Modeling diagnostics of trioxide dialuminum content in gas-aerosol medium

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ABSTRACT

The analysis of the calculation results of extinction coefficient, scattering coefficient, and absorption coefficient of aerosol, as well as transmission function under the joint and separate impact of components of mixture containing trioxide dialuminum was carried out. The spectral features of the optical characteristics of the medium at various parameters of particle size distribution function were illustrated.

Aerosol, dialuminum trioxide, water vapor, optical characteristics.

1. INTRODUCTION

An occurrence of aluminum oxide particles in the rocket engine plume is due to as the use of solid fuel with aluminium particles and possible partial micro destruction in the propulsion system. In both cases, it is necessary to carry out the remote monitoring of the amount of the dialuminum trioxide. This requires analysis of the extinction of the sensing laser radiation in the gas-aerosol medium (engine plume) that has previously been considered in our papers [1, 2]. However, these papers do not discuss a role of the size distribution function.

The numerical studies of the optical radiation beam transmitted through a polydisperse medium should take into account both the molecular absorption of and the aerosol extinction. To study the aerosol extinction, it is necessary to consider a model for a single particle. This model should allow us to determine the dependence of the light scattering characteristics on the parameters of incident radiation and parameters of a scatterer. The calculations of the aerosol optical characteristics are based on Mie theory [3]. The problem of scattering of a plane wave on a sphere is a universal, and its solution is used at numerical modeling of the media with large and small particles of various shapes (including non-spherical particles). For calculating the numerical characteristics of the radiation extinction by a system of preferentially oriented crystals, it is necessary to use more complicated techniques (in particular, the discrete dipole approximation, the geometric optics, the physical optics, and combinations thereof) that take into account the anisotropy in the light scattering providing an occurrence of the polarization effect in extinction [4-7].

2. METHOD OF CALCULATION

Let us consider a gas-aerosol medium that contains water vapor and the randomly oriented particles of the dialuminum trioxide Al_2O_3. To calculate the optical characteristics of the polydisperse medium, taking into account the distribution of particle sizes, let us consider the integral expressions determining the coefficients of the radiation extinction (α_{ext}), scattering (α_{sca}), and absorption (α_{abs}) as:

$$\alpha_{ext} = \int_a S_{ext}(a) \cdot N(a)\, da \ , \qquad (1\,a)$$

$$\alpha_{sca} = \int_a S_{sca}(a) \cdot N(a)\, da \ , \qquad (1\,b)$$

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$$\alpha_{\mathrm{abs}} = \int_a S_{\mathrm{abs}}(a) \cdot \mathrm{N}(a)\, da \ , \tag{1 c}$$

where S_{ext}, S_{sca}, and S_{abs} are the extinction, scattering, and absorption cross-sections for an individual particle. In this paper, S_{ext}, S_{sca}, and S_{abs} have been determined using Mie theory. To calculate these characteristics, there are used the following input parameters: the sphere radii a, the complex refractive index $\tilde{n} = n + i \cdot \chi$ (n is the refractive index, χ – the absorption index), and the incident radiation wavelength λ. In Eqs. (1 a) – (1 c), N(a) is distribution function of the particle sizes. A lot of experimental studies of the atmospheric polydisperse media at various temperatures show that the particle size distribution function has a prominent maximum. The modified gamma distribution adequately describes the natural and anthropogenic aerosols [8]:

$$\mathrm{N}(a) = \mathrm{C}\frac{\mu^{\mu+1}}{\mathrm{G}(\mu+1)}\frac{1}{a_m}\left(\frac{a}{a_m}\right)^{\mu}\exp\left(\frac{-\mu\, a}{a_m}\right). \tag{2}$$

Eq. (2) contains the following parameters: C is the concentration of particles in the volume element; a_m is the particle size, corresponding to the maximum of the function N(a); μ is a dimensionless parameter, which characterizes the steepness of slopes at the maximum of N(a); G(μ+1) is the gamma function. As a rule, the average radius of particles ($\overline{a}$) is used to analyze the numerical or experimental data. For the modified gamma distribution (2), the average radius $\overline{a}$ can be expressed in terms of μ and a_m as: $\overline{a} = a_m(1 + 1/\mu)$ (see Ref. 6).

The following expressions are used to calculate the transmission function (hereafter TF):

$$\mathrm{T_a} = \exp(-\alpha_{\mathrm{ext}} \cdot h)\ , \tag{3 a}$$

$$\mathrm{T_g} = \exp(-\mathrm{K_{mol}} \cdot \eta \cdot h)\ , \tag{3 b}$$

$$\mathrm{T_{com}} = \mathrm{T_a} \cdot \mathrm{T_g}\ . \tag{3 c}$$

Here T_a is the aerosol TF, T_g is the gas TF, and T_{com} is TF, accounting the common influence of the gas and aerosol components; K_{mol} is the molecular absorption coefficient; η is the partial pressure of a gas and h is a trace length. The gas absorption coefficient is calculated using the line-by-line technique, which is based on the use of databases on the spectral line parameters (DSLP) for the atmospheric and trace gases. For standard temperatures, the well-known the databases ”HITRAN 2012” [9] is most complete. It was included as an archive in the authors' information-computational system "TRAVA" [10]. We used this software package to calculate the absorption coefficient of the small gases of different nature at standard and high temperatures.

3. RESULTS AND DISCUSSION

Let us consider an influence of the chemical composition of particles on the wavelength dependence of the extinction coefficient in IR range. In Fig. 1a the wavelength dependencies of the extinction coefficient calculated for various refractive indexes are shown. From this figure it is seen that in the case of a greater difference in values of n from the optical properties of soft particles (for soft particles $n \approx 1$), there is a more prominent curve $\alpha_{ext}(\lambda)$ (compare the curves 1 and 3 in Fig. 1a), features which appear brighter in the region of wavelengths commensurate with the average particle size. Obviously, the more is the values of the absorption index (χ), the more smoothed structure $\alpha_{ext}(\lambda)$ is formed (see Fig. 1b).

The calculations of the IR radiation extinction by the aerosol, which contains the dialuminum trioxide, take into account the wavelength dependence of the Al_2O_3 complex refractive index $\tilde{n}(\lambda) = n(\lambda) + i \cdot \chi(\lambda)$, where λ is the incident radiation wavelength. The optical properties of Al_2O_3 were taken from Ref. 11. The results of calculations of the optical characteristics of the engine emissions allow us to estimate a contribution of the Al_2O_3.particles to the radiation extinction.

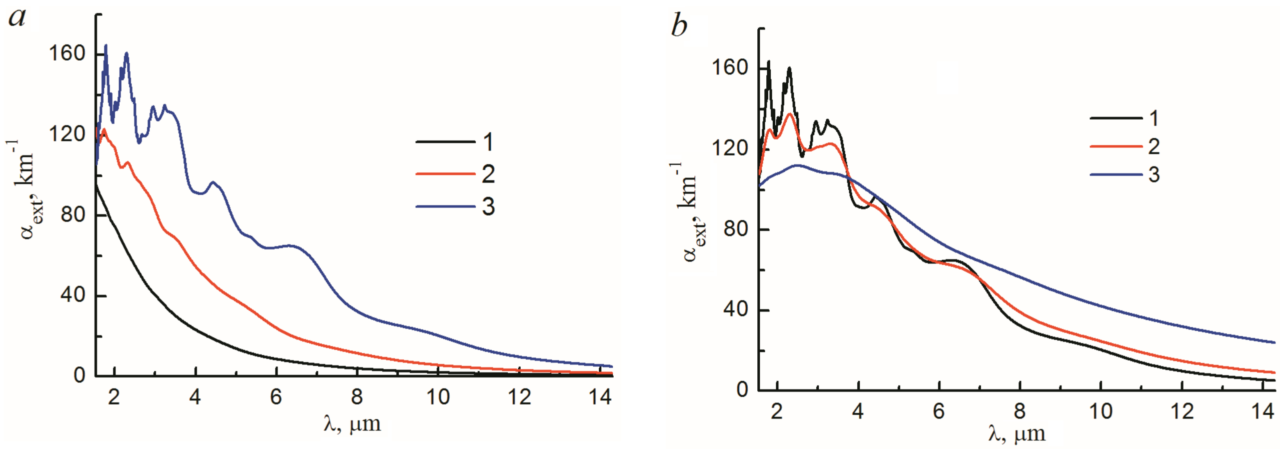

Fig. 1. The extinction coefficient $\alpha_{ext}(\lambda)$ for $\bar{a}$ =1 μm, C =10^7 l^{-1}, μ=5. (*a*): 1 – *n*=1.3, χ=0; 2 – *n*=1.5, χ=0, 3 – *n*=1.9, χ=0. (*b*): 1 – *n*=1.9, χ=10^{-3}; 2 – *n*=1.9, χ=10^{-1}; 3 – *n*=1.9, χ=0.5.

For the IR spectral range, Fig. 2 illustrates the calculated wavelength dependencies of the extinction coefficient, scattering coefficient, and absorption coefficient at μ=1 and μ=30. Fig. 2 shows that the radiation scattering is the dominant contribution to the radiation extinction for λ < 8 μm. According to information from paper [11], the Al_2O_3 absorption index χ takes the values within the [0.1 – 1.44] interval for the wavelengths λ > 9 μm. For this case, the contribution of the radiation absorption to the radiation extinction is increased. However, if a medium contains the dialuminum trioxide particles with a large variation in the sizes (for example, if μ=1), for the particles, which have sizes comparable with the radiation wavelength, the contribution of the light scattering is important even at high values of χ (see Fig. 2*a*).

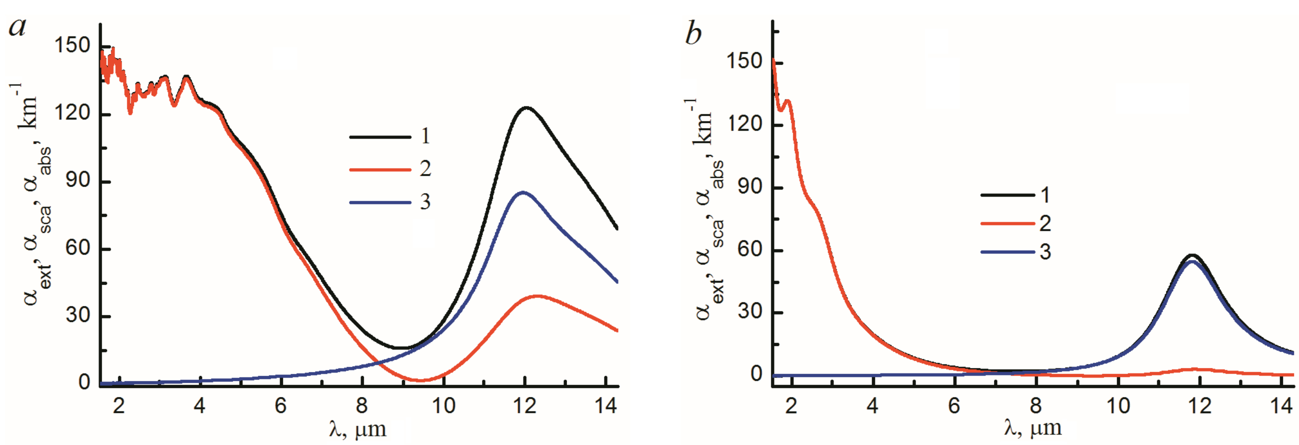

Fig. 2. The extinction coefficient: 1 – $\alpha_{ext}(\lambda)$, the scattering coefficient: 2 – $\alpha_{sca}(\lambda)$, and the absorption coefficient: 3 – $\alpha_{abs}(\lambda)$ at $\bar{a}$ =1 μm, C =10^7 l^{-1}, $\tilde{n} = \tilde{n}(\lambda)$ for Al_2O_3 (see Ref. 11). (*a*) μ=1, (*b*) μ=30.

Fig. 3 illustrates the features of the wavelength dependencies of the optical properties of a medium, which contains an ensemble of particles with various parameters of the particle size distribution function. We considered the trace length *h* =10 *m*. Figs. 3*a*, 3*c*, and 3*e* show the calculated wavelength dependences of the extinction coefficient while Figs. 3*b*, 3*d* and 3*f* show the calculated transmission function at various values of μ, which determines the width of the size distribution function. The less the value of μ, the higher is the particle sizes dispersion. It is clear that the increase of the

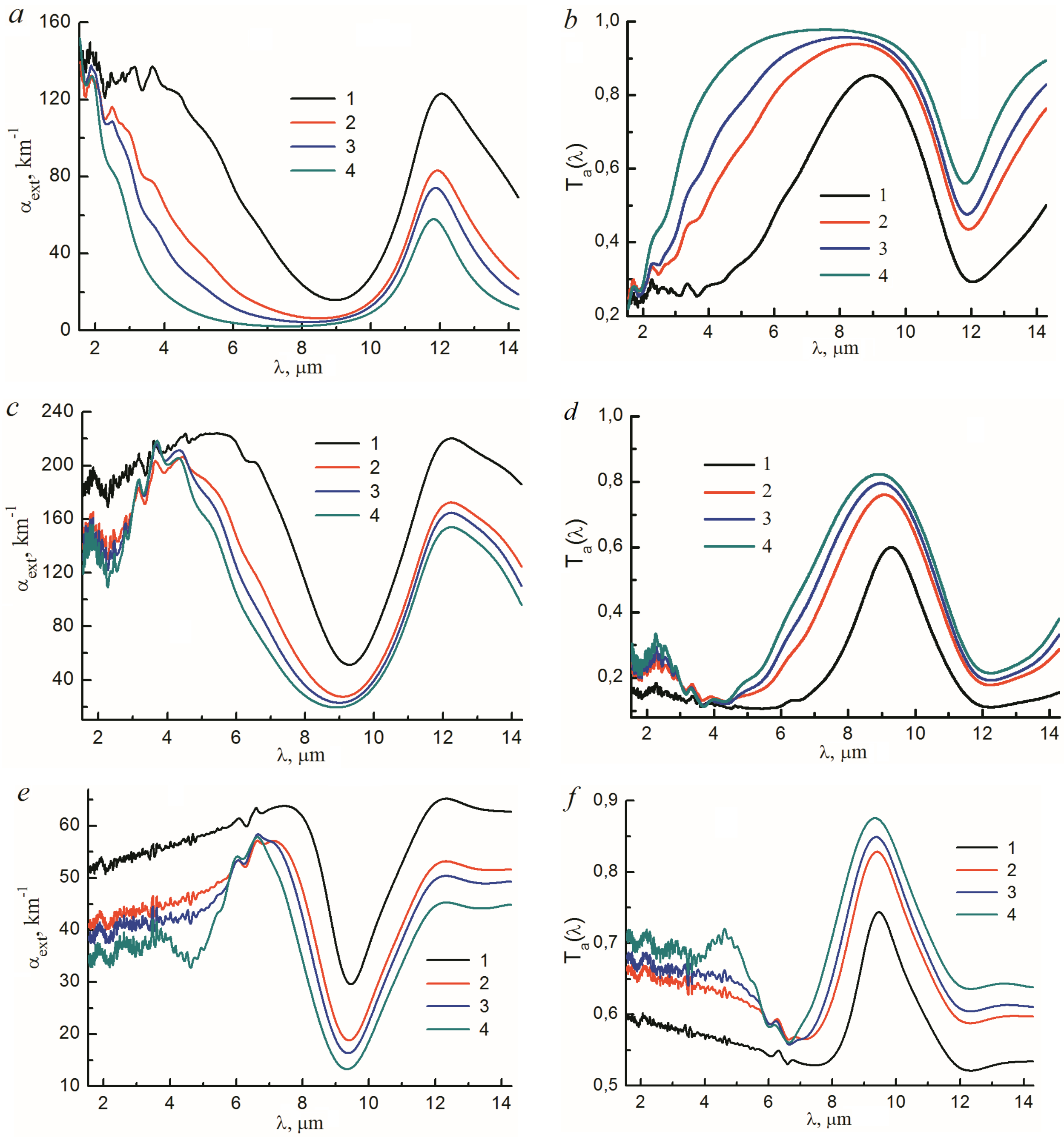

Fig. 3. The wavelength dependences of the extinction coefficient ($\alpha_{ext}(\lambda)$) and the transmission function ($T_a(\lambda)$) at $\tilde{n} = \tilde{n}(\lambda)$ for Al_2O_3 (see Ref. 11). 1 – μ=1, 2 – μ=5, 3 – μ=10, 4 – μ=30. (*a*): $\alpha_{ext}(\lambda)$ and (*b*) $T_a(\lambda)$ for $\overline{a}$ =1 μm, C=10^7 l^{-1}; (*c*): $\alpha_{ext}(\lambda)$ and (*d*) $T_a(\lambda)$ при $\overline{a}$ =2 μm, C=$4\cdot10^6$ l^{-1}. (*e*): $\alpha_{ext}(\lambda)$ and (*f*) $T_a(\lambda)$ при $\overline{a}$ =5 μm, C = $2\cdot10^5$ l^{-1}.

particle sizes results in the increase of the extinction coefficient (or the decrease of the transmission function). The features of the $\alpha_{ext}(\lambda)$ and $T_a(\lambda)$ (such as the locations of the maximum and minimum) are determined by the wavelength dependence of $\tilde{n}(\lambda)$ for Al_2O_3. The higher an average size of particles, the narrower is the wavelength interval for localization of a minimum of $\alpha_{ext}(\lambda)$ and a maximum of $T_a(\lambda)$. The curves in Fig. 3 show that the particle size dispersion can significantly affect the extinction coefficient and the transmission function. A larger spread of particle sizes leads to a decrease in position of the maximum and minimum of the $T_a(\lambda)$ function. The increase of value of the size distribution parameter μ results in an extension of the wavelength range where the minimum of $\alpha_{ext}(\lambda)$ and the maximum of $T_a(\lambda)$ are located. When the incident radiation wavelength is comparable with the average particle size and the μ parameter takes high values, an explicit fine structure of the $\alpha_{ext}(\lambda)$ and $T_a(\lambda)$ functions occurs. However, when the particle size dispersion increases, these functions are smoothed (compare the curves 1 and 4 in Figs. 3*c* – 3*f*).

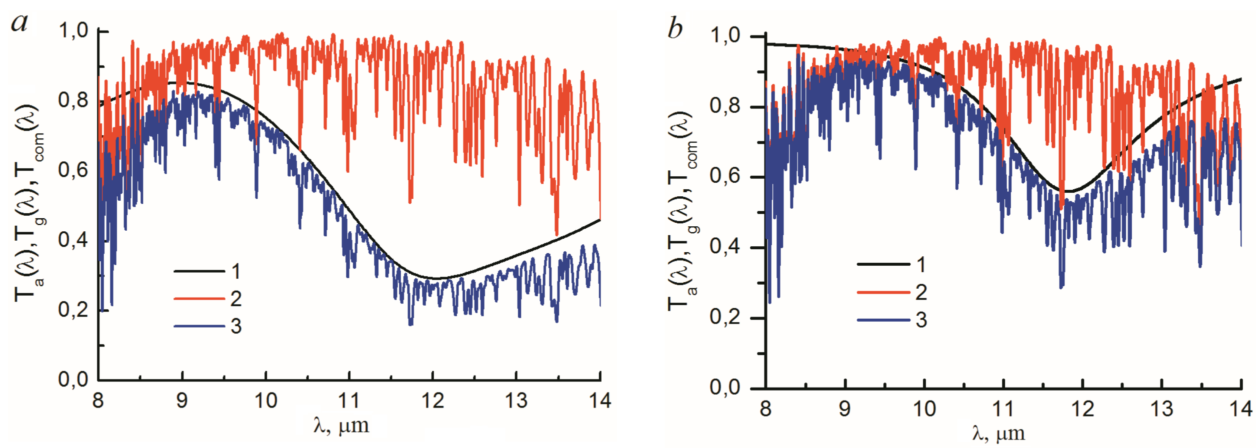

Fig. 4. The transmission function of the gas-aerosol medium at h=10 m, η=0.03 *atm* for water vapor (H_2O), T=1000 K, $\tilde{n} = \tilde{n}(\lambda)$ for Al_2O_3 (see Ref. 11), $\bar{a}$ =1 μm, C=10^7 l^{-1}: 1 – $T_a(\lambda)$, 2– $T_g(\lambda)$, 3 – $T_{com}(\lambda)$. (*a*) μ = 1, (*b*) μ=30.

Let us consider a gas-aerosol medium and study a separate and cooperative effects of the gas absorption and aerosol extinction on the transmission function. We suppose that our medium contains water vapor (gas component) and the spherical particles of the dialuminum trioxide (aerosol component). The curves in Fig. 4 show the wavelength dependencies of the transmission functions $T_{com}(\lambda)$, $T_g(\lambda)$ and $T_a(\lambda)$ (see Eqs. 3*a*, 3*b*, and 3*c*). These curves illustrate a contribution of each component to the common radiation extinction of the gas-aerosol medium. From Fig. 4 it is seen that, for the interval of 10 – 12 μm wavelength, the transmission of the considered gas-aerosol mixture is determined mainly by the dispersed component. In our work [12] it is proposed criterion of the need to consider the cooperative effect of the molecular absorption and aerosol scattering on calculations of IR transmission function. This information can be used to determine the limit values of the trioxide dialuminum particle concentration and effective radius that allow one to estimate a contribution of the gas and aerosol components to the radiation extinction.

4. CONCLUSION

The work demonstrates the effect of microphysical and optical parameters of the particles on the peculiarities of the spectral dependence of the extinction characteristics. These features should be considered when analyzing the data of the transmission of the gas-aerosol medium. In the 10 – 12 μm spectral range, the principal contributor to the molecular absorption is water vapor. Note that in this range, the continuous absorption considerably exceeds the selective absorption of the radiation. Accordingly, the overall spectral pattern in this region of wavelengths is completely determined by the behavior of the dependence of the extinction for aerosol component that allows one to evaluate the magnitude of variation of particle sizes. The measurements of the radiation extinction at a laser wavelength where the water vapor has a maximum absorption will allow one to determine quantitatively a maximum concentration of Al_2O_3.

Acknowledgments

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References

[1] Voitsekhovskaya, O.K., Shefer, O.V., Kashirskii, D.E., "Optical Characteristics of Aerosol Trioxide Dialuminum at the IR Wavelength," Proc. SPIE 9680, 96803A-1–96803A-6 (2015).

[2] Voitsekhovskaya, O.K., Kashirskii, D.E., Egorov, O.V., Shefer, O.V., "Modeling absorption spectra for detection of combustion products of jet engines by laser remote sensing," Appl. Opt. 55(14), 3814–3823 (2016).

[3] Bohren, C.F., Huffman, D.R., [Absorption and scattering of light by small particles], Wiley, New York, 530 p. (1983).

[4] Shefer, O., Popov, A., "Extinction and small angle scattering by thin plate crystals," Appl. Opt. 49(8), 1434–1445 (2010).

[5] Yang P., Wendish M., Bi L., Kattawar G., Mischenko M., Hu Y., "Dependence of extinction cross-section on incident polarization state and particle orientation," J. Quant. Spectr. Rad. Trans. 112, 2035–2039 (2011).

[6] Shefer O., "Numerical study of extinction of visible and infrared radiation transformed by preferentially oriented plate crystals," J. Quant. Spectr. Rad. Trans. 117, 104–113 (2013).

[7] Shefer, O., "Extinction of radiant energy by large atmospheric crystals with different shapes," J. Quant. Spectr. Rad. Trans. 178, 350–360 (2016).

[8] Volkovitskii, O.A., Pavlova, L.N., Petrushin, A.G., [Optical properties of ice clouds], Gidrometeoizdat, Leningrad, 200 p. (1984).

[9] Rothman, L.S., Gordon, I.E., Babikov, Y., and et. al., "The HITRAN–2012 molecular spectroscopic database," J. Quant. Spectr. Rad. Trans. 130, 4–50 (2013).

[10] Voitsekhovskaya, O.K., Voitsekhovskii, A.V., Egorov, O.V., Kashirskii, D.E., "Optical-physical methods of remote diagnostics of high-temperature gas media," Proc. SPIE 9292, 929211 (2014).

[11] Kischkat, J., Peters, S., Gruska, B., and et. al.,"Mid-infrared optical properties of thin films of aluminum oxide, titanium dioxide, silicon dioxide, aluminum nitride, and silicon nitride," Appl. Opt. 51(28), 6789–6798 (2012).

[12] Voitsekhovskaya, O.K., Shefer, O.V., Kashirskii, D.E., "Criterion of the need to consider the cooperative effect of the molecular absorption and aerosol scattering on calculations of IR transmission function," Proc. SPIE 9292, 92923M-1–92923M-8 (2014).