On thermodynamic dependence of coefficients in expansion of radiation characteristics into exponential series

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The method for determining one-parameter approximation formulas for atmospheric transmission functions in given spectral intervals, which was proposed earlier, used exact expressions for coefficients of expansion of the studied functions in exponential series and was intended for height distribution of temperatures and pressures in standard atmospheric models. In this paper, we find an approximation for coefficients of expansion into exponential series as functions of temperature and pressure for the whole range of temperatures and pressures observed in the atmosphere. This approximation can be applied to any height distribution of thermodynamic parameters. Possibilities of the approximation are illustrated by some examples with calculation of radiation flows caused by CO_2 absorption in a band of 15 μm.

Introduction

Before appearance of multitude *line-by-line* calculations, radiation flows were calculated with the use of the models of absorption bands and different ways to replace absorption on heterogeneous paths by absorption on equivalent homogeneous ones.

In spite of all accuracy advantages of the *line-by-line* method (when a proper form of the spectral line contour is used) in comparison with band models, it consumes a significant computation time. Therefore, the absorption coefficients, calculated by the *line-by-line* method at different pressures and temperatures, are used, as a rule, in radiation blocks of climatic models to find coefficients of expansion of transmission functions in exponential series with a small number of terms.[1,2] Then they are applied in calculations of radiation characteristics and implicitly contain information about thermodynamic dependences of the absorption coefficient.

Another way to take into account the dependence of expansion coefficients in exponential series on the temperature and pressure is to obtain approximation formulas for them, which, to a certain extent, mean a return to models of absorption along equivalent homogeneous paths. A similar way was realized by Chou et al.,[3] who obtained the so-called one-parameter approximation formulas for transmission, being a function of only a reduced absorbing mass. These formulas are sums of exponential terms, which are not connected directly with the above-mentioned expansions of radiation parameters in exponential series. Nevertheless, they are very convenient for application in radiation blocks because of their simplicity and universality. In particular, they are used in the climatic model of the Institute of Numerical Mathematics of the Russian Academy of Sciences.[4] The formulas[3] do not describe absorption at large heights sufficiently well because of difficulties in calculation of transmission at low pressure. The authors of Ref. 5 failed to obtain similar formulas for ozone in a band of 9.6 μm, therefore they used interpolation tables. Besides, it is desirable to have more adequate formulas to estimate the absorption caused by line wings in some parts of the spectrum, in particular, in the H_2O interval of 8–20 μm.

The possibility to obtain one-parameter approximation formulas for coefficients of expansion of radiation characteristics into exponential series in arbitrary spectral intervals for a given height distribution of thermodynamic parameters within the frames of standard models of the atmosphere was shown earlier.[6,7]

In this paper, we study the possibility to approximate coefficients of expansion into exponential series depending on the temperature and pressure applicable to an arbitrary height distribution of thermodynamic parameters.

1. One-parameter approximation formulas for transmission

In Ref. 3, one-parameter scaling reduces a heterogeneous path to an equivalent homogeneous path with selected pressure p_r and temperature T_r. The transmission along such a path depends only on the reduced amount of a matter. The absorption coefficient at an arbitrary pressure and temperature is extrapolated from the absorption coefficient at the selected pressure and temperature:

$$k_\nu(p,T) = k_\nu(p_r,T_r)(p/p_r)^m f(T,T_r), \qquad (1)$$

where m is a positive number close to 1; f is the multiplier that takes into account the temperature change. Transmission of a layer with arbitrary p, T,

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and absorbing mass u averaged over the zenith angle θ ($\theta = \cos^{-1}\mu$), is defined by the formula

$$\tau_\nu(u,p,T) = 2\int_0^1 \exp\left[-k_\nu(p,T)u/\mu\right]\mu\,d\mu. \quad (2)$$

In one-parameter scaling, transmission is reduced to

$$\tau_\nu(u,p,T) \approx \tau_\nu(w) = 2\int_0^1 \exp\left[-k_\nu(p_r,T_r)w/\mu\right]\mu\,d\mu, \quad (3)$$

where w is the reduced absorbing mass:

$$w = u(p,p_r)^m f(T,T_r). \quad (4)$$

As is seen from comparison of Eqs. (1) and (4), scaling of the absorption coefficient is equivalent to scaling of the absorbing mass.

The functions of transmission from the layer j_1 to the layer j_2, used in calculations of radiation flows,[3] have the form of a sum of exponential terms

$$\tau(j_2;j_1) = \sum_{i=1}^{m} c_i \exp\left(-1.66 k_i^{(j_s)} w(j_2,j_1)\right), \quad (5)$$

where $k_i^{(j_s)} = n^{(j_s)} k_{i-1}^{(j_s)}$ are constants; $w(j_1,j_2)$ is the corresponding absorbing mass. Approximation formulas of the form (4), where u is the amount of the absorbing substance; p and T are pressure and temperature of the considered atmospheric layer;

$$f(T,T_r) = 1 + a(T-T_r) + b(T-T_r)^2 \quad (6)$$

are used in Ref. 3 for the CO_2 absorbing masses.

Numerical coefficients in Eqs. (4)–(6) were obtained in Ref. 3 for each of the spectral intervals for a given division of the IR range into 10 spectral intervals $j_s = 1, ..., 10$.

2. Approximation formulas for coefficients of expansion of transmission functions into exponential series

For a homogeneous path, expansion of transmission functions into exponential series means the existence of the expression[1,2]

$$P(x) = \frac{1}{\Delta\omega}\int_{\omega'}^{\omega''} e^{-x\kappa(\omega)}d\omega = \sum_\nu b_\nu e^{-xs(g_\nu)}. \quad (7)$$

The coefficients of expansion into exponential series are usually calculated by the minimization methods, and the abscissas of the exponential series and coefficients of the terms are obtained from a purely numerical procedure (see, for instance, Ref. 8). In addition, there is a way that yields exact analytical expressions for parameters of an exponential series in the case when the spectral interval, the number of terms, and type of the quadrature formula are preset.[9] Here, only $s(g)$ depend on thermodynamic parameters. For instance, for the transmission function in the case of a homogeneous medium (7), the expression for $g(s)$, which is the inverse to $s(g)$, has the form

$$g(s) = \frac{1}{\Delta\omega}\int_{\kappa(\omega)\le s} d\omega, \quad \omega \in [\omega',\omega''], \quad (8)$$

convenient for numerical realization. Exact theoretical expressions for coefficients of expansion of the studied functions into exponential series $g(s)$ have been obtained for heterogeneous paths, overlapping spectra, integrals with a source function, and radiation flows.

The existence of exact formulas for expansion of radiation characteristics into exponent series makes it possible deal with approximation of thermodynamic dependences of the expansion coefficients. The coefficients for $s(g)$ are smooth functions of altitude (Fig. 1), and this permits one to hope that the coefficients of expansion in different layers relatively simply depend on the temperature and pressure.

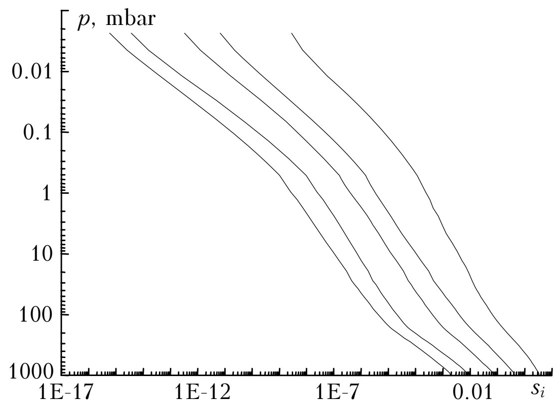

Fig. 1. Coefficients of expansion into exponential series: their behavior depending on altitude for CO_2 in the summer atmosphere of middle latitudes in the spectral interval of 720–800 cm^{-1} (5 terms in the expansion). The step by the frequency in the *line-by-line* calculation is $\Delta\omega = 0.01\ cm^{-1}$.

It can be supposed[6] that the coefficients of expansion of $s_i^{(j_r)}$ in the layer j_r for some average pressure p_r and temperature T_r can be used to obtain $s_i^{(j)}$ in other layers through formulas similar to Eq. (4):

$$s_i^{(j)} = s_i^{(j_r)} A\rho_{CO_2}(j)\left(1 + 0.0184(T_j - T_r) + 0.000112(T_j - T_r)^2\right)(p_j/p_r)^{0.5}, \quad (9)$$

where $s_i^{(j)}$ are coefficients of expansion into exponential series for transmission functions, weighted with the Planck function; j is a number of a layer; i is a number of an expansion term; A is a varied parameter; ρ is the density.

Figure 2 presents the results of calculation by formula (9) at $A = 1.25$ in comparison with other ways of calculation. It is an acceptable agreement between different ways of calculation up to altitudes of about 50 km.

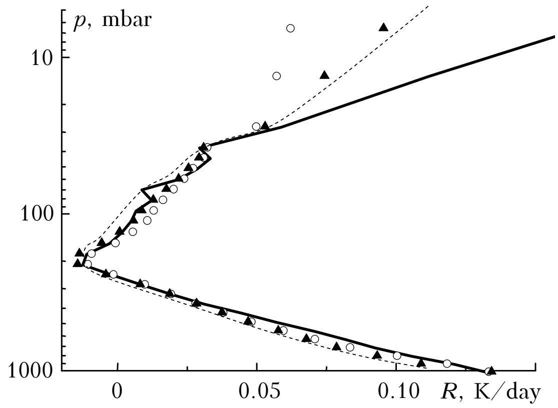

Fig. 2. The rate R of CO_2 cooling in range 720–800 cm^{-1} obtained by different ways of calculation for the summer atmosphere of middle latitudes (33 layers): *line-by-line* calculation with a step of 0.002 cm^{-1} (——); calculation by exponential series (8) with 5 terms of the series (o); calculation by the formulas from Ref. 3 (------); calculation by the approximation formulas (9) at A = 1.25 (▲).

To select parameters in coefficients of expansion, the program of non-linear deviance minimization was used. The approximating expression was given as a function of parameters k_1, k_2, ... and variables $s_i^{(j_r)}$. It was found that the approximation of logarithms of the expansion coefficients is preferable to the coefficients themselves.

Figure 3 presents the cooling rates that were obtained by the expression

$$\log_{10} s_i^{(j_L)} = (i+1)\, i^{k_1} (p_{j_L}/p_r)^{(k_2 i^2 + k_3 i + k_4)} \times \\ \times \left(1 + (T_{j_L} - T_r)^2\right). \qquad (10)$$

The values: p_r = 300 mbar, T_r = 250 K were kept as in Ref. 3. The value of the temperature factor is of low importance here. Despite the desirable approximation exactness was not reached, the cooling rate variation with altitude qualitatively reflects its character in *line-by-line* calculations.

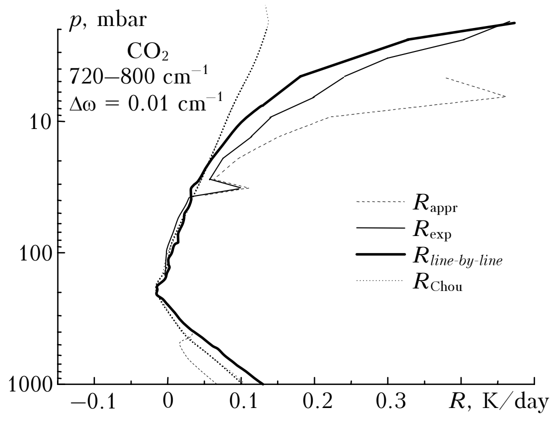

Fig. 3. The behavior of the cooling rate with growing altitude for different ways of calculation. *Line-by-line* calculation with the Foigt contour truncated by 10 cm^{-1}.

3. Approximation formulas for *s(g)* with arbitrary dependence on temperature and pressure

The earlier obtained results demonstrated a possibility to obtain one-parameter approximation formulas for coefficients of expansion into exponential series in arbitrary spectral intervals for certain models of the atmosphere. The approximation expressions for absorbing masses reducing them to some average temperature and pressure can be extended to coefficients of expansion into the exponential series:

$$s(g,p,T) = F(p,T,p_r,T_r)\, s(g,p_r,T_r), \qquad (11)$$

where $s(g,p_r,T_r)$ are coefficients of expansion at a fixed temperature and pressure; $s(g,p,T)$ are coefficients for arbitrary temperature and pressure.

If we construct a table of absorption coefficients for several values of temperature and pressure in a given spectral interval, find the corresponding expansion coefficients for s_i, and construct successful approximation formulas by these s_i, then these formulas should be applicable to any model of the atmosphere.

Table of absorption coefficients and corresponding s_i was constructed for temperatures from 170 to 370 K (41 values) and pressures from 1000 to $5 \cdot 10^{-6}$ mbar (32 values). However, in this case the fitting was not sufficient. Therefore, some pairs "temperature – pressure", not typical for the Earth's atmosphere, were removed from Table. The number of temperature and pressure points decreased from 1312 to 336: 12 values of temperature with a step of 5 K were obtained for each of the chosen 28 values of pressure. They overlap the spread in temperatures typical for models of the atmosphere. Figure 4 presents the values of the maximal and minimal temperatures used for each altitude against the background of standard model temperatures.[10]

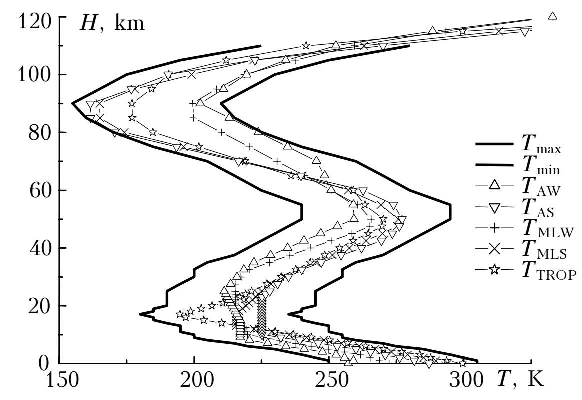

Fig. 4. Intervals of the altitude-dependent temperatures, used in calculation of initial for fitting absorption coefficients and corresponding $s(g)$ together with standard model temperatures.

The following expression was considered to be convenient for approximation of s_i obtained within the framework of the described Table:

$$s_i(p,T) = 10^f \left(Q(T)/Q(T_r)\right) s_i(p_r,T_r), \quad (12)$$

where

$$f = K_0 + \frac{K_2}{T_s} + \frac{K_1 \log p_s}{\log 10} - x_i\left(K_6 + \frac{K_8}{T_s} + \frac{K_7 \log p_s}{\log 10}\right) - \frac{\log x_i}{\log 10}\left(K_3 + \frac{K_5}{T_s} + \frac{K_4 \log p_s}{\log 10}\right). \quad (13)$$

In Eq. (13) $T_s = T/T_r$; $p_s = p/p_r$; Q, $Q(T_r)$ are relative statistical sums for the corresponding temperatures; x_i are abscissas of the Gaussian points. The coefficients $K_0, ..., K_8$, own for each considered spectral interval, are calculated by minimization of the deviance. In addition to Eq. (12), a simpler expression

$$s_i(p,T) = 10^f \left(Q(T)/Q(T_r)\right) \quad (14)$$

with the function f of the form (13) was used for fitting as well. In fact, this expression means transition from the idea of layer selection to the usual approximation of s_i depending on the temperature and pressure. The question, which variant is preferable, requires an additional study. The conducted calculations testify that one or another way can be better depending on the spectral interval. In general, exactness of the fitting is nearly the same. The quality of the fitting is shown in Fig. 5.

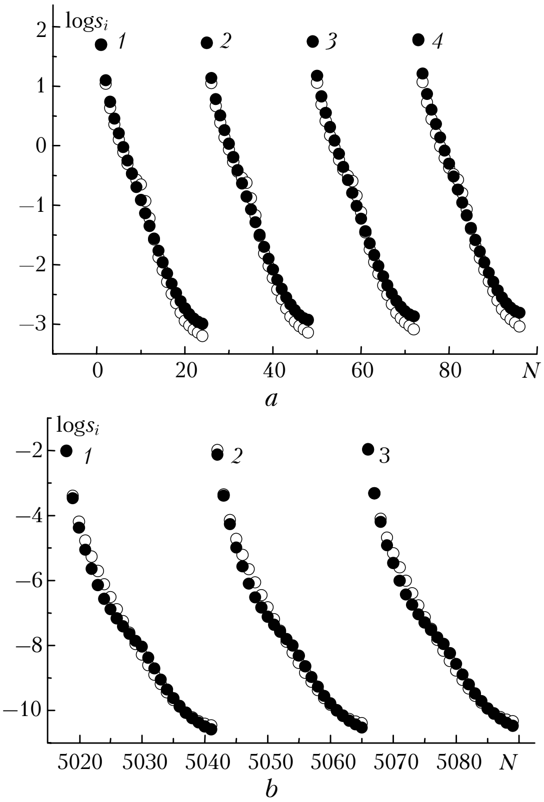

Fig. 5. Comparison of coefficients of expansion of s_i in exponential series, initial and obtained as a result of approximation for CO_2 absorption in the interval 720–800 cm^{-1}; N is the number of a point in the sequence of the values $s_i(p, T)$: curves *1–4* are for T = 250, 255, 260, 265 K, respectively, and p = 1000 mbar (*a*); curves *1–3* for T = 250, 255, and 265 K, respectively, and p = 0.2 mbar (*b*).

The groups of points s_i refer to pairs of values (p, T). In the general case, the values of s_i decrease with fall of the pressure and grow with increase of the temperature. The variants *a*, *b* were taken from the beginning and the end of Table of (p, T), respectively. In this case, the expression (14) was applied for fitting.

Figure 6 presents the values of radiation flows calculated by exponential series and with approximation of s_i by Eq. (14).

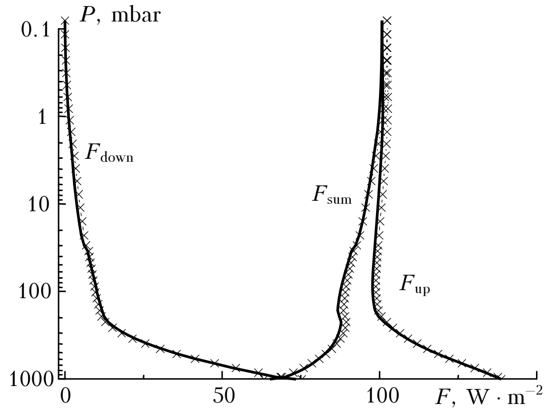

Fig. 6. Values of CO_2 radiation flows in the interval of 720–800 cm^{-1} for the summer atmosphere in middle latitudes (MLS), calculated by exponential series (the curve) and with approximation of s_i by the expression (14) (crosses).

Figure 7 presents the results of comparison of altitude profiles of the cooling rates in the interval 720–800 cm^{-1} calculated by different ways for the standard summer atmosphere of middle latitudes.

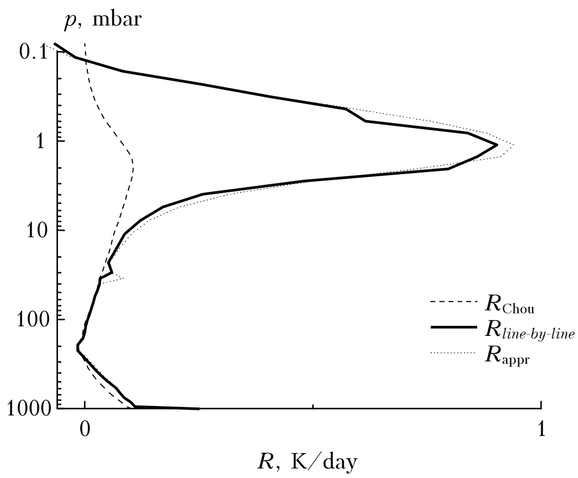

Fig. 7. Cooling rate for CO_2 in the interval 720–800 cm^{-1} for the summer atmosphere of middle latitudes, calculated by formulas of Chou,[3] *line-by-line* method, and by the approximation formulas (14).

The approximation formulas (13) for the coefficients of expansion into an exponential series with 24 terms well agree with the results of our *line-by-line* calculation at a step of 0.01 cm^{-1}.

Conclusion

Approximation expressions for absorbing masses reducing them to some average temperature and pressure can be extended to coefficients of expansion into exponential series.

Approximating expressions for the coefficients of expansion of flows into an exponential series are functions depending on the pressure p and the temperature T, abscissas of the Gaussian points, and fitting parameters. The parameters can be selected by the use of programs of non-linear minimization of deviance.

The way, by which the approximation expressions are obtained, can be applied to arbitrary spectral intervals and permits one to take into account peculiarities of the absorption line contour, including line wings.

The obtained approximation expressions for the coefficients of expansion into exponential series are applicable to atmospheric models with an arbitrary distribution of the temperature and pressure.

Thus, for an arbitrary altitude distribution of thermodynamic parameters, the approximation of coefficients of expansion into exponential series depending on the temperature and pressure has been shown. The results of calculations demonstrate the efficiency of the method in obtaining approximation formulas and a good accuracy of their application to calculating the rate of cooling.

Acknowledgements

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