# Use of lacunarity parameter in analysis of the errors in atmospheric transmittance inhomogeneities calculated using exponential series

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We analyze, by making use of the lacunarity parameter, the errors in calculating the atmospheric transmission functions by exponential series. It is shown that these errors are determined by the first two moments of the distribution of the absorption coefficients, over the spectral range considered, and their values do not exceed 1% almost through the entire optical range. The only exception is a narrow spectral interval near the ozone absorption band at 9.6 μm, where the error may reach 4% for some atmospheric paths.

## Introduction

The expansion of the transmission function caused by molecular absorption into an exponential series is now widely used in solving the radiative transfer equation. Such an approach, called the $k$-distribution method, allows solution to be obtained of a wide variety of problems in numerical calculations: it describes the transmission function with high accuracy (the difference from the line-by-line results is, on the average, ~ 1%), involves a small number of parameters (the number of terms in the series usually does not exceed 5 to 7), and has the exponential functional dependence, which provides for its easy and convenient use in various computational schemes, in particular, when multiple scattering is considerable.[1]

The method of $k$-distribution is based on the transformation of the spectrally integral transmission of a homogeneous medium

$$T_\nu = \frac{1}{\Delta\nu}\int_{\Delta\nu}\exp\{-k(\nu)L\}\mathrm{d}\nu \qquad (1)$$

to the form

$$T_g = \int_0^1 \exp\{-k(g)L\}\mathrm{d}g\,, \qquad (2)$$

where $k(\nu)$ is the molecular absorption coefficient being a fast-oscillating function of the argument $\nu$; $L$ is the path length; $\nu$ is the wave number; $k(g)$ is a piecewise-continuous, monotonically increasing function of the argument $g$, which can be interpreted as an absorption coefficient in the space of cumulative wave numbers $g$ [see Ref. 1].

For an inhomogeneous path, the following formal definition of the optical thickness of a medium layer in the space of cumulative wave numbers is used in the literature:

$$\tau(g, z_0, z) = \int_{z_0}^{z} k(g,h)\mathrm{d}h\,, \qquad (3)$$

where $k(g, h)$ has the meaning of the absorption coefficient with the cumulative wave number $g$ at the height $h$. The value of $k(g, h)$ can be calculated based on $k(\nu, h)$. Fulfillment of Eq. (3) in the case of one absorbing gas was checked many times (for more details, see Ref. 5), and it was found that Eq. (3) is valid, if the approximation of $k$-correlation meaning the similarity of absorption spectra at different heights is fulfilled.

However, standard methods of application of exponential series face the problem of overlapping of absorption bands. Band overlapping in the problems of radiative transfer through the earth's atmosphere is understood in a narrower meaning than in spectroscopy, namely, only as overlapping of absorption bands belonging to different gases. In simulation of transmission of a mixture of gases, the so-called product rule is widely used. In such a case, the transmission function of a gas mixture is represented as a product of the transmission functions formed due to absorption by individual gases.

In Refs. 2–4 it was found that the error of this approximation is small, if the following conditions are fulfilled:

(a) the spectral range is wide enough and includes at least several lines of each gas;

(b) line positions of two gases are random and not connected by some functional dependence;

(c) the partial pressure of the buffer gas is much higher than that of the absorbing gases. With these conditions true, it was established that the approximation error has a random character, and

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deviations from the line-by-line calculation may be both positive and negative.[6] Despite the product rule provides for the rather high accuracy of calculation of the transmission functions, when using the $k$-distribution it leads to the catastrophic increase in the number of terms in the series, which grows exponentially with the increase of the number of absorbing gases.

In Refs. 1 and 5, a new technique is proposed for using the exponential series: first, the molecular absorption coefficients are calculated by the line-by-line method for the mixture of gases, and then the series parameters are estimated. In this case, there is no need in using the product of transmission functions. However, if a gas mixture in the inhomogeneous atmosphere is considered, parameterization errors may arise. This is connected with the fact that the accuracy of the model (3) of the absorption spectrum of the medium decreases along the path, in particular, with the increase of a temperature inhomogeneity.[7]

In Ref. 8 the criterion for estimating the accuracy of transmittance calculation by Eq. (3) for the nonisothermal atmosphere based on the concept of lacunarity of an optical spectrum was qualitatively justified. The lacunarity of the function $k(\nu)$ is connected with its first statistical moments as follows:

$$\Lambda = \frac{M_2\{k(\nu)\}}{M_1^2\{k(\nu)\}}. \qquad (4)$$

The aim of this work was to find a quantitative criterion for estimating the accuracy of transmittance calculation using Eq. (4) for the case of nonisothermal inhomogeneous atmosphere, whose dominant absorbing components are $H_2O$, $CO_2$, $O_3$.

## Justification of the quantitative criterion

The error $\delta$ in the transmittance of an inhomogeneous atmosphere calculated by the $k$-distribution method can be estimated as:

$$\delta = |\, T_\nu(L) - T_g(L)\,|\,. \qquad (5)$$

For estimates we use the model of a plane stratified atmosphere, assuming the layers to be so thin that the optical thickness $\tau(\nu, L) \ll 1$. In this case, the transmission function of the entire inhomogeneous atmospheric path can be represented in the following form:

$$T_\nu(L) = \frac{1}{\Delta\nu}\int_{\nu_1}^{\nu_2}\exp\left[-\sum_{i=1}^{N}k(\nu,L_i)\Delta L_i\right]d\nu \approx$$

$$\approx 1 - \left\langle\sum_{i=1}^{N}k(\nu,L_i)\Delta L_i\right\rangle_\nu +$$

$$+\frac{1}{2}\left\langle\sum_{i=1}^{N}\sum_{m=1}^{N}k(\nu,L_i)\Delta L_i k(\nu,L_m)\Delta L_m\right\rangle_\nu, \qquad (6)$$

where the parameters $L_m$, $\Delta L_m$ characterize the position and thickness of $m$th layer.

Formally, the transition into the space of cumulative frequencies is equivalent to the change of the integration variables in Eq. (1): $\nu \to k$, where $k \equiv k(\nu)$ is the absorption coefficient of the medium. For an inhomogeneous path, such a change is possible, if the frequency dependence of the absorption coefficients of individual layers of the inhomogeneous path $k(\nu, L_i)$ is similar, that is, the following condition is fulfilled:

$$k(\nu, L_i) = c_i k(\nu, L_1), \qquad (7)$$

where $c_i$ are the frequency-independent parameters. Introduce designations for the mean value of the absorption coefficient, its variance, and the correlation coefficient, as follows:

$$\bar{k}_i = \frac{1}{\Delta\nu}\int_{\nu_1}^{\nu_2}k(\nu,L_i)d\nu\,,$$

$$\sigma_i^2 = \frac{1}{\Delta\nu}\int_{\nu_1}^{\nu_2}k^2(\nu,L_i)\,d\nu\,,$$

$$R_{ij} = \frac{1}{\sigma_i\sigma_j}\frac{1}{\Delta\nu}\int_{\nu_1}^{\nu_2}k(\nu,L_i)k(\nu,L_j)d\nu.$$

If the condition (7) holds, Eq. (6) takes the form

$$T_g(L) \approx 1 - \sum_{i=1}^{N}\bar{k}_i\Delta L_i + \frac{1}{2}\sum_{i=1}^{N}\sum_{m=1}^{N}\sigma_i\sigma_m\Delta L_i\Delta L_m. \qquad (8)$$

It is obvious that the error in the transmittance of an inhomogeneous atmosphere calculated by the $k$-distribution method based on the transformation (8) into the space of cumulative frequencies is determined by the accuracy with which the condition (7) holds.

In this case, the estimate of the error in the transmittance of an inhomogeneous atmosphere calculated by the $k$-distribution method can be obtained in the following way:

$$\delta \approx \frac{1}{2}\sum_{i,j=1}^{N}\bar{k}_i\bar{k}_j\sqrt{\Lambda_i}\sqrt{\Lambda_j}\Delta L_i\Delta L_j\left|(1 - R_{ij})\right|. \qquad (9)$$

The above equations show that the approximation of $k$-correlation is valid, if the spectra at different heights correlate, that is, $R_{ij} = 1$.

The earth's atmosphere is not optically thin. In this case, it is impossible to obtain the correlation coefficient in the explicit form, as in Eqs. (5) and (9). Nevertheless, it can be shown[9] that the spectral dependence $k(g, L)$ is fully determined by the function $g(k, L)$, which can be interpreted as the distribution function of the molecular absorption coefficient $k(\nu, L)$

$$k(g) = g^{-1}(k)\,, \qquad (10)$$

where $g^{-1}(k)$ is the function inverse to $g(k)$. For an inhomogeneous atmosphere, we should analyze the distribution function of the optical thickness $g(\tau)$. If it keeps constant with height, then the approximation of $k$-correlation is valid.

## Simulated results

The transmittance was calculated in the spectral regions where such gases as (a) $H_2O$, (b) $CO_2$, (c) $CO_2$+$H_2O$, (d) $O_3$, (e) $CO_2$+$H_2O$+$O_3$ absorb. These gases were chosen because $H_2O$, $CO_2$, and $O_3$ are the main absorbers of IR radiation, the mixtures considered above describe all possible combinations of the spatial variability of optically active gases, since water vapor is concentrated near the ground, carbon dioxide is a uniformly distributed gas, and the ozone concentration increases with height, reaching its maximum at the heights of 25–30 km.

Some results obtained by a computer simulation are shown in Figs. 1–4. Figures 1a and 2a depict the fragments of the atmospheric absorption spectra as functions of height. From a comparison of these spectra one can see that in the first case the spectral structure at different heights is similar. For the mixture of $H_2O$, $CO_2$, and $O_3$ we can see two significantly different height ranges with different structures of the spectrum. In addition, the mean value of the $CO_2$ absorption coefficient (Fig. 1b) rapidly decreases with height, while for the mixture we can see two height peaks in the mean absorption coefficient: one near the ground and at the heights of 20–25 km (Fig. 2b).

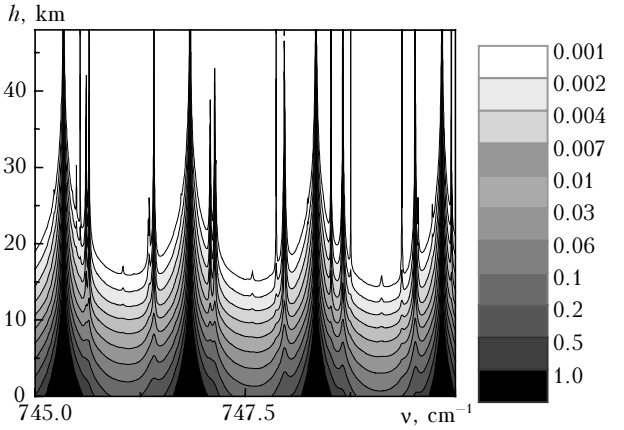


**Fig. 1a.** Height and spectral dependence of the $CO_2$ molecular absorption coefficient, in $km^{-1}$ (fragment of the spectrum).

Our analysis has shown that it is just these two factors that determine the error in the transmission functions calculated using exponential series. We have calculated the transmission functions for different paths by the direct line-by-line method and using exponential series. In the case of carbon dioxide the maximum value of the error did not exceed 0.5% (Fig. 1d), and in the case of the gas mixture it achieved 4.3%. In the case of $CO_2$ absorption, the paths originating from the atmospheric top led to larger errors than the paths originating from the atmospheric bottom, while for the gas mixture the situation was quite opposite.

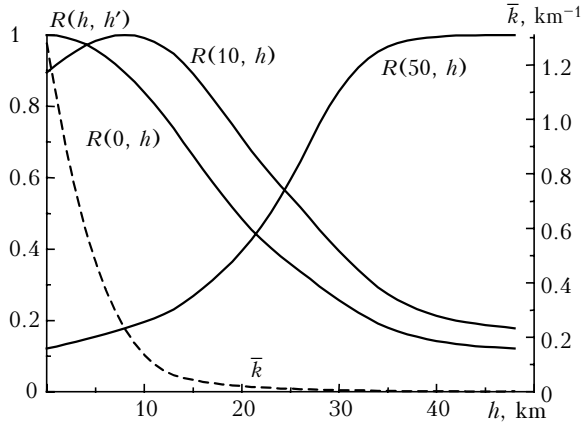


**Fig 1b.** Correlation between absorption coefficients at different heights.

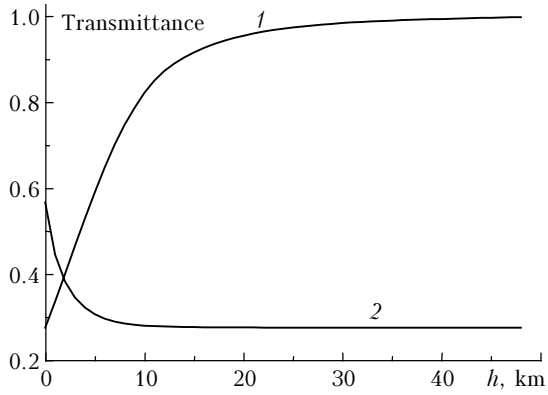


**Fig. 1c.** Calculation of atmospheric transmittance by the line-by-line method. Vertical paths: fixed upper boundary $h_{up}$ = 50 km, variable lower boundary (*1*); fixed lower boundary $h_{low}$ = 0 km, variable upper boundary (*2*). Spectral range of 740–760 $cm^{-1}$.

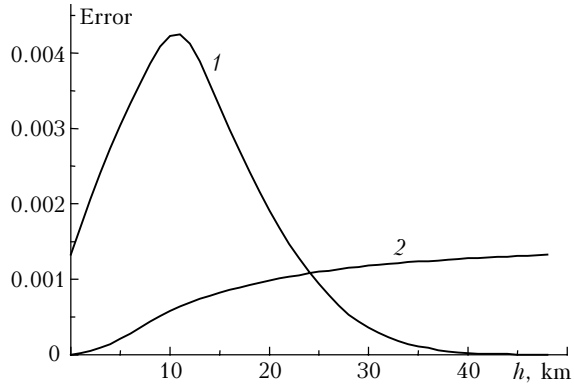


**Fig. 1d.** Error of transmittance calculation by the $k$-distribution method. Designations are the same as in Fig. 1c.

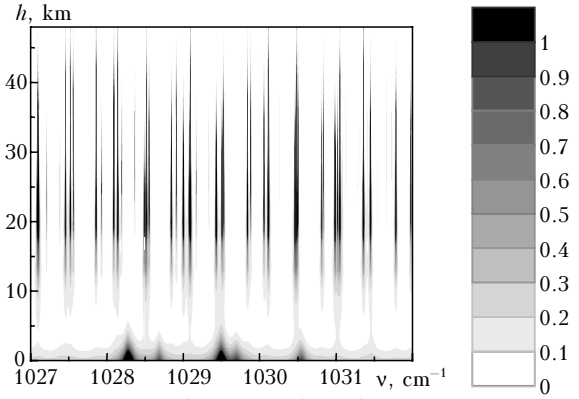


**Fig. 2a.** Height and spectral dependence of the molecular absorption coefficient in the gas mixture of $H_2O$, $CO_2$, and $O_3$, in $km^{-1}$.

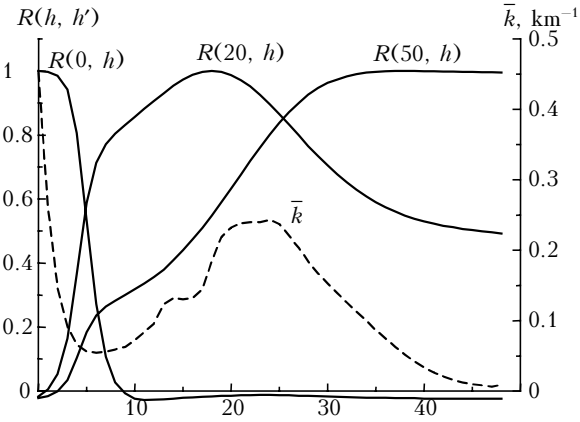


**Fig. 2b.** Correlation between absorption coefficients at different heights.

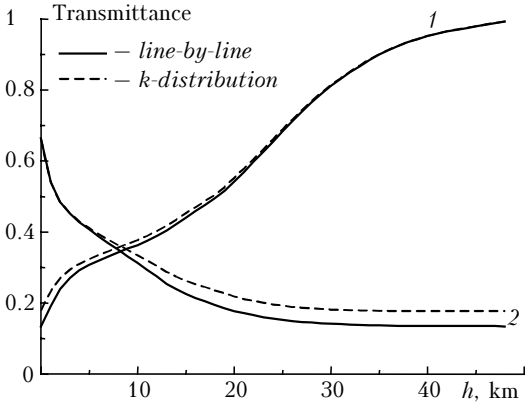


**Fig. 2c**. Calculation of atmospheric transmittance by the line-by-line method (solid curve) and by the $k$-distribution method (dashed curve). Designations are the same as in Fig. 1c. Spectral range of 1027–1032 $cm^{-1}$.

To obtain qualitative estimates, we calculated the lacunarity and the correlation coefficients $R_{ij}$ between the volume absorption coefficients $k(h)$ (measured in $km^{-1}$) at different heights $h_i$, $h_j$. It is seen from Fig. 3 that the height dependence of the lacunarity parameter for different gases is similar. Moreover, the simulation showed that in the two ranges depicted in Figs. 1*a* and 2*a* the height dependence of the lacunarity parameters calculated for the $CO_2$ spectra turned out to be close. Therefore, we drew only one curve in the figure.

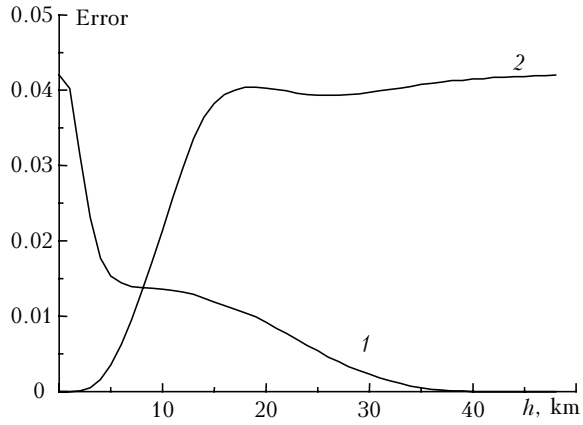


**Fig. 2d**. Error of transmittance calculation by the $k$-distribution method. Designations are the same as in Fig. 1c.

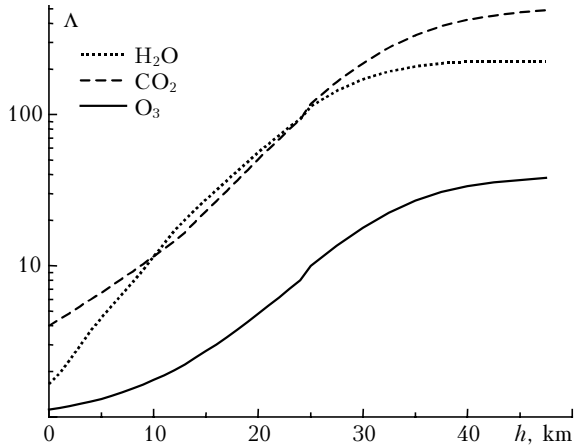


**Fig. 3.** Height dependence of the lacunarity parameter for different absorbing gases in the spectral range of 1027–1032 $cm^{-1}$.

The lacunarity parameter characterizing the degree of modulation of the absorption spectrum proved to be strongly dependent on the air pressure and varied with height in inverse proportion to the halfwidth of the absorption line. From the method of models of absorption bands,[10] we know that the transmission function is determined by two parameters, one of which is connected with the mean intensity of absorption lines (the first moment of distribution of the absorption coefficients), while another one is connected with the mean values of the line halfwidth and strength, which can be related to the lacunarity parameter. This agrees with the results of our previous paper,[7] where it was shown that the parameters of expansion of the transmission function into the exponential series could be related to the moments of distribution of the absorption coefficient.

While revealing the quantitative criterion for estimation of the error of the expansion into the exponential series for the inhomogeneous atmosphere,

we have analyzed the vertical behavior of the absorption coefficients $k(h)$, the lacunarity parameters $\Lambda(h)$, and the correlation coefficients $R_{ij}$. The absorption coefficient of $H_2O$ decreases most quickly with height as compared to that of other gases. In the case of absorption by the $CO_2$, the volume absorption coefficient also decreases with height, and the optical thickness is determined by a relatively thin lower atmospheric layer, within which the correlation coefficient is close to unity. For ozone and the mixture of the three gases, the vertical profile of the absorption coefficient is significantly different and different atmospheric layers contribute to the optical thickness.

As was already mentioned the character of the height dependence of the lacunarity parameter for different gases is similar. Therefore, the differences in the vertical profiles of $\bar{k}(h)\sqrt{\Lambda(h)}$, entering into Eq. (9), are mostly determined by the difference in the vertical profiles of the absorption coefficients. Figure 4 shows the height dependence of the product $\bar{k}(h)\sqrt{\Lambda(h)}$, while Figs. 1*b* and 2*b* show the correlation coefficients for different gases.

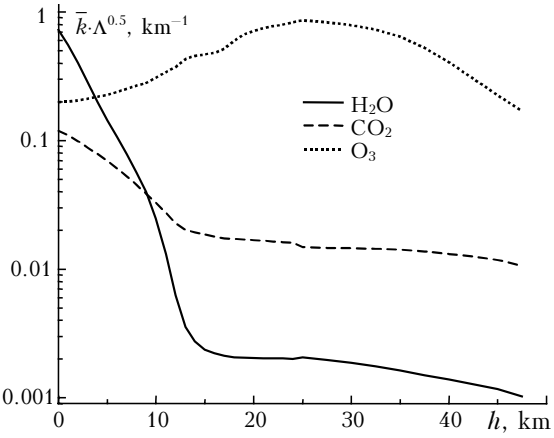


**Fig. 4.** Height dependence of the mean absorption coefficient multiplied by the lacunarity parameter for different absorbing gases in the spectral range of 1027–1032 cm$^{-1}$.

The simulation has demonstrated that the largest values of the correlation coefficients $R_{ij}$ were observed in the case of absorption by a single gas, while the smallest values characterized the absorption by the mixture of the gases $H_2O$, $CO_2$, and $O_3$. Thus, the weak height dependence of $\bar{k}(h)\sqrt{\Lambda(h)}$, on the one hand, and strong variability of the correlation coefficients $R_{ij}$, on the other hand, led to marked errors in the transmission functions calculated using exponential series.

## Conclusions

The simulation has shown that the approximation of $k$-correlation works well almost in the entire optical region, and the error in the transmission functions calculated by the $k$-distribution method does not exceed 1%. The only exception is the narrow spectral range near the ozone band at 9.6 μm, where water vapor and carbon dioxide absorb along with the ozone. In this case, for some paths through the entire atmosphere, the error of the exponential series expansion may reach 4%. This error is determined by the facts that layers at significantly different heights contribute to absorption, the shape of the absorption spectrum transforms with height, and the correlation coefficient between the absorption coefficients decreases quickly as the height increases.

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