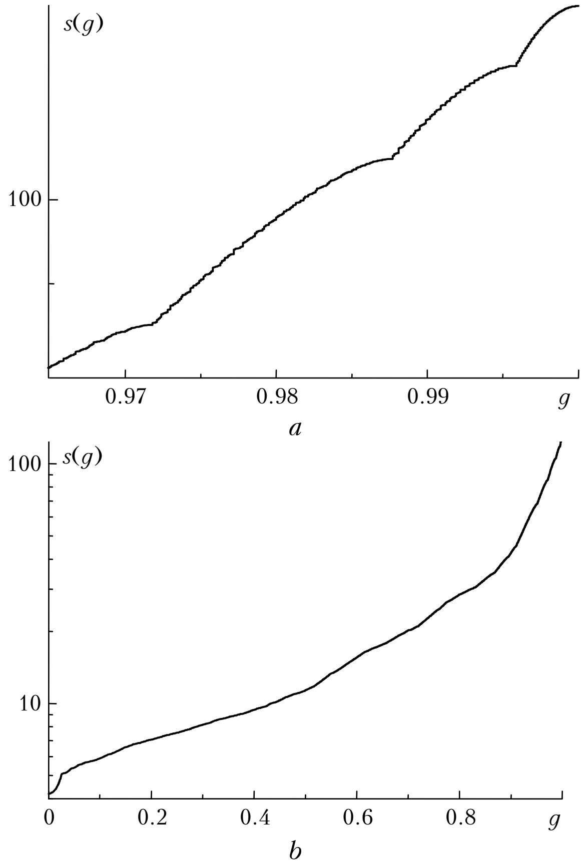

Fig. 12. The transmission function of CO_2 in the range 780–880 cm^{-1}, the total pressure p = 1000.0 mbar, the step is 10^{-3} cm^{-1}; (*a*) is the interval of g close to maximum; (*b*) is the interval of g at [0,1].

Conclusion

Earlier, the authors have developed an original approach for obtaining the expansions of radiation values in the exponential series based on the theory of Dirichlet series (Refs. 3–5 and the references). Using this approach, the analytical expressions were derived for the expansion coefficients of transmission functions in the exponential series through the absorption coefficients for homogeneous (see Eq. (3)) and inhomogeneous media, for integrals with the source function, as well as directly for radiation fluxes. In addition to purely calculational advantages as compared with obtaining $s(g)$ by minimization, the analytical expressions of the type (3) have made it possible to perform a detailed analysis of characteristics of k-distribution coefficients.

Thus, based upon the determination (3) of g, as a sum of frequency ranges, in which $\kappa(\omega) < s$, we managed to derive formulae for coefficients of exponent series of s(g) in case of one line with Lorentz, Doppler, and Voigt contours. Analysis of derivative function of $s(g)$ has revealed a more detailed structure of this curve. It turns out that at a general increasing character its points of inflection correspond to line maxima, that can have an effect on the calculation accuracy at small pressures.

The structure of $s(g)$ at small pressures has made it possible to write the asymptotic estimation for the integral, presenting the transmission function in case of one line and an arbitrary number of lines. The calculations made for CO_2 absorption in the 15 μm range have shown that the asymptotic estimations can be used in the wide pressure range, where their results coincide with *line-by-line* calculations, having the advantage in the simplicity of the formulae and in the assumption of the calculation time.

On the whole, the obtained results have shown that the mathematical approaches in some cases can yield the interesting results and favor the understanding better than the direct numerical simulation.

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