Step-by-step technique for taking into account thermal radiation scattering by aerosol formations in the atmosphere. Part 3. Applications to mathematical modeling of measurements

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Some capabilities of the algorithm, described in previous parts of this paper, are presented and applied to mathematical modeling of measurements under conditions of taking into account the problem of effective calculations of monochromatic intensity and the instrumental function convolution. Basic methods for the calculations are outlined. A new technique of fast calculations and the corresponded modification of the algorithm described in the second part of this paper are suggested.

Introduction

The method of successive approximations for the problems of the thermal radiation scattering in the atmosphere and the corresponding algorithm for calculation of monochromatic radiation were considered in two first parts of the paper.[1,2] When mathematically modeling measurements by real devices, a necessity appears of calculation of the convolution of the obtained monochromatic radiation intensity with the instrumental function (functions) of the device.[3] The following formula can be written in the approximation of the effect of only the spectral instrumental function on the results of measurements:

$$I(\Delta\nu, z, \vartheta, \varphi) = \int_{\nu_1}^{\nu_2} I(\nu', z, \vartheta, \varphi) y(\nu') d\nu' \Big/ \int_{\nu_1}^{\nu_2} y(\nu') d\nu', \qquad (1)$$

where (z, ϑ, φ) are the height, nadir angle, and azimuth of vision[1]; $y(\nu)$ is the instrumental function of the measuring device; $I(\Delta\nu, z, \vartheta, \varphi)$ is the intensity at the device output (the parameter to be modeled); $I(\nu, z, \vartheta, \varphi)$ is the monochromatic intensity with the frequency ν at the device input. The intensities of polarized radiation[2] in Eq. (1) are replaced with the Stokes vectors, and the instrumental function $y(\nu)$ is replaced with the corresponding matrix 4×4. Formula (1) should be written for each component of the Stokes vector, and the necessary component in the denominator results from multiplication of the matrix $y(\nu)$ by the unit vector. Thus, accounting for polarization introduces no new problems into modeling of measurements, and only for briefness we will further use the scalar form of the formula (1).

As was noted,[1] at the preset characteristics of the device, namely, the instrumental function $y(\nu)$ and the boundaries ν_1 and ν_2 of the spectral range $\Delta\nu$ determined by this function, the problem is formally reduced to calculation of the monochromatic intensity $I(\nu, z, \vartheta, \varphi)$. The corresponding algorithm for the considered method of successive approximations was presented in Ref. 2. However, as is well known, when applying the quadrature formulas to the nominator of Eq. (1), some difficulties appear due to strong oscillations of the monochromatic intensity $I(\nu, z, \vartheta, \varphi)$ caused by the selective molecular absorption, that puts the problem of integration in Eq. (1) out of the framework of a purely technical problem and requires a development of effective integration algorithms. This is especially important when taking into account the scattering, where calculation of the monochromatic intensity is also quite complicated and cumbersome.[1,2] Below, the available algorithms are briefly outlined and a new technique for calculation of the integral (1) is proposed. Note that the restrictions on the interval $\Delta\nu$ being implicitly present in some algorithms do not decrease their generality, because the integral over any interval $\Delta\nu$ as large as one likes can be divided into a sum of integrals over the required small intervals.

Most presented algorithms were used by the author in practical calculations.

Non-monochromatic approximation

If the integration interval $\Delta\nu$ is sufficiently small, a change of all values can be neglected, except for the volume absorption coefficient. Disregarding the scattering, we come to the widely used approximation of the non-monochromatic transmission function,[3] when the integral (1) is calculated only for an individual transmission function of the molecular absorption (see Eq. (3) in Ref. 1), and the mean values of other parameters on $\Delta\nu$ are used. The intensity at the device output is calculated taking into account these values as in the monochromatic case.

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When taking into account the scattering, we cannot separately integrate the operators with respect to frequency for the intensity written in the form of the series in terms of the scattering and reflection multiplicities (Eqs. (20) and (23) from Ref. 1). However, it doest not mean that the use of the non-monochromatic approximation is impossible in principle. All depends on particular problems, spectral intervals, and requirements to the calculation accuracy. In the algorithm presented in Ref. 2, the operator of the direct radiation $T_0(j, j', k')$ and the single scattering albedo $\omega_0[\tau(j)]$ are to be integrated by Eq. (1).

Two cases can be distinguished, when the non-monochromatic approximation is sufficiently accurate: a significant predominance of absorption over scattering ($\omega_0 \to 0$) in the limit providing for the mathematically correct case of the absence of scattering, and *vise versa*, a significant predominance of scattering over absorption ($\omega_0 \to 1$) in the limit excluding the effect of the absorption selectivity.

A choice of irregular grid of integration

Obviously, for optimization of calculation of the nominator in Eq. (1), a step of integration must be chosen with accounting for the particular peculiarities of the spectral dependence of the intensity $I(\nu, z, \vartheta, \varphi)$. The quadrature trapezoid formula with the step duplication is convenient for reaching a sufficient accuracy of integration. Let $Y = \int_a^b f(x)\mathrm{d}x$ and the initial grid x_i, $i = 1,\ldots,N$ ($x_1 = a$, $x_N = b$) be preset. Then

$$Y_m = Y_{m-1}/2 + \sum_{i=1}^{N-1} \Delta_{i,m} \sum_{k=1}^{2^m-1} f(x_i + (2k-1)\Delta_{i,m}),$$

$$Y_0 = \frac{1}{2}\sum_{i=1}^{N-1} (f(x_{i+1}) + f(x_i))\Delta_{i,0},$$

$$\Delta_{i,m} = (x_{i+1} - x_i)/2^m. \qquad (2)$$

Iterations by Eq. (2) should be terminated at $|Y_m - Y_{m-1}| < \varepsilon$, where ε is the parameter determining the accuracy of calculations. The algorithm (2) is very convenient because at any quantity of iterations the function $f(x)$ is calculated at each point of the integration grid only once, and it is not necessary to store corresponding values in the computer memory.

When applying formula (2) to calculating the integral (1), the main problem is to choose the initial frequency grid ν'_i, $i = 1, \ldots, N$. Very simple and quite effective technique is to choose as ν'_i either central frequencies of the absorption lines inside the interval $\Delta\nu$, or the frequencies in the middle between them (or both). Indeed, in this case taking into account all spectral peculiarities related to each absorption line is guaranteed. The choice of the central frequencies is effective at a weak absorption, and middle ones — at a strong absorption. A similar but more complicated way for choosing ν'_i was proposed in Ref. 4, where for each line the own frequency grid was set with essentially different steps in its center, periphery, and wings.

Monte Carlo method

The integrals of the form (1) are ideally suitable for calculations by the Monte Carlo method. Indeed, by definition of the integral of probability (Stieltjes) the identity is true:

$$I(\Delta\nu, z, \vartheta, \varphi) \equiv \mathbf{M}_{\psi(\nu)}[I(\nu, z, \vartheta, \varphi)],$$

$$\psi(\nu) = y(\nu) \Big/ \int_{\nu_1}^{\nu_2} y(\nu')\mathrm{d}\nu', \qquad (3)$$

which asserts that the sought intensity is the mathematical expectation of the monochromatic intensity, the frequency of which is interpreted as a random value distributed on the interval $[\nu_1, \nu_2]$ with the probability density $\psi(\nu)$ calculated for the instrumental function of the device $y(\nu)$ by Eq. (3). Thus, by modeling the frequency as a random value and setting the accuracy of calculations, the integral (1) can be quite effectively calculated, that has been realized.[4,5] The algorithm for computer modeling of the random frequency and estimating the accuracy of integration is described in Ref. 5.

A disadvantage of the Monte Carlo method is a presence of a random error in calculations, as a rule, of the order of one percent; however, if it is used for calculation of only scattered thermal radiation, which usually is an insignificant fraction of the direct radiation, it can be efficient in the high-accuracy calculations. Note that the Monte Carlo method is free of restrictions on the integration interval width. This allows us to consider it to be applicable, in principle, to very wide spectral intervals, for example, in the problems of atmospheric energetics.

Method of integration with respect to the absorption coefficient (*k*-method)

This method is one of the well-known and widely used methods. It is actually associated with passing from integration with respect to frequency in Eq. (1) to integration with respect to the probability density of appearance in the interval $[\nu_1, \nu_2]$ of values of the volume absorption coefficient or its profile for the inhomogeneous atmosphere. Other parameters therewith are assumed to be constant on the interval of integration or, as, for example, for the instrumental function, their probability density together with the volume absorption coefficient can be evaluated. The described technique allows us to decrease many times the number of nodes of the quadrature formula in the

calculation by Eq. (1), because the probability density is a non-oscillating function.

The foundations of the *k*-method are given, in particular, in Ref. 3, and its applications to different problems can be found, for example, in Refs. 6–8. In comparison with other considered techniques for integration of Eq. (1), the *k*-method is much more complicated, besides, it requires significant preliminary calculations. From the standpoint of practical realization of the calculation algorithms, these facts can be considered as disadvantages of the *k*-method, because not only the calculation time needs optimization, but also the time necessary for development of the corresponding software.

Note also that, although the *k*-method can be especially convenient for the problems with fixed parameters (particular device and spectral interval), its efficiency significantly decreases (because of cumbersome preliminary calculations) in scientific problems, where it is necessary to study the calculated intensity as a function of variations of different atmospheric parameters including those, which determine the volume absorption coefficient. Due to these facts, we consider the *k*-method in calculations of thermal radiation scattering only as an alternative, which has no *a priori* advantages over other methods.

Variation approximation at integration with respect to frequency

The proposed method for calculation of the integral (1) is ideologically close to the *k*-method, but does not require any preliminary calculations. Like the *k*-method, it is based on grouping the grid nodes not upon the principle of closeness of frequencies ν, but upon the principle of closeness of the values of the integrand.

Let the interval $[\nu_1, \nu_2]$ be sufficiently small so that one can neglect spectral dependences of all parameters inside it, except for the volume absorption coefficient $\kappa(\nu)$ (it may be molecular or summarized with the aerosol one). In each particular calculation of Eq. (1), all atmospheric parameters (profiles of temperature, pressure, concentrations of the absorbing gases, aerosol characteristics) are set and fixed. Hence, when calculating the monochromatic intensity $I(\nu, z, \vartheta, \varphi)$, the profile $\kappa(\nu, z)$ depends only on the frequency ν. Let the intensity $I(\nu'_i, z, \vartheta, \varphi)$ corresponding to the vertical profile $\kappa(\nu'_i, z)$ have been calculated by the quadrature trapezoid formula (2) or by the Monte Carlo method (3). Let us store the intensity and the profile values, but remove the data on frequency, that means, pass to $I_i(z, \vartheta, \varphi)$ and $\kappa_i(\nu)$. When calculating the next frequency ν'_j, $\kappa(\nu'_j, z)$ may become quite close to $\kappa_i(z)$, for example, for all z

$$| \kappa(\nu'_j, z) - \kappa_i(z) | < \varepsilon, \qquad (4)$$

where ε is some parameter determining the method's accuracy. Then, instead of calculating $I(\nu'_j, z, \vartheta, \varphi)$ by the scattering algorithm, we use the variation approximation:

$$I(\nu'_j, z, \vartheta, \varphi) = I_i(z, \vartheta, \varphi) + \int_{z_0}^{z_\infty} \frac{\delta I_i(z', \vartheta, \varphi)}{\delta \kappa_i(z')} [\kappa(\nu_j, z') - \kappa_i(z')] \mathrm{d}z'. \qquad (5)$$

Naturally, in real calculations the integral in Eq. (5) is replaced with the quadrature sum, and the variation derivative $\delta I_i(z', \vartheta, \varphi) / [\delta \kappa_i(z')]$ – with the vector of the intensity partial derivatives with respect to the volume absorption coefficient at each node of integration.

General logic of the algorithm is very simple. As each node of integration in Eq. (1) with respect to frequency is passed, $\kappa(\nu'_j, z)$ is compared with all $\kappa_i(z)$, $i = 1, \ldots, L$, stored in the computer memory, and if i, for which the condition of closeness (4) is fulfilled, is found, then the sought intensity of the scattered radiation $I(\nu'_j, z, \vartheta, \varphi)$ is calculated by Eq. (5) much faster than by the algorithm from Ref. 2. Otherwise, if the condition (4) failed to fulfill for all $\kappa_i(z)$, $i = 1, \ldots, L$, then $I(\nu'_j, z, \vartheta, \varphi)$ is calculated by the algorithm from Ref. 2, and the calculation results for

$$I_{L+1}(z, \vartheta, \varphi) \equiv I(\nu'_j, z, \vartheta, \varphi),$$

$$\frac{\delta I_{L+1}(z, \vartheta, \varphi)}{\delta \kappa_{L+1}(z)} \equiv \frac{\delta I(\nu'_j, z, \vartheta, \varphi)}{\delta \kappa(\nu', z)} \text{ and } \kappa_{L+1}(z) = \kappa(\nu'_j, z)$$

are stored in the computer memory.

The storing does not introduce difficulties into calculations due to the modern resources of computers.

The condition of closeness (4) is not optimal. Indeed, it is reasonable to require a greater closeness of the profiles at the heights, where the dependence of the intensity on $\kappa(z)$ variations is strong, and a less closeness, where the dependence is weak. Similarly, the peculiarities of the instrumental function of the device must be also taken into account. This leads to the following "weight" modification of the closeness condition:

$$\left| (\kappa(\nu'_j, z) - \kappa_i(z)) \frac{\delta I_i(z, \vartheta, \varphi)}{\delta \kappa_i(z)} y(\nu'_j) \right| < \varepsilon.$$

A new point in the proposed method is a necessity of calculation, together with the scattered radiation intensity, of its partial derivatives with respect to the volume absorption coefficient. But the calculation can be simply performed by the algorithm from Ref. 2. The corresponding formulas are briefly presented below, in which all notations[1,2] and numbering the operations of the algorithm[2] are kept. Operations, which are not changed through calculations of derivatives, are omitted.

1. *Derivatives of the direct radiation intensity.* Let the integration interval from z_0 to z_∞ be divided into nodes z_m, $m = 1, \ldots, M$ and let δ_m be the corresponding weights of the quadrature formula

(positive or negative). Then we have for the transmission function (1) from Ref. 1:

$$\frac{\partial P_\kappa(\nu, z_1, z_2, \vartheta)}{\partial \kappa(\nu, z_m)} = -\frac{\delta_m}{\cos\vartheta} P_\kappa(\nu, z_1, z_2, \vartheta), \qquad (6)$$

and, taking into account Eq. (6), for the direct radiation intensity (2), (3) from Ref. 1

$$\frac{\partial I(\nu, z_2, \vartheta, \varphi)}{\partial \kappa(\nu, z_m)} = I(\nu, z_1, \vartheta, \varphi) P_\sigma(\nu, z_1, z_2, \vartheta) \frac{\partial P_\kappa(\nu, z_1, z_2, \vartheta)}{\partial \kappa(\nu, z_m)} -$$

$$-B_e[\nu, T(z_m)] P_\sigma(\nu, z_m, z_2, \vartheta) \frac{\partial P_\kappa(\nu, z_m, z_2, \vartheta)}{\partial \kappa(\nu, z_m)} +$$

$$+\sum_{k=m}^{M} B_e[\nu, T(z_k)] P_\sigma(\nu, z_k, z_2, \vartheta) \frac{\partial P_\kappa(\nu, z_k, z_2, \vartheta)}{\partial z_k \partial \kappa(\nu, z_m)} \delta_k .$$

2. *Derivatives of the quadrature formula weights for integration with respect to the optical depth.* They must be calculated, because the variable of integration in the algorithm[2] is the optical depth, but not the height. The particular form of $\partial d(j, j_1, j_2)/\partial\kappa(\nu, z_m)$ depends on representation of $d(j, j_1, j_2)$ through the nodes of integration in the used quadrature formula. Then, for the recommended trapezoid formula[2] we have:

$$\frac{\partial d(j, j_1, j_2)}{\partial \kappa(\nu, z_m)} = \frac{1}{2}\left(\frac{\partial \tau(j+1)}{\partial \kappa(\nu, z_m)} - \frac{\partial \tau(j-1)}{\partial \kappa(\nu, z_m)}\right),$$

if $\min(j_1, j_2) < j < \max(j_1, j_2)$,

$$\frac{\partial d(j, j_1, j_2)}{\partial \kappa(\nu, z_m)} = \frac{1}{2}\left(\frac{\partial \tau(j+1)}{\partial \kappa(\nu, z_m)} - \frac{\partial \tau(j)}{\partial \kappa(\nu, z_m)}\right),$$

if $j = \min(j_1, j_2)$,

$$\frac{\partial d(j, j_1, j_2)}{\partial \kappa(\nu, z_m)} = \frac{1}{2}\left(\frac{\partial \tau(j)}{\partial \kappa(\nu, z_m)} - \frac{\partial \tau(j-1)}{\partial \kappa(\nu, z_m)}\right),$$

if $j = \max(j_1, j_2)$. Then, according to the definition of the optical depth[1]:

$$\frac{\partial \tau(j')}{\partial \kappa(\nu, z_m)} = \delta_m, \text{ if } z_m \geq z_{j'}$$

and

$$\frac{\partial \tau(j')}{\partial \kappa(\nu, z_m)} = 0, \text{ if } z_m < z_{j'}.$$

4. *Derivatives of the initial source function:*

$$\frac{\partial B_0(l, j, k)}{\partial \kappa(\nu, z_m)} = \frac{\omega_0[\tau(j)]}{\alpha[\tau(j)]} B_e\{\nu, T[\tau(j)]\} \frac{\partial \tau(j)}{\partial \kappa(\nu, z_m)} .$$

5. *Derivatives of the direct radiation operator:*

$$\frac{\partial T_0(j, j', k')}{\partial \kappa(\nu, z_m)} = -\frac{T_0(j, j', k')}{\eta(k')}\left(\frac{\partial \tau(j')}{\partial \kappa(\nu, z_m)} - \frac{\partial \tau(j)}{\partial \kappa(\nu, z_m)}\right).$$

6. *Derivatives of the single scattering operator:*

$$\frac{\partial T_1(l, l', j, k, j', k')}{\partial \kappa(\nu, z_m)} = -T_1(l, l', j, k, j', k') \times$$

$$\times\left(\frac{1}{\alpha[\tau(j)]} \frac{\partial \tau(j)}{\partial \kappa(\nu, z_m)} + \frac{1}{\eta(k')}\left(\frac{\partial \tau(j')}{\partial \kappa(\nu, z_m)} - \frac{\partial \tau(j)}{\partial \kappa(\nu, z_m)}\right)\right).$$

8–11. Calculation of the derivatives in these operations of the algorithm is reduced to the elementary differentiation of sums and products, so the corresponding formulas are not presented here.

Algorithms for fast calculation of the volume absorption coefficient

Let us briefly consider the techniques for acceleration of calculation of the integral (1) through application of special algorithms for calculating the volume absorption coefficient. As is known, most time for its calculation is consumed to summing the spectral lines

$$\kappa(\nu, z) = \sum_{k=1}^{N[\nu_3, \nu_4]} C_{m(k)}(z) S_k[T(z)] f_k[\nu, \nu_k, p(z), T(z)], \quad (7)$$

where k is the number of a spectral line, $C_{m(k)}$ is the concentration of the mth absorbing gas, p is the pressure, S_k is the intensity, f_k is the function of the spectral line contour centered at ν_k. In Eq. (7), all N lines are summed in the spectral interval $[\nu_3, \nu_4]$, which, in general case, is much wider than $[\nu_1, \nu_2]$ in Eq. (1).

The well-known and quite effective technique for acceleration of calculations by Eq. (7) is approximation of the contribution of the line wings, at which the sum of the terms of the series (7) situated quite far from the boundaries of the integration interval $[\nu_1, \nu_2]$ is replaced with polynomial in terms of pressure. The polynomial's coefficients depend on the type of gas and the temperature. They are precalculated for a prescribed set of temperatures, and then, when calculating by Eq. (7), are interpolated to a particular $T(z)$. This approximation algorithm in the form convenient for practical realization can be found in Refs. 5 and 9.

Another effective technique that can be used both in combination with wing contribution approximation or without it, is the line selection. Indeed, line intensities in Eq. (7) usually differ by some orders of magnitude, therefore, weaker lines can be excluded from the sum without loss of the calculation accuracy. A simple selection algorithm was proposed in Ref. 10. Setting in Eq. (7) $\nu = \nu_1$, and then $\nu = \nu_2$ and numbering the lines outside the interval $[\nu_1, \nu_2]$ in the order of increasing their contribution into the sum (7), we can successively exclude the first numbers (i.e., the weakest lines) until the error in calculations of Eq. (7), related to the excluding, exceeds the preset value. We can either preliminary look over different model variants of the temperature, pressure, and concentration profiles of absorbing gases or take into account the fact that the greatest contribution

into the sum (7) is reached at minimal temperature, maximal pressure and concentration of the gas[3] and perform either selection for these conditions or individual selection for each model condition. Note that application of the line selection has resulted in almost tenfold acceleration of calculations by the algorithm realized by the author in Ref. 11.

The above-described technique makes it possible to select lines only outside the interval $[\nu_1, \nu_2]$. One should be careful when selecting lines inside the interval of integration, because the contribution of even weak line at a frequency close to its center ν_k can be significant. Here we recommend a simple technique suitable for particular applied problems with rigidly set parameters of calculation. The lines inside $[\nu_1, \nu_2]$ are successively excluded from Eq. (7), starting from the weakest ones but at temperatures, pressures and concentrations corresponding to their maximal contribution into the sum (7). And we estimate the procedure effect on the accuracy of not the volume absorption coefficient (7), but the modeled intensity (1).

Conclusions

The considered optimization techniques together with analogous techniques mentioned in Ref. 2 provide for development and computer realization of the effective and fast algorithms for modeling measurements of the thermal radiation, which take into account aerosol scattering and are suitable for both scientific-research and applied calculations.

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