

Use of k -distribution method for solution of shortwave radiative transfer equation in a spatially inhomogeneous atmosphere

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We describe an approach to treatment of molecular absorption in solving, by use of the Monte Carlo method, the radiation transfer equation for the case of spatially inhomogeneous aerosol-gaseous media. The approach is based on expansion of the broadband transmission function in an exponential series. Theoretical and numerical analysis has been performed to check the applicability of the expansion in exponential series for spatially inhomogeneous atmospheres. The numerical simulation performed showed high efficiency of this method, because thus obtained results are close within 0.2% accuracy to the results calculated using line-by-line technique while consuming 350 times shorter computer time.

In recent years, many well known specialists from the atmospheric optics community have been involved in the problem on propagation of non-monochromatic radiation in multicomponent media with complicated and spatially variable absorption spectra of individual components,¹⁻¹⁰ as, for example, in studying interaction of solar optical radiation with the Earth's atmosphere for the weather and climate prediction models. This study requires improved data on the fine structure of absorption spectra of gaseous atmospheric constituents (because the aerosol component of the atmosphere has much weaker spectral variations and needs no further detail). Upon improvement in detail, the task is then achieved by solving the stationary transfer equation for each wavelength, with a subsequent integration over a specified spectral interval. This method is called the line-by-line technique.

Unfortunately, while seemingly simple and asymptotically exact, this method is very expensive even with modern computers. This stimulated the development of alternative methods of compiling large bulks of spectroscopic information, based on the expansion of a broadband transmission function in an exponential series. It provides high-efficiency calculations of the frequency-integrated characteristics of radiation propagated through a spatially homogeneous multicomponent gas and aerosol medium. However, for a spatially inhomogeneous medium, the successive analysis was made only for the molecular atmosphere.¹⁻³ This paper discusses the applicability of exponential series technique to multicomponent spatially inhomogeneous atmosphere with the account of scattering effects.

The solution of transfer equation for inhomogeneous scattering and absorbing atmosphere will be considered for a standard formulation of the problem under the assumption that the underlying surface is absolutely black. Generalization to a more practical case of a

reflecting surface can be obtained through solution of standard problem.⁴ For simplicity of presentation, only aerosol scattering and molecular absorption will be considered. The conclusions below will also be valid if aerosol absorption and molecular scattering are taken into account. The integral equation with the generalized kernel will be presented as⁵:

$$z(\mathbf{x}) = \int_{\mathbf{x}} k(\mathbf{x}', \mathbf{x}) z(\mathbf{x}') d\mathbf{x}' + \Psi(\mathbf{x}), \quad (1)$$

where $z(\mathbf{x})$ is the sought function defined as collision density related to the intensity of radiation by the following equation:

$$I(\mathbf{r}, \boldsymbol{\Omega}) = |\mu| S z(\mathbf{r}, \boldsymbol{\Omega}) / \beta_{\text{ext}}(\mathbf{r}); \quad (2)$$

here, \mathbf{x} is phase space of coordinates and directions; $\mathbf{x} = (\mathbf{r}, \boldsymbol{\Omega})$; μ is the secant of solar zenith angle; S is the solar constant; and β_{ext} is the extinction coefficient. The generalized kernel in (1) is defined by⁵:

$$k(\mathbf{x}', \mathbf{x}) = \beta_{\text{ext}}(\mathbf{r}) \frac{\bar{\omega}(\mathbf{r}') f(\mathbf{r}, \boldsymbol{\Omega}, \boldsymbol{\Omega}') \exp\{-\tau_s(\mathbf{r}, \mathbf{r}')\}}{|\mathbf{r} - \mathbf{r}'|^2} \delta\left(\boldsymbol{\Omega} - \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|}\right), \quad (3)$$

where $\bar{\omega}(\mathbf{r}')$ is the single scattering albedo; $f(\mathbf{r}, \boldsymbol{\Omega}, \boldsymbol{\Omega}')$ is the scattering phase function; and $\tau_s(\mathbf{r}, \mathbf{r}')$ is the optical depth.

The source distribution density $\Psi(\mathbf{x})$ for a standard problem formulation is

$$\Psi(\mathbf{x}) = \beta_{\text{ext}}(\mathbf{r}) \exp\{-\tau_s(\mathbf{r}, \mathbf{r}_\infty)\} \delta(\boldsymbol{\Omega} - \boldsymbol{\Omega}_\infty). \quad (4)$$

The solution of integral equation (1) can be presented as Neumann series

$$z = \sum_{i=1}^{\infty} K^i \Psi. \quad (5)$$

The existence of solution, as well as related issues, are discussed elsewhere.⁵ For a convenience, the expressions (3) and (4) are written as

$$k(\mathbf{x}', \mathbf{x}) = \beta_{\text{ext}}(\mathbf{r}) \frac{\beta_{\text{sct}}^a(\mathbf{r}')}{\beta_{\text{ext}}(\mathbf{r}')} \exp\{-\tau(\mathbf{r}, \mathbf{r}')\} k_0(\mathbf{x}', \mathbf{x});$$

$$\Psi(\mathbf{x}) = \beta(\mathbf{r}) \exp\{-\tau(\mathbf{r}, \mathbf{r}_\infty)\} \Psi_0(\mathbf{x}),$$

where

$$k_0(\mathbf{x}', \mathbf{x}) = \frac{f(\mathbf{r}, \boldsymbol{\Omega}, \boldsymbol{\Omega}') \exp\{-\tau_a(\mathbf{r}, \mathbf{r}')\}}{|\mathbf{r} - \mathbf{r}'|^2} \delta\left(\boldsymbol{\Omega} - \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|}\right);$$

$$\Psi_0(\mathbf{x}) = \exp\{-\tau_a(\mathbf{r}, \mathbf{r}_\infty)\} \delta(\boldsymbol{\Omega} - \boldsymbol{\Omega}');$$

β_{sct}^a is the aerosol scattering coefficient; and τ and τ_a are the optical depths due to molecular absorption and aerosol scattering, respectively. It should be noted that $\Psi_0(\mathbf{x})$ and $k_0(\mathbf{x}, \mathbf{x}')$ do not include molecular scattering contribution.

Let us consider two first terms of the series (5)

$$K\Psi = \int_X k(\mathbf{x}_1, \mathbf{x}) \Psi(\mathbf{x}_1) d\mathbf{x}_1 = \beta_{\text{ext}}(\mathbf{x}) \times$$

$$\times \int_X k_0(\mathbf{x}_1, \mathbf{x}) \Psi_0(\mathbf{x}_1) \beta_{\text{sct}}^a(\mathbf{r}_1) \exp\{-\tau(\mathbf{r}_1, \mathbf{r}_\infty) - \tau(\mathbf{r}_1, \mathbf{r})\} d\mathbf{x}_1,$$

$$K^2\Psi = \int_{XX} k(\mathbf{x}_1, \mathbf{x}) k(\mathbf{x}_2, \mathbf{x}_1) \Psi(\mathbf{x}_2) d\mathbf{x}_1 d\mathbf{x}_2 =$$

$$= \beta_{\text{sct}}(\mathbf{x}) \int_X k_0(\mathbf{x}_1, \mathbf{x}) k_0(\mathbf{x}_2, \mathbf{x}_1) \Psi_0(\mathbf{x}_2) \beta_{\text{sct}}^a(\mathbf{r}_1) \beta_{\text{sct}}^a(\mathbf{r}_2) \times$$

$$\times \exp\{-\tau(\mathbf{r}_2, \mathbf{r}_\infty) - \tau(\mathbf{r}_1, \mathbf{r}) - \tau(\mathbf{r}_2, \mathbf{r}_1)\} d\mathbf{x}_1 d\mathbf{x}_2. \quad (7)$$

Expressions for other terms of the series can be obtained in similar way. In frequency integration of the intensity of radiation described by formula (5), it is possible to separate out the transmission function due to molecular absorption. For this, the width of the spectral interval $\Delta\nu$ must be chosen such that the solar constant and scattering coefficient can be considered constant within it. In this case it is possible to remove from the integrand all factors independent of the optical depth τ . With the account of Eqs. (6) and (7), the radiation intensity will include factors proportional to the transmission function

$$T_j = \frac{1}{\Delta\nu} \int_{\Delta\nu} \exp\{-\tau_j(\nu)\} d\nu, \quad (8)$$

where $\tau_j(\nu)$ is optical depth of the j th term of the series (5). In particular, $\tau_2(\nu)$ has the form

$$\tau_2(\nu) = \tau(\mathbf{r}_2, \mathbf{r}_\infty) + \tau(\mathbf{r}_1, \mathbf{r}) + \tau(\mathbf{r}_2, \mathbf{r}_1).$$

For a homogeneous path, the optical depth is related to molecular absorption coefficient by

$$\tau_j(\nu) = \beta_{\text{abs}}^m(\nu) L_j,$$

where L_j is the total path length. Owing to functional dependence of the transmission on wavelength, it is possible to perform Laplace transform⁶ to the space of cumulative frequencies g , in which the transmission function becomes

$$T_j = \frac{1}{\Delta\nu} \int_0^1 \exp\{-\beta_{\text{abs}}^m(g) L_j\} dg, \quad (9)$$

where $\beta_{\text{abs}}^m(g)$ can be interpreted as the absorption coefficient in the space of cumulative frequencies g . Indeed, the functions $\beta_{\text{abs}}^m(\nu)$ and $\beta_{\text{abs}}^m(g)$ have the same set of values and both functions are continuous. For each $\beta_{\text{abs}}^m(\nu)$ value in the space of frequencies ν , there is also an equal coefficient $\beta_{\text{abs}}^m(g)$ in the cumulative frequency domain (with the reverse being also true). The only significant difference is that, whereas $\beta_{\text{abs}}^m(\nu)$ rapidly oscillates, $\beta_{\text{abs}}^m(g)$ is a monotonically increasing function of the argument g . Application of quadrature formulas to (9) yields a short (5 to 10 terms) exponential series

$$T_j = \sum_{i=1}^n C_i \exp\{-\beta_{\text{abs}}^m(g_i) L_j\}, \quad (10)$$

where C_i and g_i are the coefficients and nodes of the corresponding quadrature formulas. Most simple and efficient are Gaussian quadratures, which with no more than six series terms, provide for quite accurate calculation of the transmission functions to within 1% accuracy.

The above-mentioned method of calculation of the transmission function gives accurate results using a small number of absorption coefficients $\beta_{\text{abs}}^m(g_i)$ at preselected frequencies. Since transformation from (8) to (9) is integral in form, and the monochromatic coefficients $\beta_{\text{abs}}^m(\nu)$ and $\beta_{\text{abs}}^m(g)$ are not explicitly related, these preselected frequencies can be determined only after the spectrum $\beta_{\text{abs}}^m(\nu)$ is calculated and converted to $\beta_{\text{abs}}^m(g)$.

With the account of formula (8), all steps of derivation Eqs. (1)–(10) can be reverted to give transfer equation (1) with the only difference that the absorption coefficient will now be defined in cumulative frequency domain and will be a smooth function there. Using this trick, one can solve the transfer equation for a small number of preset frequencies g_i , and then sum the solutions with weights C_i .

For an inhomogeneous path, the above inferences will be valid if the relations hold for all τ_j in the cumulative frequency domain:

$$\tau_1(g_i) = \tau(g_i, \mathbf{r}_1, \mathbf{r}_\infty) + \tau(g_i, \mathbf{r}_1, \mathbf{r}),$$

$$\tau_2(g_i) = \tau(g_i, \mathbf{r}_2, \mathbf{r}_\infty) + \tau(g_i, \mathbf{r}_1, \mathbf{r}) + \tau(g_i, \mathbf{r}_2, \mathbf{r}_1).$$

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This is possible if the optical depth is related to the absorption coefficient in the cumulative frequency domain in the same way as in the wavenumber space, namely

$$\tau(g_i) = \int_r \beta_{\text{abs}}^m(g, \mathbf{r}) d\mathbf{r}.$$

This approximation was frequently used for calculation of transmission function of molecular nonscattering atmosphere¹⁻³ and was shown to be accurate to within 1%.

In addition, it should be noted that the constancy of the solar constant within Δv is not generally true. To weaken this limitation, the transmission function can be redefined as⁷

$$T = \int_{\Delta v} S(v) \exp\{-\tau(v)\} dv / \int_{\Delta v} S(v) dv;$$

while the transmission function for an inhomogeneous atmosphere can also be expressed in terms of the series (10), where the number of terms does not depend on the spectral behavior of the solar constant assumed.⁷ Thus, over spectral intervals (Δv) as wide as 100 cm^{-1} or wider, the radiative transfer equation can be solved quite accurately using 5-6 series terms.

The next step in validation of the exponential series as a method of few-parameter description of the molecular absorption in solution of direct atmospheric-optics problems would be a change to scattered fluxes of optical radiation, since essentially not all atmospheric-optical situations can be described quite accurately in terms of the transmission function.

Prior to this step, it is necessary to clarify the realizability of these algorithms, i.e., the possibility using them as a part of already existing methods of solution of stationary (nonstationary) radiative transfer equation for estimation of scattered (including multiply scattered) radiative fluxes in problems of propagation of optical radiation in scattering and absorbing media. These include approximations of the lowest orders of scattering, small-angle, diffuse, and other approximations, or Monte Carlo method. The Monte Carlo method is asymptotically exact method of solution of radiative transfer equation (RTE) with controllable accuracy and, as such, it is superior to other techniques. Indeed, by means of it, and using the line-by-line method, one can not only estimate the accuracy of the line-by-line treatment of the molecular absorption for scattered radiative fluxes in the absorption bands (provided, of course, that it is compatible with internal structure of the Monte Carlo method), but also estimate the utility of alternative approximate RTE solution techniques for these same purposes.

These arguments, as well as the available experience of solution of different atmospheric optics problems by Monte Carlo method,⁸ have been the basis for the following problem formulation, that would made it possible to ascertain the compatibility of the above atmospheric absorption treatment with the method of statistical tests and its efficiency. Of course, this should be done with the account of numerical character of Monte Carlo solutions and, hence, complexity of the generalization of obtained numerical results.

We will confine ourselves to a simplest model scheme requiring modest computer resources on the basis of Intel Pentium Celeron 333 processor, to explore tentatively the possibility of incorporating the above-mentioned k -distribution method in algorithms of direct Monte Carlo simulation of unscattered and diffuse radiation propagation. Moreover, it is reasonable to estimate the efficiency of new solutions in comparison with results calculated by traditional (line-by-line) method in a simplified situation first, before making a decision on whether or not to investigate their applicability limits in a wider range of both optical-geometrical aspects of the problem formulation, and different Monte Carlo schemes used to solve more complex atmospheric-optical problems.

We chose to solve the problem of illumination of the Earth's surface in a plane parallel model of the atmosphere-surface system. It was assumed that solar radiation is incident normally on the top of the atmosphere. The xoy plane coincides with purely absorbing underlying surface, while oz axis points to the radiative source (Fig. 1).

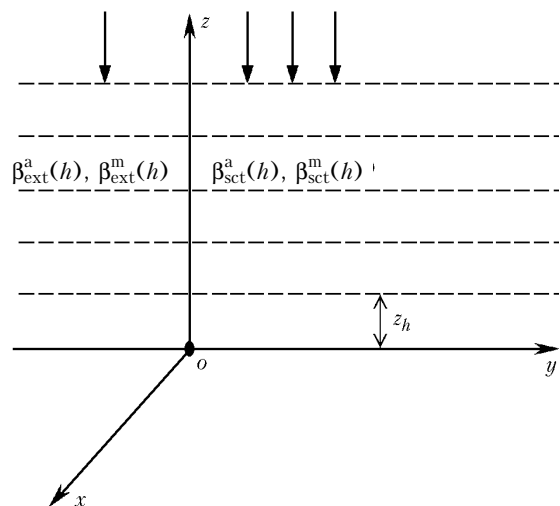


Fig. 1. Geometry of the experiment.

The integrated optical properties of the molecular-aerosol atmosphere were specified using a set of altitude profiles of the scattering and absorption coefficients. The scattering phase functions were specified from look-up tables as "weighted" aerosol-gaseous phase functions determined from the formula (see, e.g., Ref. 9):

$$f(\theta) = \frac{\beta_{\text{sct}}^a}{\beta_{\text{sct}}} f^a(\theta) + \frac{\beta_{\text{sct}}^m}{\beta_{\text{sct}}} f^m(\theta),$$

where β_{sct}^a and β_{sct}^m are the aerosol and molecular-scattering coefficients in the j th layer; $\beta_{\text{sct}} = \beta_{\text{sct}}^a + \beta_{\text{sct}}^m$; and $f(\theta)$, $f^a(\theta)$, and $f^m(\theta)$ are "weighted" aerosol and molecular scattering phase functions, respectively.

The atmosphere was assumed to be stratified: in the height range 0-25 km the layer thickness was 1 km, in the range 25-50 km it was 5 km. Water vapor

was assumed to be the main molecular absorber. The purpose was to estimate the surface irradiance in the wavelength interval 0.943–0.952 μm (or 10500–10600 cm^{-1}).

The model of atmospheric optical properties was chosen such that it imitates the physical situation, in which scattered radiation would be a substantial portion of the total irradiance, and in which the control line-by-line calculations on Intel Pentium Celeron 333 computer could be made at a modest cost without computer failures. Therefore, the meteorological visibility in the near-ground layer of the aerosol atmosphere was taken to be 8 km. As an example, Figure 2 presents an altitude profile of aerosol extinction coefficient, while Figure 3 shows the spectral dependence of the water vapor absorption coefficient in the near-ground atmospheric layer.

In terms of integrated optical characteristics, the model chosen here assumes the optical depth due to aerosol scattering to be $\tau_a = 1.42$, molecular scattering contribution $\tau_m = 0.0107$, the spectrally mean optical depth due to molecular absorption $\tau = 1.44$, and the total optical depth $\tau_s = 2.8707$.

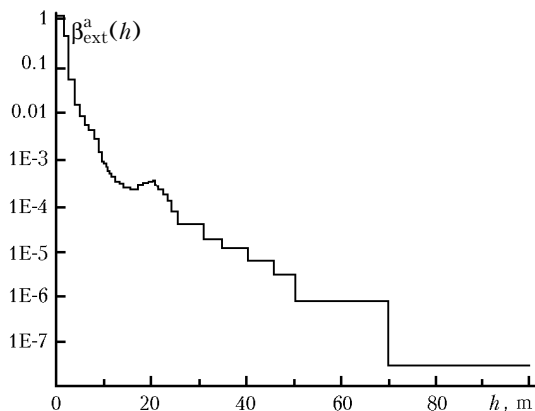


Fig. 2. Vertical profile of the aerosol extinction coefficient.

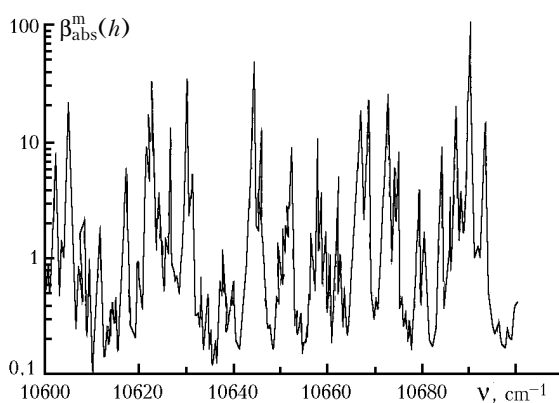


Fig. 3. Absorption spectrum of water vapor.

A straightforward Monte Carlo code is used to simulate radiation propagation in a molecular-aerosol

atmosphere, chosen for its simplicity and low computer demands when used to calculate illumination of the Earth's surface at a given wavelength λ .⁵

Test line-by-line calculations for the model atmosphere considered above have shown that, on the average, 13.32 s of computer time was required to simulate irradiance E_j (where subscript j indicates wavelength of radiation in the wavelength interval 0.943–0.952 μm) with the rms calculation error of $\varepsilon \approx 0.1\%$. For a correct account of the spectral dependence of water vapor absorption coefficient in the region of 1 μm , calculations with the step $\lambda = 10^{-2} \text{ cm}^{-1}$ (comparable with the half-width of a spectral line), i.e., 10000 Monte Carlo runs, are required. Then, the integrated irradiance E is calculated from the formula:

$$E = \Delta\lambda \sum_{j=0}^N E_j S(\lambda_j), \quad (11)$$

where $N = 10000$; $\Delta\lambda = 0.01 \text{ cm}^{-1}$; $S(\lambda_j)$ is the spectral solar constant; E_j is the fraction of the initial unit irradiance, reaching the Earth's surface at a given wavelength.

We note that 37 h of computer time was spent to simulate 10000 E values. Increasing the discretization step $\Delta\lambda$, i.e., by decreasing the number N of wavelengths, at which calculations are made, could reduce the total computer time. However, this leads to uncontrollable error in the irradiance estimate (Fig. 4).

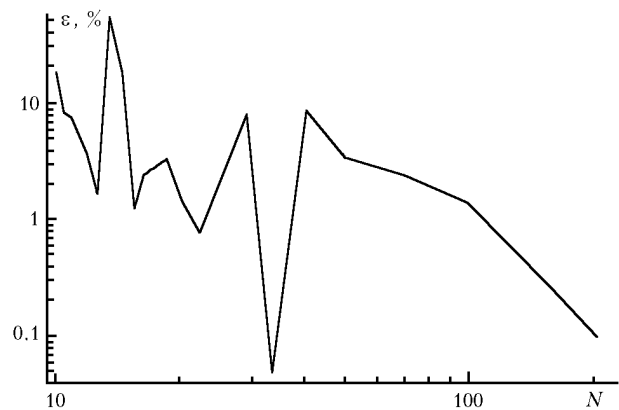


Fig. 4. Relative error of calculations of the surface irradiance versus number N of wavelengths chosen from the initial wavelength interval 0.943–0.952 μm and used for the computation.

This is because the molecular absorption coefficient strongly varies (see its spectrum in Fig. 3) with the wavelength.

Alternatively, the irradiance was calculated using exponential series to account for the absorption by H_2O molecules in the same wavelength range 0.943–0.952 μm ; for this, we have used no more than 10 Monte Carlo estimates of E_j for specially selected wavelengths, and summed them up according to the following formula:

$$E = \Delta\lambda \sum_{j=1}^n C_j E_j S(\lambda_j), \quad (12)$$

where C_j are the coefficients of Gaussian quadratures. For $n = 10$, calculation from this formula (plus obtaining Monte Carlo solutions) has required no more than 5 min of computer time. At the same time, the estimate by Eq. (12) has small relative error, remaining within 0.2% of line-by-line calculations based on formula (11). In addition, we have performed calculations using exponential series with different numbers of terms (Fig. 5). The simulation results have shown that, in the studied spectral interval, sufficiently high accuracy is achieved with 6–7 series terms when Gaussian quadratures are used.

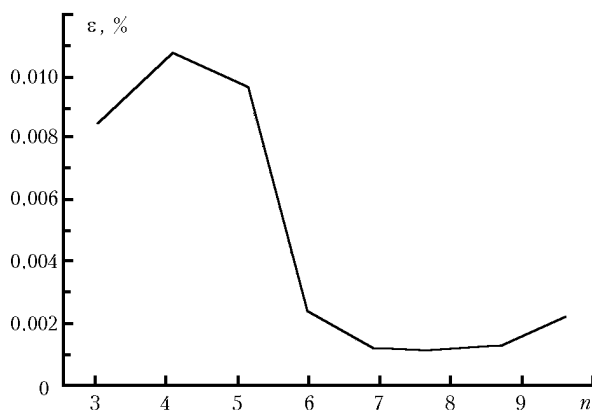


Fig. 5. Surface irradiance computation error versus the number of Gaussian quadratures.

To test the molecular absorption model used in our calculations, we compared the model results with independent data obtained by Fomin (Table 1).¹⁰ From the Table it is seen that the calculations disagree by no more than 0.44%, a good mark of the model realism.

The errors depicted in Fig. 5 turned out to be smaller than in Table 1. However, there is no contradiction here. Our analysis has shown that the discrepancy between our calculations and those by Fomin is mostly caused by different quadratures used for numerical integration over the optical depth. Thus, the use of exponential series leads to less uncertainty than the discretization error.

We conclude by noting that the chosen atmospheric optical model produced quite strong scattering on the path from top to bottom of the atmosphere. According to line-by-line calculations, contribution of scattered radiation to irradiance E is 30%. This suggests that, in the treatment of water vapor absorption along the scattered photon trajectories, large errors in Monte Carlo estimates of irradiance were very likely, but not appeared.

Table 1. Downward fluxes in the spectral range 10000–10500 cm^{-1} , calculated by k -distribution and line-by-line methods¹⁰ for absorption by water vapor under conditions of midlatitude summer atmosphere. Solar zenith angle is 10°

Height,	Downward fluxes, W/m^2		Relative
	k -distribution method	Line-by-line ¹⁰	
0	27.11	26.99	0.44
1	29.30	29.20	0.34
5	34.48	34.45	0.09
10	35.72	35.69	0.08
70	35.76	35.76	0.00

Thus, in this formulation of the problem, the use of a new treatment of the molecular absorption of the atmosphere to calculate surface irradiance in the absorption band 0.943–0.952 gave more than a factor of 350 gain in the efficiency for a 0.2% loss in accuracy of estimates. This makes grounds to believe that, with the method of parameterization of spectroscopic information on atmospheric molecular absorption proposed here, the problem of accounting for scattering (including multiple-scattering) effects in the atmosphere on radiative fluxes in wide spectral intervals can be successfully solved.

The efficiency and accuracy of this method in solving more complex atmospheric-optics problems will be the subject of future studies.

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