Relationship between the error in transmittance calculation for the inhomogeneous atmosphere by the *k*-distribution method and spectrum lacunarity

Yu.V. Kistenev,[1] Yu.N. Ponomarev,[2] K.M. Firsov,[2] and D.A. Gerasimov[3]

[1]Siberian State Medical University, Tomsk
[2]Institute of Atmospheric Optics,
Siberian Branch of the Russian Academy of Sciences, Tomsk
[3]Tomsk State University

Received December 30, 2002

It is shown that lacunarity characterizing a molecular absorption spectrum as a multifractal allows estimation of the error in the method of *k*-functions for multicomponent inhomogeneous gas media without cumbersome line-by-line calculations.

The specific features of climate simulation problems impose rather strict requirements on the accuracy and speed of radiative blocks.[1,2] Therefore, significant efforts of investigators have been aimed at the development of efficient methods for parameterization of characteristics of molecular and aerosol extinction that enter into the radiative transfer equation that would allow one to reach a compromise between the computational time and accuracy.

Molecular absorption spectra of atmospheric gases are characterized by high selectivity as compared to aerosol extinction spectra. The characteristic scale of variation of the molecular absorption coefficient is 10^{-1} cm^{-1}. Besides, the number of spectral lines to be taken into account is large. Thus, for example, in the HITRAN-2000 database the total number of absorption lines exceeds 10^6. Therefore, direct methods for calculating characteristics of molecular absorption are very computationally expensive and unacceptable in solution of general atmospheric circulation problems.

Now an efficient method has been developed for parameterization of molecular absorption characteristics – the *k*-distribution method.[1–5] Initially, the *k*-distribution method was based on band models, and its advantage was in the fact that it allowed the transmission function to be represented as an exponential series. Evolving, this method became free from restrictions connected with the model representations, and today it can be considered as a modification of the line-by-line method. To obtain an exponential series, integral transformation of the transmission function of the medium is used[4]:

$$T_{\Delta\nu} = \frac{1}{\Delta\nu}\int_{\Delta\nu} \exp\{-k(\nu)L\}\mathrm{d}\nu = \int_0^1 \exp\{-k(g)L\}\mathrm{d}g\,, \qquad (1)$$

where $k(\nu)$ is the molecular absorption coefficient; L is the path length; ν is the wave number, cm^{-1}; $k(g)$ can be treated as an absorption coefficient in the space of cumulative wave numbers g (Ref. 5). In Eq. (1) $k(\nu)$ is a rapidly oscillating function, and $k(g)$ is a monotonically increasing piecewise continuous function. Applying quadrature equations of numerical integration to the second integral in Eq. (1), we can readily obtain a short exponential series.

The function $k(g)$ can be calculated based on $k(\nu)$. For this purpose, it is necessary to find the distribution function for values of the absorption coefficient $g(k)$:

$$g(k) = \frac{1}{\nu_2 - \nu_1}\int_{\nu_1}^{\nu_2} U(\nu)\mathrm{d}\nu\,, \qquad (2)$$

where

$$U(\nu) = \begin{cases} 1, & k(\nu) < k \\ 0, & k(\nu) > k \end{cases}.$$

It follows from Eq. (2) that $g(k)$ is a monotonically increasing function; therefore, inverting $g(k)$, we can calculate $k(g)$:

$$k(g) = g^{-1}(k), \qquad (3)$$

where $g^{-1}(k)$ is the inverse function.

Since $k(g)$ is connected with the distribution function of the absorption coefficient, this method is referred to in the literature as the *k-distribution method.*

In our earlier paper,[5] it was shown that the *k*-distribution method allows molecular absorption to be correctly taken into account in solving the radiative transfer equation in the scattering and absorbing atmosphere through the single scattering albedo and the optical depth. The only approximation to be fulfilled is *correlation of the k-distribution*,[7] which allows the optical depth and the absorption coefficient to be connected in a natural way in the space of cumulative wave numbers:

0235-6880 / 03 / 03 247-04 $02.00

$$\tau(g,z_0,z) = \int_{z_0}^{z} k(g,h)\mathrm{d}h , \qquad (4)$$

where $k(g, h)$ has the meaning of the absorption coefficient at the height h and the cumulative frequency g.

Equation (4) is violated in an inhomogeneous atmosphere. This is connected with the fact that the distribution function $g(k)$ varies with height. In the case of an inhomogeneous atmosphere, Eq. (2) should include the optical depth in place of the absorption coefficient, and the distribution function of the optical depth of the inhomogeneous atmosphere differs from the distribution function of the absorption coefficient, and the wider is the difference, the larger is the error of calculation by Eq. (4).

Now there are no objective criteria for applicability of the approximation (4), therefore to check it in the studied spectral intervals, it is necessary to perform voluminous calculations of the transmission function for variations of the vertical temperature profiles and the concentration of gaseous constituents.

Reference 6 gives qualitative justification to the criterion of estimation of the accuracy in calculation of transmission using the approximation (4) for the nonisothermal atmosphere based on the applicability of the concept of lacunarity of an optical spectrum (for estimations of lacunarity of optical spectra see Ref. 8).

In this paper, we study the quantitative relationship between the error of calculating the transmittance of an inhomogeneous atmosphere by the k-distribution method and the spectrum lacunarity. To find the quantitative criterion of applicability of the k-distribution method to an inhomogeneous atmosphere, the model of two-layer nonisothermal medium with the layer temperature $Ò_i$ and the thickness L_i (i = 1, 2) is used.[6] Figure 1 exemplifies transformation of the absorption spectrum of the medium layers in the space of wave numbers and cumulative wave numbers.

The exact $T_{\Delta\nu}$ and approximate (in the approximation of k-correlation) T_g values of the transmission function were calculated by the equations:

$$T_{\Delta\nu} = \int_0^1 \exp\{-\tau(g)\}\mathrm{d}g ,$$

$$T_g = \int_0^1 \exp[-k(g,T_1)L_1 - k(g,T_2)L_2]\mathrm{d}g .$$

The coefficients $k(g, T_1)$ and $k(g, T_2)$ were found for each layer by Eqs. (2)–(3), and $\tau(g)$ was calculated as

$$g(\tau) = \frac{1}{\nu_2 - \nu_1}\int_{\nu_1}^{\nu_2} U(\nu)\mathrm{d}\nu ,$$

where

$$U(\nu) = \begin{cases} 1, & k(\nu,T_1)L_1 + k(\nu,T_2)L_2 < \tau \\ 0, & k(\nu,T_1)L_1 + k(\nu,T_2)L_2 > \tau \end{cases} .$$

The error of calculation was determined as

$$\varepsilon = \sup_{L_1,L_2}\left|T_{\Delta\nu} - T_g\right| .$$

The absorption coefficients for atmospheric CO_2 were calculated in the spectral region of 3450–3770 cm^{-1}, the line assumed to have the Voigt shape, the intensities of spectral lines for the given temperatures (300–1000 K) were taken from the CDSD database[9] (Carbon Dioxide Spectroscopic Databank), that was kindly present at our disposal by V.I. Perevalov. The spectral resolution varied from 10 to 100 cm^{-1}.

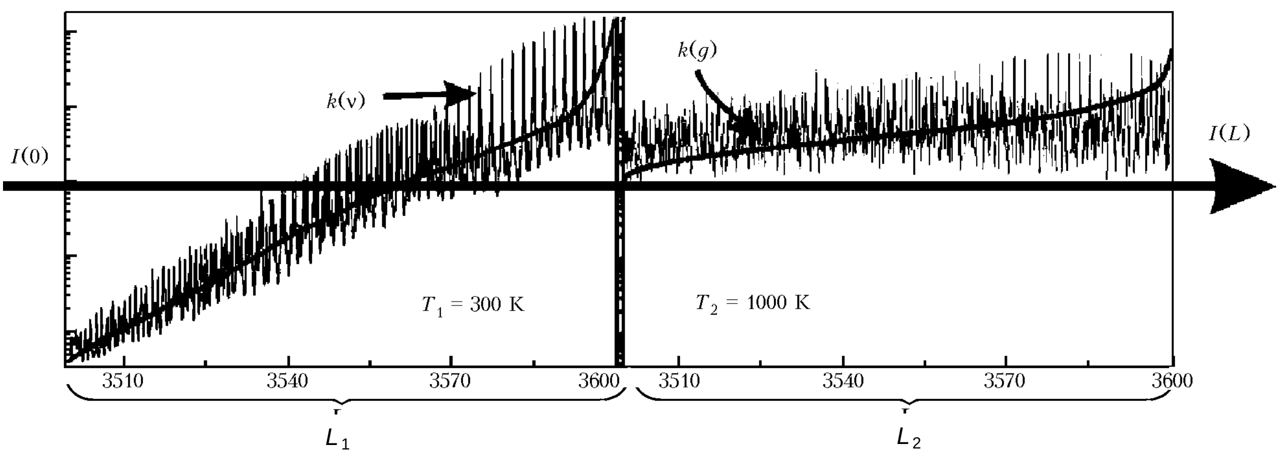

Fig. 1. Radiation propagation through a two-layer medium.

Figure 2 depicts typical dependence of the error in calculation of the transmission function by the method of *k*-correlation on the difference between the temperature of the first and second layers.

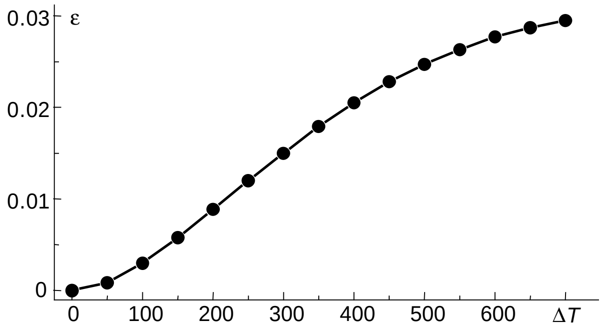

Fig. 2. The error in calculation of transmittance for the two-layer medium by the *k*-distribution method as a function of the temperature difference between the layers (temperature of the first layer is 300 K). Spectral range of 3500–3600 cm^{-1}.

It can be seen from Fig. 2 that the error increases with the increasing temperature difference between the layers. Note that the temperature is not a universal criterion because this error is largely caused by variation of the distribution function of the absorption coefficient. Statistical criteria are most adequate for estimation of the variability of the transmission function. In Ref. 6 it was shown that spectrum lacunarity can be such a criterion. The spectrum lacunarity is expressed through the first two distribution moments of the absorption coefficient and characterizes not only the statistical properties of the distributions, but also their symmetry (scale and translational).

This paper presents calculations of higher lacunarities:

$$\Lambda_n(k) = \frac{M_{n+1}\{k(\nu,T)\}}{\left[M_1\{k(\nu,T)\}\right]^{n+1}}, \qquad n = 1,\ 2,\ 3\,.$$

Figure 3 depicts the results of lacunarity calculation for n = 1, 2, 3 and the spectral range of 3500–3600 cm^{-1}.

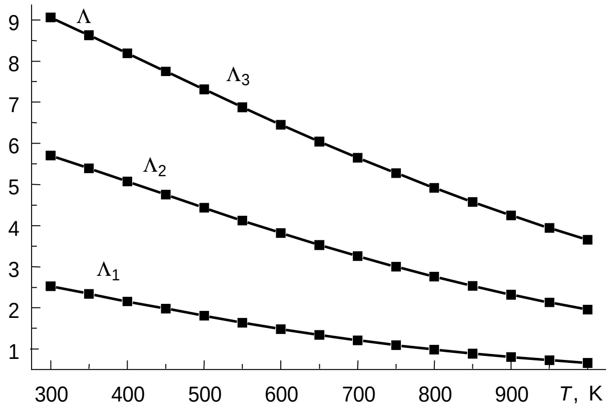

Fig 3. Temperature dependence of lacunarity parameters $\Lambda_n(k)$ calculated for the Ñ Î$_2$ absorption spectrum in the range of 3500–3600 cm^{-1}.

It can be seen from Fig. 3 that the temperature dependence of the first three lacunarity moments is identical. The similar pattern was observed also for lacunarity moments calculated based on the distribution function of spectral line intensity. For Ñ Î$_2$ in the spectral range of 3450–3770 cm^{-1} for averaging intervals varying from 10 to 100 cm^{-1}, the regularities similar to those shown in Fig. 3 were observed. For this reason, as the main characteristic of temperature variability of the distribution function of the absorption coefficient or the distribution function of the spectral line intensity, it is possible to use lower-order lacunarity $\Lambda_1(k)$.

Simulation performed by us showed that the error in calculation of medium transmittance is functionally related to the lacunarity parameter characterizing the gas mixture as a whole (Fig. 4).

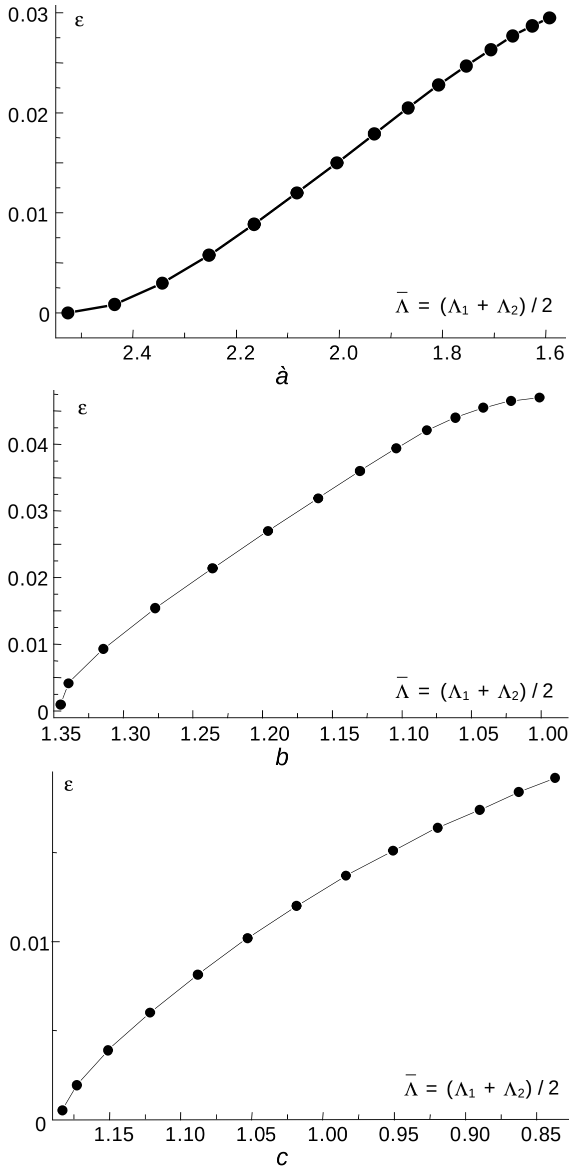

Fig. 4. Dependence of the error in calculation of the transmission function on the lacunarity parameters: range of 3500–3600 cm^{-1} (*a*), 3600–3620 cm^{-1} (*b*), and 3700–3710 cm^{-1} (*c*).

It should be noted that the dependences obtained for all the cases were well described by the linear regression (the correlation coefficient R was 0.99), which is convenient for practical applications.

Thus, the lacunarity parameter depending on the temperature and characterizing the spectrum as a multifractal allows one to estimate the error of the k-distribution method for multicomponent inhomogeneous gas media without performing cumbersome line-by-line calculations.

Acknowledgments

This work was partly supported by the Russian Foundation for Basic Research, Grant No. 01–05–65152à.

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