Calculating the Natural Atmospheric Radiation Using the General Circulation Model of the Earth's Lower and Middle Atmosphere

B. N. Chetverushkin^{*a*}, I. V. Mingalev^{*b*}, *, E. A. Fedotova^{*b*}, K. G. Orlov^{*b*}, V. M. Chechetkin^{*a*,*c*,*d*}, and V. S. Mingalev^{*b*}

^aKeldysh Institute of Applied Mathematics, Russian Academy of Sciences, Moscow, 125047 Russia ^bPolar Geophysical Institute, Russian Academy of Sciences, Murmansk, 183010 Russia ^cNational Research Nuclear University Moscow Engineering Physics Institute MEPhI, Moscow, 115409 Russia ^dNational Research Center Kurchatov Institute, Moscow, 123182 Russia

> **e-mail: mingalev_i@pgia.ru* Received June 24, 2019; revised June 24, 2019; accepted September 9, 2019

Abstract—The paper describes a block for calculating the Earth's natural atmospheric radiation in the IR range developed for the general circulation model simulating the lower and middle atmosphere. This block uses the new parametrization of molecular absorption in the frequency range from 10 to 2000 cm^{-1} at the altitude ranging from the Earth's surface to 76 km. The algorithm for constructing this parametrization takes into account the change in the gas composition of the atmosphere with altitude and has some other significant advantages. In addition, for the numerical solution of the radiation transfer equation, the discrete ordinate method and the computational zenith angle grid with the step of about nine degrees are used. The results of the line-by-line calculations of the Earth's internal atmospheric radiation field are compared with the results of the calculations performed using parametrization, and it is shown that the presented parametrization is accurate in the lower and middle atmosphere both in the absence of clouds and in the presence of cloud layers with a significant optical thickness.

Keywords: general circulation model, parameterization of molecular absorption, atmospheric radiation, calculation of radiation field

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1. INTRODUCTION

Computing the atmospheric radiation field in the infrared (IR) range is required to calculate the rate of heating the atmosphere by radiation when modeling the general circulation of the Earth's atmosphere. In this case, the higher the accuracy of calculating the heating rate the higher the quality of the modeling of the general circulation of the atmosphere.

At altitudes of more than 20 km, the absorption lines of atmospheric gases become narrow and the coefficient of molecular absorption changes quickly with the change in frequency. Therefore, in order to guarantee the accuracy of 1% and better when calculating the radiation intensity, the frequency resolution should be approximately 0.001 cm⁻¹. Calculations with such a high frequency resolution are called line-by-line calculations and their computational cost is too high to be affordable in general atmospheric circulation models both at present and in the foreseeable future. For this reason, general circulation models of planetary atmospheres employ a variety of simplified methods for the rapid calculation of radiation fluxes [1-18].

The main idea of these methods is that the real dependence of the molecular absorption coefficient on frequency is replaced by the model dependence that is more convenient for calculations. In this case, narrow spectral channels are grouped based on a special algorithm and each group is replaced by a single wide model channel. As a result, several million narrow spectral channels are replaced by several tens or several hundreds of model channels, for each of which the radiation transfer equation is numerically solved. The procedure for constructing these model channels is called constructing the parametrization of molecular absorption. In order to verify the accuracy of the constructed parameterization, the results of calculating the radiation field in the model channels are compared to the results of the line-by-line calculations.

It should be noted that at the altitudes of 0-70 km it is necessary to take into account the change in the gas composition of the Earth's atmosphere with altitude. Below the altitude of 15 km, the contribution of water vapor to the coefficient of molecular absorption is significant and the contribution of ozone is small. Above 20 km, the role of water vapor decreases and the contribution of ozone increases. Therefore, the absorption spectra at low and high altitudes are not correlated.

One of the methods for constructing parameterization is the k-correlation method [1-17], which, in turn, is one of the variants of the Lebesgue method for the frequency averaging of the absorption cross sections [19]. In the k-correlation method, the transmission function for the selected frequency interval and the given altitude interval is represented as the sum of a series of exponentials, and each term of this series is assigned its own model channel. Two assumptions are also used: (1) when solving the radiation transfer equation, it suffices to know the distribution function of the absorption coefficient (k-distribution), and (2) the distribution function of the absorption coefficients changes slightly with altitude. The latter assumption is substantially violated for the altitude range of 0 to 70 km.

Previously, numerous different parametrizations of molecular absorption in the Earth's atmosphere had been developed in the frequency range of 10 to 3000 cm^{-1} , containing from several dozens to 150-200 model channels [5–17]. A common feature of these parameterizations is that they all ensure accurate (within 0.5K/day) calculations for the rates of heating and cooling of the atmosphere due to natural radiation at the altitudes of the troposphere and lower stratosphere (up to about 20 km). At the altitudes exceeding 25 km, the accuracy of these parameterizations significantly deteriorates. The method of constructing the parametrization proposed in [11] provides the best accuracy for the given number of model channels but its implementation is quite laborious since it requires a significant number of fitting calculations for each model channel. It should be noted that due to the improving computer speed, at present, parameterizations containing 500–1000 model channels provide fairly acceptable performance.

This paper presents a description of a block for calculating the Earth's atmospheric radiation in the IR range, which was designed for the general circulation model of the lower and middle atmosphere developed by the authors of this work. The dynamic core of this model is described in [20]. In the presented block for calculating the natural radiation of the Earth's atmosphere, a new parameterization of molecular absorption is used in the frequency range from 10 to 2000 cm⁻¹ in the altitude range from the Earth's surface to 76 km, in which there are 280 model channels. The method for constructing this parameterization was presented by the authors in [21]. This method takes into account the change in the atmospheric gas composition with altitude, does not require fitting calculations for each model channel, and its software implementation is relatively simple compared to other algorithms. In addition, this method differs from the *k*-correlation method and does not use the distribution function of the absorption coefficient.

The model block presented in this work has two important features. The first feature is that the numerical solution of the radiation transfer equation is based on the discrete ordinate method and the computational zenith angle grid with the constant step of nine degrees. This enables accurate calculation of the radiation field in the presence of cloud layers with a significant optical thickness. It should be noted that in all known models simulating the general circulation of the Earth's atmosphere and weather forecast, the two-stream approximation [11-17] is used in calculating the field of atmospheric radiation, which obviously cannot provide good computation accuracy in the presence of cloud layers. The second important feature of the presented block is that all calculations are carried out on GPUs using massively parallel computing. This provides a good calculation speed.

The accuracy of the presented block was checked using line-by-line calculations performed with a frequency resolution of 0.001cm⁻¹. The molecular absorption coefficient of atmospheric gases was calculated using the HITRAN 2012 spectroscopic database [22] based on the standard theory, according to which the contributions of various absorption lines are summarized when cutting the lines' wings at a distance of 25 cm⁻¹ from the center of the line and taking into account the continuous absorption of water vapor and carbon dioxide, which was specified using the empirical model MT CKD [23].

To verify the accuracy of their line-by-line calculations, the authors compared the results of these calculations with the results of the line-by-line calculations performed by other scientific groups as part of the international project Continual Intercomparison of Radiation Codes (CIRC, https://circ.gsfc.nasa.gov) and made sure that for the same optical parameters of the atmosphere, the calculated fluxes coincided with the accuracy of at least 1%.

The authors also compared the results of the line-by-line calculations of the Earth's atmospheric radiation field with the results of calculations performed using the presented model block and showed that this block provided good calculation accuracy in the lower and middle atmosphere both in the absence of clouds and in the presence of cloud layers with a significant optical thickness.

2. ORGANIZATION OF CALCULATIONS AND NUMERICAL SOLUTION OF THE RADIATION TRANSFER EQUATION

In our model, a computational grid uniform in spherical geographical coordinates is used, in which the integer grid nodes closest to the poles are removed from the poles altitudinally by half-a-step [20]. The altitude grid step is 200 m, and the altitude of the upper boundary of the simulation domain above the ocean level in the current version of the model is $z_{max} = 76$ km. For each integer node of the computational grid on the Earth's surface, a vertical column of grid nodes located above it is considered. In this column of grid nodes, for each spectral channel, the field of the atmospheric radiation is calculated within the approximation of a flat and horizontally uniform atmosphere. In this case, the one-dimensional spatial equation for the transfer of the natural radiation is numerically solved using the modification of the discrete ordinate method developed by the authors, which is described in detail in [24].

For writing this equation, we denote by u the cosine of the angle between the direction of the photon momentum and the vertical direction. This angle will be referred to as the zenith angle. Sometimes it is counted downward. By z we denote the altitude above the Earth's surface in the vertical column of the atmosphere, in which the radiation field is calculated. Also for this column we denote by T(z) the temperature of the atmospheric gas at altitude z; by I(v, z, u) we designate the radiation intensity with frequency v and the zenith angle, the cosine of which is equal to u at altitude z; $\sigma(v, z)$ and $\omega(v, z)$ are the volumetric attenuation (extinction) and single-scattering albedo coefficients of the atmospheric gas at altitude z for the radiation with frequency v; and by $B(v,T) = 2hv^3c^{-2}(\exp(hv/(k_B T)) - 1)^{-1}$, we denote the Planck function in which h is Planck's constant, k_B is the Boltzmann constant, and c is the light velocity.

The transport equation of the atmospheric radiation in the considered column can be written as

$$\frac{u}{\sigma(v,z)}\frac{dI(v,z,u)}{dz} = -I(v,z,u) + (1 - \omega(v,z))B(v,T(z)) + \frac{\omega(v,z)}{4\pi}\int_{-1}^{1}I(v,z,w)\left(\int_{0}^{2\pi}\chi(v,z,m(w,u,\varphi))d\varphi\right)dw, (1)$$

where w and u are the cosines of photons' zenith angles before and after scattering, φ is the difference between the azimuthal angles of the photons before scattering and after scattering, $m(w, u, \varphi) = wu + \cos \varphi \sqrt{(1 - w^2)(1 - u^2)}$ denotes the cosine of the scattering angle, and $\chi(v, z, m)$ stands for the scattering indicatrix for radiation with frequency v at altitude z at the angle the scattering of which is m.

For Eq. (1), the following boundary conditions are used. On the upper boundary for the atmospheric radiation, the downward radiation must be zero:

$$I(v, z_{\max}, u < 0) = 0.$$
⁽²⁾

On the lower boundary, the upward radiation is composed of the incident radiation scattered by the surface and of the thermal radiation of the surface with temperature T_p . For isotropic scattering by the surface, the condition on the lower boundary has the form

$$I(v, z = 0, u > 0) = (1 - \Omega(v)) B(v, T_p) + \Omega(v) \int_{-1}^{0} I(v, z = 0, w) dw,$$
(3)

where $\Omega(v)$ is the surface albedo for radiation with frequencyv. It follows from (3) that, on the lower boundary, the intensity of the upward radiation does not depend on the zenith angle.

The discretization method for the numerical solution of Eq. (1) with boundary conditions (2) and (3) is as follows [4, 24]. A zenith angle grid is introduced. Next, the radiation field is divided into a finite number of streams, each of which is associated with a fixed zenith angle of the introduced grid. The angular integral defining the source of scattered radiation on the right-hand side of (1) is approximated by a linear combination of the streams. Equation (1) is replaced by a finite system of ordinary differential equations describing the changes in altitude observed for radiation intensities with the given zenith angles. The boundary conditions for this system follow from conditions (2) and (3). Our model uses the uniform zenith angle grid, which provides the best accuracy for the given number of nodes and is specified by the formula $u_i = \cos(\pi(i/N - 1))$, i = 0, ..., N. The current version uses 20 grid nodes (N = 19), which provides good calculation accuracy in the presence of cloud layers.

This is followed by the altitude discretization of the resulting system of ordinary differential equations. Between the altitude grid nodes, the scattering indicatrix and the single-scattering albedo are considered

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linearly dependent on the optical thickness (this dependence varies from layer-to-layer). Next, a transition is made from a system of ordinary differential equations to a system of integral equations according to the altitude connecting the radiation intensities at the nodes of the altitude and zenith angle grids on adjacent layers. After that, a transition to a system of linear algebraic equations is carried out with respect to the radiation intensity at the nodes of the zenith angle and altitude grids. This transition is performed by approximating the altitude integrals in the integral equations by analytical formulas. Our model uses the approximation method described in detail in [24].

This system of linear equations can be represented as a system of three-point vector equations for vector columns of radiation intensities at the zenith angle and altitude grid nodes $\mathbf{I}_k = (I(z_{M-k}, u_0), ..., I(z_{M-k}, u_N))^T$ (*M* is the number of the top node of the altitude grid, k = 0, ..., M):

$$\widehat{\mathbf{C}}_{0} \mathbf{I}_{0} - \widehat{\mathbf{B}}_{0} \mathbf{I}_{1} = \mathbf{F}_{0},$$

$$-\widehat{\mathbf{A}}_{k} \mathbf{I}_{k-1} + \widehat{\mathbf{C}}_{k} \mathbf{I}_{k} - \widehat{\mathbf{B}}_{k} \mathbf{I}_{k+1} = \mathbf{F}_{k}, \quad k = 1, \dots, M - 1,$$

$$-\widehat{\mathbf{A}}_{M} \mathbf{I}_{M-1} + \widehat{\mathbf{C}}_{M} \mathbf{I}_{M} = \mathbf{F}_{M},$$
(4)

in which $\hat{\mathbf{A}}_k, \hat{\mathbf{C}}_k$, and $\hat{\mathbf{B}}_k$ are the square matrices of size $(N + 1) \times (N + 1)$ and \mathbf{F}_k stands for column vectors with dimensions N + 1. The formulas by which they are calculated are given in [21].

For the numerical solution of system (4), the authors developed a special version of the Jordan–Gauss method with a two-run choice of the main element. Initially, the first run is performed, during which the matrix elements lying below diagonal \hat{C}_0 , \hat{C}_1 , ..., \hat{C}_M and all the elements of the matrixes \hat{A}_1 , ..., \hat{A}_M are reset to zero. After these calculations, the second run is performed, at the beginning of which the column vector I_M is calculated, and then the column vectors I_{M-1} , I_{M-2} , ..., I_0 are computed sequentially. This method requires fewer arithmetic operations than the matrix sweep method described in [25] and also allows the use of parallel computations.

The parallel calculations on graphic accelerators in the block calculating the Earth's atmospheric radiation in our model use the CUDA technology and are organized as follows. The run is performed over all angles of the spatial grid on the Earth's surface. For each such node, a CUDA function is invoked, which calculates the radiation field in the vertical column above this node in all the model channels. These calculations are divided into blocks. Each block is executed on one GPU multiprocessor and performs calculations for one model channel. The number of blocks is equal to the number of model channels.

Inside the block, the computational threads first calculate the arrays of optical parameters at the altitude grid nodes, and then carry out calculations for the first run, in which each row of the matrices $\hat{\mathbf{A}}_k, \hat{\mathbf{C}}_k$, and $\hat{\mathbf{B}}_k$ is processed by its own computational thread. Then, the computational threads carry out the calculations of the second run, in which each row of matrices $\hat{\mathbf{C}}_k$ and $\hat{\mathbf{B}}_k$ obtained after the first run is processed by its own computational thread. This method of organizing calculations enables fairly effi-

3. PARAMETERIZATION CONSTRUCTION

cient loading of the graphics accelerator.

In order to construct the parametrization, the entire spectral section in the range of 10 to 3000 cm⁻¹ is divided into intervals with a width of 100 to 500 cm⁻¹, which will be called averaging intervals. In each averaging interval, the narrow spectral channels are combined according to various algorithms into wide model channels, which are also called resonance carriers [19]. The main idea of the new algorithm [20] is to construct the model channels in two stages. At the first stage, the altitude of the first sorting is selected in the range of 5 to 17 km in order to take into account the absorption lines of the water vapor. All the narrow channels from the averaging interval are divided into groups so that the molecular absorption coefficients of the narrow channels within each group would be sufficiently close to each other at this altitude and at altitudes of 0 to 20 km. At the second stage, the second sorting altitude is selected in the range of 40 to 55 km in order to take into account the ozone absorption lines. Each group of narrow channels obtained after the first sorting is divided into N_2 subgroups so that the molecular absorption coefficients of the narrow channels within each subgroup are sufficiently close to each other at this altitude and at altitudes of 0 to 20 km. The narrow channels included into N_2 subgroups so that the molecular absorption coefficients of the narrow channels within each subgroup are sufficiently close to each other at this altitude and at altitudes of 0 to 76 km. The narrow channels included in one subgroup are combined into one model channel. This yields N_1N_2 model channels per averaging interval.

Let us denote by *T* and *P* the temperature and pressure of atmospheric gas; by v, the frequency; by *z*, the altitude from the surface of the Earth; by $K^{\text{mol}}(T, P, v)$, the volumetric coefficient of molecular absorption of the atmospheric gas, which for the given molecular composition of this gas is a function of temperature, pressure, and frequency; and it is calculated according to the standard theory using the HITRAN 2012 spectroscopic database [22] taking into account the continuous absorption of water vapor and carbon dioxide, which can be specified using the empirical models, for example, MT CKD [23].

In this study, we used the following algorithm for constructing the model channels. We consider the averaging interval $[v_{\min}, v_{\max}]$, from 100 to 500 cm⁻¹ wide, which we divide into narrow channels with the frequency v_i . Inside the channels, the optical parameters can be assumed to be constant. Then we select some average dependences of the temperature T(z), pressure P(z) of the atmospheric gas, and partial pressures of water vapor $P_{vap}(z)$ and ozone $P_{oz}(z)$ on the altitude. Next we construct the grid for altitude z_k in which the numbering begins on the upper boundary of the atmosphere and the grid of pressure $P_k = P(z_k)$, $P_0 < ... < P_k < P_{k+1} < ... < P_{\max}$, and specify the values of the average temperature profile of atmospheric gas at the nodes of this grid: $T_{k,0} = T(z_k) = T(P_k)$. It should be noted that the choice of the steps of the pressure grid should provide acceptable accuracy for the interpolation of the optical parameters. The calculations performed by the authors show that in order to achieve good accuracy, it is sufficient to use the grid steps of 200 m at altitudes less than 10 km and grid steps of 400 m at altitudes higher than 10 km.

For each node of the pressure grid P_k , we construct a uniform grid of temperature values with step ΔT using the formulas

$$T_{k,l} = T_{k,0} + l\Delta T, \quad l = -L, ..., L,$$
 (5)

while step ΔT and number L are selected so that all possible atmospheric gas temperatures at pressure P_k fall inside the interval $[T_{k,0} - L\Delta T, T_{k,0} + L\Delta T]$ and provide the acceptable accuracy of the interpolation of the optical parameters with respect to temperature. The calculations performed by the authors show that to fulfill these conditions in the lower and middle atmosphere, it is sufficient to take $\Delta T = 10$ K and L = 10 if it is assumed that $\Delta T = 5$ K, then the interpolation accuracy remains practically unchanged but if we take $\Delta T = 20$ K, the accuracy markedly deteriorates at altitudes higher than 20km.

First, the altitude of the first sorting is selected in the range from 5 to 15 km where narrow channels are combined into groups such that the same optical parameters of the narrow channels included in the same group are close to each other in the lower atmosphere. Our calculations show that the best accuracy is achieved when z_{C1} is selected in the range from 10 to 15km.

At this altitude, for the fixed values $P(z_{C1})$, $T(z_{C1})$, $P_{vap}(z_{C1})$, and $P_{oz}(z_{C1})$, we calculate the minimum and maximum values of the molecular absorption coefficient for all narrow channels from the averaging interval: $K_{C1,min} = \min_{i} K^{mol}(z_{C1}, v_i)$ and $K_{C1,max} = \max_{i} K^{mol}(z_{C1}, v_i)$. In the interval $[K_{C1,min}, K_{C1,max}]$, we introduce the grid of values of the volumetric molecular absorption coefficient uniform on a logarithmic scale that is given by the following formulas:

$$K_{C1,0} = K_{C1,\min}, \quad K_{C1,N_1} = K_{C1,\max}, \quad K_{C1,j} = (K_{C1,0})^{(1-j/N_1)} (K_{C1,N_1})^{(j/N_1)}.$$
(6)

This grid divides the line into N_1 parts. After constructing this grid, narrow channels are sorted into groups that are combined into wide model channels according to the following rule. All narrow channels for which the condition $K^{\text{mol}}(h_{C1}, v_i) \in (K_{C1,j-1}, K_{C1,j}]$ is satisfied are combined in the group with number *j*. We denote by N_j the number of narrow channels included in this group; and by $\Omega_j = (i_{j,1}, \dots, i_{j,N_j})$, a list of numbers of these narrow channels recorded in ascending order.

Next, we select the altitude of the second sorting z_{C2} ranging from 40 to 55km, in which narrow channels are combined into model channels such that the same optical parameters of the narrow channels included in one model channel are close to each other not only in the lower but also in the middle atmosphere. The performed calculations show that the best accuracy is achieved when the range from 45 to 50 km is selected. At this altitude of sorting, each group of narrow channels obtained at the first sorting is sub-divided into subgroups.

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For the fixed values $P(z_{C2})$, $T(z_{C2})$, $P_{vap}(z_{C2})$, and $P_{oz}(z_{C2})$ we calculate the minimum and maximum values of the molecular absorption coefficients for all narrow channels included in set Ω_j : $K_{C2,\min}(j) = \min_{i \in \Omega_j} K^{mol}(z_{C2}, v_i)$, $K_{C2,\max}(j) = \max_{i \in \Omega_j} K^{mol}(z_{C2}, v_i)$. In the interval $[K_{C2,\min}, K_{C2,\max}]$, we introduce a grid uniform on the logarithmic scale that is given by the following formulas:

$$K_{C2,j,0} = K_{C2,\min}(j), \qquad K_{C2,j,N_2} = K_{C2,\max}(j), \qquad K_{C2,j,m} = (K_{C2,j,0})^{(1-m/N_2)} (K_{C2,j,N_2})^{(m/N_2)}.$$
(7)

This grid divides the line into N_2 parts. After constructing this grid, all the narrow channels from the set Ω_j , for which the condition $K^{\text{mol}}(z_{C2}, v_i) \in (K_{C2, j, m-1}, K_{C2, j, m}]$ is fulfilled, are combined into the model channel with indices *j* and *m*.

We denote by $N_{j,m}$ the number of narrow channels included in this model channel; and by $\Omega_{j,m} = (i_{j,1}, \dots, i_{j,N_{j,m}})$, a list of numbers of these narrow channels recorded in ascending order. The total width of the narrow channels included in the considered model channel is $N_{j,m} \Delta v$, where $\Delta v = 0.001 \text{ cm}^{-1}$ is the width of the narrow channels. For each node of the pressure and temperature grid, the Lebesgue measure of narrow channels is set through the values of the Planck function B(T, v) in these channels equal to $B(T_{k,l}, v_i) \Delta v$, and the Lebesgue measure of each model channel with indices *j* and *m* is set by the formula

$$\mu(j,m,T_{k,l}) = \Delta \nu \sum_{i \in \Omega_{j,m}} B(T_{k,l},\nu_i),$$

in which the summation is carried out over all the narrow channels included in the considered model channel. Next, the ratio of the Lebesgue measure to the width of the narrow channels is determined, i.e.

$$M(j,m,T_{k,l}) = \frac{1}{\Delta v} \mu(j,m,T_{k,l}), \qquad (8)$$

and the Lebesgue-averaged value of the Planck function is calculated by the formula

$$B(j, m, T_{k,l}) = \frac{1}{N_{j,m}} M(j, m, T_{k,l}).$$

Then, for the considered model channel and the pressure and temperature grid nodes, we calculate the Lebesgue-averaged absorption and scattering cross sections and scattering indicatrices for the water vapor molecules, ozone, and air molecules without water vapor and ozone, as well as for the medium-sized background and cloud aerosol particles.

The Lebesgue-averaged absorption cross sections for air molecules without water vapor and ozone for the model channel with indices *j* and *m* are calculated by the formula

$$\sigma_{\mathrm{air,ab}}(j,m,T_{k,l},P_k) = \frac{1}{M(j,m,T_{k,l})} \sum_{i \in \Omega_{j,m}} \sum_{\alpha} q_{\alpha} \sigma_{\mathrm{mol,ab},\alpha}(T_{k,l},P_k,\nu_i) B(T_{k,l},\nu_i),$$
(9)

where index α denotes one of the five sorts of molecules N₂, N₂O, O₂, CO₂, and CH₄, which are taken into account in the calculations, q_{α} is the volumetric share of molecules of the sort α , $\sigma_{\text{mol},ab,\alpha}$ is the absorption cross section of a molecule of this sort. At the same time, the absorption cross section of the CO₂ molecule is calculated taking into account the continuum absorption. The volumetric fractions of the molecules of these sorts are considered constant.

The Lebesgue-averaged value of the absorption cross section of the water vapor molecules for the model channel with indices j and m is calculated by the formula

$$\sigma_{\text{vap,ab}}(j,m,T_{k,l},P_k,P_{\text{vap}}) = \frac{1}{M(j,m,T_{k,l})} \sum_{i \in \Omega_{j,m}} \sigma_{\text{mol,ab,vap}}(T_{k,l},P_k,P_{\text{vap}},\nu_i) B(T_{k,l},\nu_i),$$
(10)

where P_{vap} is the partial pressure of water vapor and $\sigma_{mol,ab,vap}$ stands for the absorption cross section of a water vapor molecule, which is calculated taking into account the continuum absorption.

The Lebesgue-averaged value of the ozone molecule's absorption cross section for the model channel with indices *j* and *m* is calculated by the formula

$$\sigma_{\text{oz,ab}}(j,m,T_{k,l},P_k,P_{\text{oz}}) = \frac{1}{M(j,m,T_{k,l})} \sum_{i \in \Omega_{j,m}} \sigma_{\text{mol,ab,oz}}(T_{k,l},P_k,P_{\text{oz}},\nu_i) B(T_{k,l},\nu_i),$$
(11)

where P_{oz} is the ozone partial pressure and $\sigma_{mol,ab,oz}$ is the ozone absorption's cross section.

It should be noted that the dependence of the absorption cross section of the water vapor molecule on the partial pressure of this vapor and the dependence of the absorption cross section of the ozone molecule on the partial pressure of ozone can be neglected for the following reason. These sections depend on partial pressures only in terms of the half-width of the Lorentz contour line. Since the relative contribution of the partial pressure of water vapor to the total air pressure does not exceed 0.01 and the same contribution for ozone does not exceed 0.0000001, an increase in the half-width of the line due to the collisions of water vapor molecules with air molecules. Similarly, since the relative contribution of the partial pressure of ozone to the total air pressure does not exceed 0.0000001, an increase in the half-width of the line due to the collisions of the total air pressure does not exceed 0.0000001, an increase in the half-width of the line due to the collisions of the partial pressure of ozone to the total air pressure does not exceed 0.0000001, an increase in the half-width of the line due to the partial pressure of ozone to the total air pressure does not exceed 0.0000001, an increase in the half-width of the line due to the collisions of the partial pressure of ozone to the total air pressure does not exceed 0.0000001, an increase in the half-width of the line due to the collisions of ozone molecules with each other can also be neglected compared to the increase in the half-width of the line due to the collisions of ozone molecules with each other can also be neglected compared to the increase in the half-width of the line due to the collisions of ozone molecules with each other can also be neglected compared to the increase in the half-width of the line due to the collisions of ozone molecules with air molecules.

The Lebesgue-averaged value of the absorption cross section for one background aerosol particle for the model channel with indices *j* and *m* is calculated by the formula

$$\sigma_{\mathrm{as,ab}}(j,m,T_{k,l}) = \frac{1}{M(j,m,T_{k,l})} \sum_{i \in \Omega_{j,m}} \sigma_{\mathrm{p,ab,as}}(\mathsf{v}_i) B(T_{k,l},\mathsf{v}_i), \tag{12}$$

where $\sigma_{p,ab,as}$ are the size-averaged absorption cross sections of one particle of the background aerosols.

The Lebesgue-averaged value of the absorption cross section of cloud aerosol particles for the model channel with indices j and m is calculated by the formula

$$\sigma_{\mathrm{cl,ab}}(j,m,T_{k,l}) = \frac{1}{M(j,m,T_{k,l})} \sum_{i \in \Omega_{j,m}} \sigma_{\mathrm{p,ab,cl}}(\mathbf{v}_i) B(T_{k,l},\mathbf{v}_i), \tag{13}$$

where $\sigma_{p,ab,cl}$ is the size-averaged absorption cross section of a single particle of cloud aerosols.

The Lebesgue-averaged value of the scattering cross section for all types of air molecules for the model channel with indices j and m is calculated by the formulas

$$\sigma_{\text{air,sc}}(j, m, T_{k,l}, P_k) = \frac{1}{M(j, m, T_{k,l})} \sum_{i \in \Omega_{j,m}} \sigma_{\text{mol,sc}}(T_{k,l}, P_k, \nu_i) B(T_{k,l}, \nu_i),$$
(14)

where $\sigma_{mol,sc}$ is the absorption cross section of a single molecule, which is calculated according to the formulas of the theory of molecular scattering [1–3].

The Lebesgue-averaged value of the scattering cross section of a single particle of background aerosols for the model channel with indices *j* and *m* is calculated by the formula

$$\sigma_{\mathrm{as,sc}}(j,m,T_{k,l}) = \frac{1}{M(j,m,T_{k,l})} \sum_{i \in \Omega_{j,m}} \sigma_{\mathrm{p,sc,as}}(\mathbf{v}_i) B(T_{k,l},\mathbf{v}_i), \tag{15}$$

where $\sigma_{p,sc,as}$ is the absorption cross section of a single particle of background aerosols averaged over the particles' size.

The Lebesgue-averaged value of the scattering cross section of a single particle of cloud aerosols for the model channel with indices *j* and *m* is calculated by the formula

$$\sigma_{\text{cl,sc}}(j,m,T_{k,l}) = \frac{1}{M(j,m,T_{k,l})} \sum_{i \in \Omega_{j,m}} \sigma_{\text{p,sc,cl}}(v_i) B(T_{k,l},v_i),$$
(16)

where $\sigma_{p,sc,cl}$ is averaged over the size of the particles' absorption cross section of a single particle of cloud aerosols.

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The Lebesgue-averaged value of the volumetric absorption coefficient for the model channel with indices j and m is calculated by the formula

$$K_{ab}(j,m,T_{k,l},P_{k},P_{vap},P_{oz}) = \frac{(P_{k} - P_{vap} - P_{oz})}{k_{B}T_{k,l}} \sigma_{air,ab}(j,m,T_{k,l},P_{k}) + \frac{P_{vap}}{k_{B}T_{k,l}} \sigma_{vap,ab}(j,m,T_{k,l},P_{k}) + \frac{P_{oz}}{k_{B}T_{k,l}} \sigma_{oz,ab}(j,m,T_{k,l},P_{k}) + n_{as}\sigma_{as,ab}(j,m,T_{k,l}) + n_{cl}\sigma_{cl,ab}(j,m,T_{k,l}),$$
(17)

where $k_{\rm B}$ is the Boltzmann constant, $n_{\rm as}$ is the concentration of the particles of the background aerosols calculated by the average size of these particles, and $n_{\rm cl}$ denotes the concentration of particles of cloud aerosols calculated from the water and iceiness of the clouds and the average size of the particles in the clouds.

The Lebesgue-averaged value of the volumetric scattering coefficient (the sum of the molecular and aerosol scattering coefficient) for the model channel with indices *j* and *m* is calculated by the formula

$$K_{\rm sc}(j,m,T_{k,l},P_k) = \frac{P_k}{k_{\rm B}T_{k,l}} \sigma_{\rm air,sc}(j,m,T_{k,l},P_k) + n_{\rm as}\sigma_{\rm as,sc}(j,m,T_{k,l}) + n_{\rm cl}\sigma_{\rm cl,sc}(j,m,T_{k,l}).$$
(18)

The Lebesgue-averaged value of the volumetric attenuation coefficient for the model channel with indices j and m is calculated by the formula

$$K_{\text{ext}}(j, m, T_{k,l}, P_k, P_{\text{vap}}, P_{\text{oz}}) = K_{\text{ab}}(j, m, T_{k,l}, P_k, P_{\text{vap}}, P_{\text{oz}}) + K_{\text{sc}}(j, m, T_{k,l}, P_k);$$

and the Lebesgue-averaged single-scattering albedo, by

$$\omega(j, m, T_{k,l}, P_k, P_{\text{var}}, P_{\text{oz}}) = \frac{K_{\text{ext}}(j, m, T_{k,l}, P_k)}{K_{\text{sc}}(j, m, T_{k,l}, P_k, P_{\text{var}}, P_{\text{oz}})}.$$
(19)

The Lebesgue-averaged values of the scattering index of a single particle of background aerosols and the scattering indicatrix of a single particle of cloud aerosols for the model channel with indices *j* and *m* are calculated by the formulas

$$\chi_{\rm as}(u, j, m, T_{k,l}) = \frac{\sum_{i \in \Omega_{j,m}} \chi_{\rm p,as}(v_i, u) \ \sigma_{\rm p,sc,as}(v_i) \ B(T_{k,l}, v_i)}{M(j, m, T_{k,l}) \ \sigma_{\rm as,sc}(j, m, T_{k,l})},$$
(20)

$$\chi_{cl}(u, j, m, T_{k,l}) = \frac{\sum_{i \in \Omega_{j,m}} \chi_{p,cl}(v_i, u) \ \sigma_{p,sc,cl}(v_i) \ B(T_{k,l}, v_i)}{M(j, m, T_{k,l}) \ \sigma_{cl,sc}(j, m, T_{k,l})} ,$$
(21)

where $\chi_{p,as}(v_i, u)$ is the scattering indicatrix of a single particle of background aerosols averaged over the particle size, $\chi_{p,cl}(v_i, u)$ is the scattering indicatrix of a single particle of cloud aerosols averaged over the particle size, and u is the cosine of the scattering angle.

The Lebesgue-averaged value of the indicatrix of air scattering together with the aerosols for the model channel with indices *j* and *m* is calculated by the formula

$$\chi(u, j, m, T_{k,l}, P_k) = \frac{1}{K_{\rm sc}(j, m, T_{k,l}, P_k)} \times \left(\frac{\chi_{\rm mol}(u)\sigma_{\rm air,sc}(j, m, T_{k,l}, P_k)P_k}{k_{\rm B}T_{k,l}} + \chi_{\rm as}(u, j, m, T_{k,l})\sigma_{\rm as,sc}(j, m, T_{k,l})n_{\rm as} + \chi_{\rm cl}(u, j, m, T_{k,l})\sigma_{\rm cl,sc}(j, m, T_{k,l})n_{cl}\right).$$
(22)

In practical calculations, the expansion of the scattering indicatrix into Legendre polynomials is often used. In order to obtain the averaged expansion coefficient of the scattering indicatrix, it is necessary in (22) to replace all the scattering indicatrices by their expansion coefficients with the same number.

This completes the process of calculating the average values of the optical characteristics at the pressure and temperature grid nodes for wide model channels. Thus, hundreds of thousands of narrow spectral channels from the averaging interval are replaced by tens or hundreds (depending on the required accuracy and calculation speed) of the wide model channels.

When modeling the general atmospheric circulation, it is necessary to calculate the radiation field in the model channels for the vertical distributions of the concentrations and temperatures of the absorbing

gases and the distributions of aerosol particles over each node of the spatial grid on the Earth's surface. Since each of these nodes at the given time instant has its own vertical distribution of concentrations and temperatures of absorbing gases and aerosol particle distributions, for each of these distributions, the vertical profiles of the optical parameters for each model channel should be promptly computed. Optimization of the calculation procedure for these profiles plays an important role. Since the averaged volumetric absorption and attenuation coefficients, as well as the single-scattering albedo, are expressed in terms of the product of the concentrations of molecules and aerosol particles by their averaged absorption and scattering cross sections, the calculation of these cross sections must be optimized

According to formulas (10) and (11), the averaged absorption cross sections of water vapor and ozone molecules formally depend on their partial pressures. For this reason, under the formal approach, it is necessary for each pressure grid node to introduce additional grids of the partial pressures of water vapor and ozone, and at the nodes of the partial pressure grid of ozone, the averaged absorption cross sections of the ozone molecules must be calculated and stored in the computer memory, and at the nodes of the partial pressure grid of ozone, the averaged absorption cross sections of ozone molecules should be calculated and stored in the computer memory. In this case, the grid steps for partial pressures should be selected so as to ensure the desired interpolation accuracy with the minimum number of grid nodes. To calculate these cross sections between grid nodes, interpolation in three variables must be used.

However, if we use the fact substantiated in the comment to formula (11) stating that the dependence of the absorption cross section of the water vapor molecule on the partial pressure of this vapor and the dependence of the absorption cross section of the ozone molecule on the partial pressure of ozone can be neglected, then it is possible to calculate and store these sections in the computer memory only for the the pressure and temperature grids, and to calculate these cross sections between the grid nodes interpolation in two variables can be used.

The described technique makes it possible to quickly calculate the optical parameters in each model channel for the arbitrary vertical distributions of the concentrations and temperatures of absorbing gases and distributions of aerosol particles. In this case, it is necessary to store in the RAM the arrays of the values of all the averaged absorption and scattering cross sections given by formulas (9)-(16) and the averaged expansion coefficients of the scattering indicatrix of cloud particles and background aerosols at the temperature and pressure grid nodes for each model channel.

The accuracy of the presented parameterization algorithm can theoretically be estimated using the following considerations. For line-by-line calculations, the grid of the altitude (optical thickness) and of the zenith angle is introduced. The intensity of the atmospheric radiation in each narrow spectral channel with frequency v_i at the nodes of this grid is recorded as a one-dimensional column vector $\mathbf{I}(v_i)$. After discretization of the radiation transport equation with respect to the altitude and zenith angle, a system of linear algebraic equations is obtained (4), which, using the vector $\mathbf{I}(v_i)$ can be written as

$$\mathbf{A}(\mathbf{v}_i)\,\mathbf{I}(\mathbf{v}_i) = \mathbf{b}(\mathbf{v}_i),\tag{23}$$

where $\mathbf{A}(\mathbf{v}_i)$ is the coefficient matrix, the elements of which are expressed in terms of the values at the nodes of the grid of the extinction coefficient's altitude, the single-scattering albedo, and the scattering indicatrix, and $\mathbf{b}(\mathbf{v}_i)$ is the vector of the right-hand sides. On solving system (23), vector $\mathbf{I}(\mathbf{v}_i)$ can be represented as $\mathbf{I}(\mathbf{v}_i) = \mathbf{A}^{-1}(\mathbf{v}_i) \mathbf{b}(\mathbf{v}_i)$, where $\mathbf{A}^{-1}(\mathbf{v}_i)$ is the matrix inverse to matrix $\mathbf{A}(\mathbf{v}_i)$. Let *N* be the number of narrow channels in the averaging interval and $\Delta \mathbf{v}$ be the width of narrow spectral channels. Then the vector of radiation fluxes at the altitude and zenith angle's grid nodes in this averaging interval obtained using the line-by-line calculations can be represented as

$$\mathbf{I}_{\text{lbl}} = \Delta \mathbf{v} \sum_{i=1}^{N} \mathbf{A}^{-1}(\mathbf{v}_{i}) \mathbf{b}(\mathbf{v}_{i}) = \Delta \mathbf{v} \sum_{j=1}^{N_{1}} \sum_{m=1}^{N_{2}} \sum_{i \in \Omega_{j,m}} \mathbf{A}^{-1}(\mathbf{v}_{i}) \mathbf{b}(\mathbf{v}_{i}).$$
(24)

For the model channel with indices *j* and *m*, the averaged optical parameters are calculated by formulas (8)–(22). These parameters define the matrix of averaged coefficients $A_{av}(j,m)$ and its inverse matrix $A_{av}^{-1}(j,m)$. The vector of radiation fluxes at the altitude and zenith angle grid nodes in the averaging interval obtained using parameterization can be represented as

$$\mathbf{I}_{nap} = \Delta \mathbf{v} \sum_{j=1}^{N_1} \sum_{m=1}^{N_2} \mathbf{A}_{av}^{-1}(j,m) \sum_{i \in \Omega_{j,m}} \mathbf{b}(\mathbf{v}_i).$$
(25)

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By subtracting (25) from (24), we obtain the formula for the difference between the flux vector calculated using the line-by-line calculations and the flux vector obtained using parameterization,

$$\mathbf{I}_{\rm lbl} - \mathbf{I}_{\rm par} = \Delta \mathbf{v} \sum_{j=1}^{N_1} \sum_{m=1}^{N_2} \sum_{i \in \Omega_{j,m}} \left(\mathbf{A}^{-1}(\mathbf{v}_i) - \mathbf{A}_{cp}^{-1}(j,m) \right) \mathbf{b}(\mathbf{v}_i).$$
(26)

It can be seen from (26) that the accuracy of the parameterization is determined by the norm of the dif-

ference of matrices $\mathbf{A}^{-1}(\mathbf{v}_i) - \mathbf{A}_{av}^{-1}(j,m)$ for the narrow channels included in the model channel with indices *j* and *m*. This norm is smaller the closer the optical parameters of the narrow channels included in one model channel are to each other over the entire range of altitudes. The presented algorithm for constructing parametrization provides the necessary proximity of these parameters over the entire range of altitudes.

4. RESULTS OF THE TEST CALCULATIONS

The authors of this work carried out the line-by-line calculations of the Earth's atmospheric radiation field in the approximation of a horizontal homogeneous atmosphere with the frequency resolution of 0.001 cm^{-1} and calculations of this field performed using parametrizations of the optical characteristics of the Earth's atmosphere in the altitude range from the Earth's surface up to 76 km. For the numerical solution of the radiation transfer equation, a variant of the discrete ordinate method was used, which was described in detail in [24]. In the calculations, the uniform altitude grid with the step of 200 m and the uniform zenith angle grid with the step of nine degrees was used, with allowance for the molecular and aerosol scattering.

The calculations used the vertical profiles of the temperature and concentrations of the main atmospheric gases calculated according to the NRLMSISE-00 empirical model for the conditions in July over the North Atlantic at a latitude of 55° and the vertical profiles of the volumetric fractions of the small gas components, normalized extinction coefficient, single-scattering albedo, and the asymmetry parameter for aerosol particles in clouds constructed from the experimental data given in the monograph [1], as well as the dependence of the extinction coefficient on the altitude of the upper, middle, and lower cloud layers at the wavelength of 0.5 μ m presented in [26]. The optical thickness of the cloud layers was taken to be large and close to the maximum observed to verify the accuracy of the parameterization. In the atmosphere, three types of background aerosols are considered: continental, marine, and stratospheric aerosols. The optical parameters of these aerosols are taken from [27].

The results of the line-by-line calculations were compared with the results of the calculations in which the following parameterization was used. The entire range of 10 to 2000 cm⁻¹ was divided into four parts: $10-500 \text{ cm}^{-1}$, $500-1000 \text{ cm}^{-1}$, $1000-1500 \text{ cm}^{-1}$, and $1500-2000 \text{ cm}^{-1}$. In the range $10-500 \text{ cm}^{-1}$, one averaging interval of 10 to 500 cm^{-1} was used, in which at first, four channels were singled out using the first sorting, which was carried out at the altitude of 15 km and then in each of these four channels six sub-channels were singled out using the second sorting, which was carried out at the altitude of 24 model channels were used in this range.

In the range $500-1000 \text{ cm}^{-1}$, two averaging intervals were used, $500-750 \text{ cm}^{-1}$ and $750-1000 \text{ cm}^{-1}$, in each of which four channels were first singled out using the first sorting, which was carried out at the altitude of 15 km, and then in each of these four channels ten subchannels were singled out using the second sorting, which was carried out at the altitude of 47 km. In total, 80 model channels were used in this range.

In the range 1000–1500 cm⁻¹, four averaging intervals were used: 1000–1125 cm⁻¹, 1125–1250 cm⁻¹, 1250–1375 cm⁻¹, and 1375–1500 cm⁻¹, in each of which four channels were first singled out using the first sorting, which was carried out at the altitude of 15 km, and then in each of these four channels, eight sub-channels were singled out using the second sorting, which was carried out at the altitude of 12 km. A total of 128 model channels were used in this range.

In the range $1500-2000 \text{ cm}^{-1}$, two averaging intervals were used, $1500-1750 \text{ cm}^{-1}$ and $1750-2000 \text{ cm}^{-1}$, in each of which four channels were first singled out using the first sorting, which was carried out at the altitude of 15 km, and then in each of these four channels, six subchannels were singled out using the second sorting, which was carried out at the altitude of 47 km. A total of 48 model channels were used in this range. Thus, 1 990 000 narrow spectral channels used in the line-by-line calculations are replaced by 280 model channels.

Figure 1 presents the upward and downward radiation fluxes in the frequency range of 10 to 2000 cm⁻¹ in a cloudless atmosphere and the heating–cooling rate of atmospheric gas due to these fluxes obtained



Fig. 1. The fluxes of upward and downward atmospheric radiation in the frequency range $10-2000 \text{ cm}^{-1}$ and atmospheric gas heating—cooling rates due to these fluxes in a cloudless atmosphere. Curve *I*, heating—cooling rate, calculated using parameterization; curve *2* obtained using line-by-line calculations. Curves *3* and *4*, fluxes of upward and downward atmospheric radiation calculated using parameterization; curves *5* and *6*, the same fluxes obtained using line-by-line calculations.

using the line-by-line calculations, as well as the calculations using parameterization. From Fig. 1 it is seen that the heating—cooling rate of atmospheric gas calculated using parameterization is very close to the same rate obtained using the line-by-line calculations. The largest deviation of about 0.2 K/day between these speeds is reached at the altitude of 48 km. The upward and downward radiation fluxes calculated using parameterization coincide with the same fluxes obtained using the line-by-line calculations with the relative error of less than 1%.

Figure 2 shows the same profiles as Fig. 1; however, they are calculated taking into account the presence of the average cloud layer with a significant optical thickness in the altitude range from 3 to 6 km, the parameters of which are given in [26]. This thickness is responsible for the significant values of the heating—cooling rate of the air inside the cloud layer. It is clear from Fig. 2 that the heating—cooling rate of atmospheric gas and the upward and downward fluxes calculated using parameterization and using the line-by-line calculations coincide accurately. The deviation between the fluxes obtained by the line-byline calculations and in the calculations using parameterization, both outside and inside the cloud layer,



Fig. 2. The fluxes of upward and downward atmospheric radiation in the frequency range $10-2000 \text{ cm}^{-1}$ and atmospheric gas heating—cooling rates due to these fluxes in the presence of the average cloud layer with significant optical thickness. Curve *1*, heating—cooling rate calculated using parameterization; curve *2*, the same rate obtained using line-by-line calculations. Curves *3* and *4*, fluxes of upward and downward atmospheric radiation calculated using parameterization; curves 5 and 6, the same fluxes obtained using line-by-line calculations.

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is less than 1%, and the deviation between the heating rates does not exceed 0.2 K/day outside the cloud layer and 0.5 K/day inside this layer. In the case of the presence of the lower or upper cloud layers with a significant optical thickness, the parameterization accuracy turned out to be the same.

The authors investigated the influence of the altitudes of the first and second sorting on the parameterization accuracy. The altitude of the first sorting was varied in the range from 5 to 20 km. It turned out that the altitude of 15 km is close to optimal. When a different altitude of the first sorting is selected, the accuracy of parameterization with the same number of model channels does not improve. The altitude of the second sort was also varied over a wide range from 35 to 60 km. It turned out that the altitudes selected in the presented altitude parametrization of the second sorting are close to optimal. Changing them did not improve the accuracy of the parameters. Also, the calculation results show that with an increase in the number of model channels compared to their number in the presented parameterization, the parameterization accuracy improves slightly, and with a decrease in this number, this accuracy deteriorates more significantly. The width of the averaging intervals in the range 100-125cm⁻¹ is optimal.

5. CONCLUSIONS

The paper describes the method for calculating the Earth's atmospheric radiation in the IR range, which is used in the radiation block of the general circulation model of the lower and middle atmosphere developed by the authors. This method employs a novel parameterization of molecular absorption in the frequency range from 10 to 2000 cm^{-1} in the altitude range from the Earth's surface up to 76 km, the construction of which takes into account changes in the atmospheric gas composition with altitude, and for the numerical solution of the radiation transfer equation, the discrete ordinate method and a computational zenith angle grid with the step of nine degrees are used.

A comparison of the results obtained by calculating the Earth's atmospheric radiation field using the radiation block of our model with the results of the line-by-line calculations show that the radiation block of our model accurately calculates the Earth's lower and middle atmosphere both in the absence of clouds and in the presence of cloud layers with a significant optical thickness.

It should be noted that the high-performance computing systems of the near future, which allow efficient adaptation of the computational algorithms in their architecture, will make it possible to model in detail the effect of solar and thermal radiation on processes in the atmosphere [28].

CONFLICT OF INTEREST

The authors declare that they have no conflicts of interest.

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