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Visualization of Radiation Scattering Indicatrix on a Polydisperse System of Spherical Particles

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Abstract

The article is devoted to solving the direct problem of light scattering on an ensemble of spherical polydisperse particles. The paper presents an algorithm for computer simulation of the optical radiation scattering indicatrix by a particle system based on the theory of G. Mie. The influence of the relative complex refractive index of scattering centers and their size distribution, wavelength and polarization state of incident light on computer models of scattering indicatrix is investigated. The practical significance of the results obtained lies in the fact that computer models of scattering indicatrix are useful in the experimental study of dispersed systems by static light scattering for the optimal choice of installation parameters and experimental conditions and, more importantly, in solving the inverse problem of the static light scattering method to restore the characteristics of nanoparticles from experimental data.

Keywords: light scattering, scattering indicatrix, computer modeling.

1. Introduction

The problem of dispersed media diagnostics with methods based on elastic light scattering targets determining the field of scattered and not the transmitted radiation by the known parameters of the probing radiation and the scattering object. Potentially, its solution can be obtained with the K. Maxwell's classical electromagnetic theory without loss of rigor, since with the elastic nature of the interaction. There is no exchange of energy between light and particles of matter. In fact, it turned out that in many cases it is extremely laborious or impossible to obtain a solution of Maxwell's equations in relation to the problem of light scattering on a single particle. And the variations in the morphology and optical properties of the particles, for which an analytical solution has been found, are very limited. Therefore, there is currently no complete theory of elastic light scattering on a single particle, and, accordingly, on an ensemble of particles. However, the existing solutions to the scattering problem and the following conclusions from them turned out to be sufficient for the formation of methods for the diagnosis of dispersed media.

G. Mie in 1908 [1] have obtained a complete analytical solution to the problem of scattering of a plane arbitrarily polarized electromagnetic wave on an isotropic and homogeneous dielectric or weakly absorbing spherical particle.

A significant contribution to the solution of the direct problem of radiation elastic scattering was made by K.S. Shifrin. In the works of K.S. Shifrin, not only a detailed study of the mathematical apparatus of the theory of G. Mie was carried out, but also the deep physical aspects of light scattering in turbid media were considered, the formulas of G. Mie were adapted to a form convenient for practical use, the first calculations were carried out and light scattering tables were compiled [2, 3].

A similar work on the systematization of the results of light scattering experimental studies in turbid media and the development of practical approximations of the theory of G. Mie was carried out by H.C. van de Hulst [4].

Analytical calculation of infinite series sum in the formulas of G. Mie for an arbitrary radius of the particle is impossible and in practice it is necessary to use methods of approximate calculation. The advent of computers has opened up fundamentally new technical possibilities for the application of G. Mie formulas in applied research. In 1969, D. Deirmendjian presents in his monograph the algorithms that allow for approximate calculation of the values of complex amplitude scattering functions according to the Mie formulas [5].

The monograph of C.F. Bohren and D.R. Huffman published in 1986 is devoted to a systematic and multifaceted presentation of the issues of scattering and absorption of light by small particles [6].

Modern research related to the direct problem of light scattering considers developing methods and finding solutions for complex shape particles. The paper [7] presents a boundary element method with hermitian interpolation for solving light scattering problems on two-dimensional nanoparticles. It is shown that in the case of a circular cylinder, the results of numerical calculations are in excellent agreement with the classical Mie solution (relative deviation of the order of 10^{-5} – 10^{-6}). With a slight increase in the counting time in comparison with the usual method of boundary elements, the accuracy of the method is increased by 1-2 orders of magnitude. In a series of Shapovalov K.A. articles, formulas were obtained and the scattering indicatrix was modeled in the Rayleigh-Hans-Debye approximation. Thus,his first works [8, 9] present a computational solutions for the amplitude and cross-section of light scattering by optically «soft» hexagonal cylindrical particles of finite length in the Rayleigh-Hans-Debye. The possibility of practical use of Rayleigh scattering for diagnostics is expanded by further published works by Shapovalov K.A. The works present calculations of scattering indicatrix for cylindrical particles with arbitrary ends [10], axisymmetric particles [11], a hexagonal pyramid and a needle-like column [12]. Currently, it is important to refer the research of V.G. Farofanov, that actively develops new mathematical methods for calculating scattering indicatrix, including in the Rayleigh-Hans-Debye approximation. His recent works have presented in particular a new solution to the problem of scattering a plane wave by a multilayer non-focal spheroid [13], the Rayleigh hypothesis and its applicability in electrostatics [14], the electrostatic problem for Chebyshev particles [15], light scattering by small pseudospheroids [16], the properties of the T-matrix in the Rayleigh approximation [17], generalized a method for separating variables in the problem of light scattering by small axisymmetric particles [18].

In this paper, the algorithm and the results of modeling the optical radiation scattering indicatrix on a system of polydisperse spherical particles are presented, the effect of the size distribution function (SDF) on the scattering pattern is shown.

2. Algorithm of optical radiation scattering indicatrix calculating models on polydisperse system of spherical particles

The scheme of the scattering elementary act is shown in Fig.1. A Cartesian three-dimensional system of coordinates (x, y, z) is considered. At the origin of the coordinate system (point 0), both a separate scattering particle and a spherical volume of various scattering particles can be located, which at the same time are in a state of continuous motion. A plane monochromatic arbitrarily polarized wave falls in the direction of the axis $0y$ and undergoes scattering at point 0. The intensity of the scattered radiation is determined in the direction of point M, remote from the center of scattering. The P_{scatt} plane formed by the observation point M and the wave vector $\mathbf{k}$ of the probing radiation is called the scattering plane. The wave vector $\mathbf{ks}$ of the scattered radiation lies in the plane of the P_{scatt}. The vector $\mathbf{ks}$ is directed with respect to the vector of the $\mathbf{k}$ by the angle θ, which is commonly referred as the scattering angle. Two components of the incident wave field strength are also considered, one of which E_{01} (complex amplitude A_{01}) is oriented perpendicular to the scattering plane, and the other E_{02} (complex amplitude A_{02}) is located in this plane. For a scattered wave, similar components of the field strength vector E_1 (complex amplitude A_1) and E_2 (complex amplitude A_2) are considered. The intensities given per unit solid angle corresponding to each of the field components are designated I_{01}, I_{02}, I_1 and I_2 respectively.

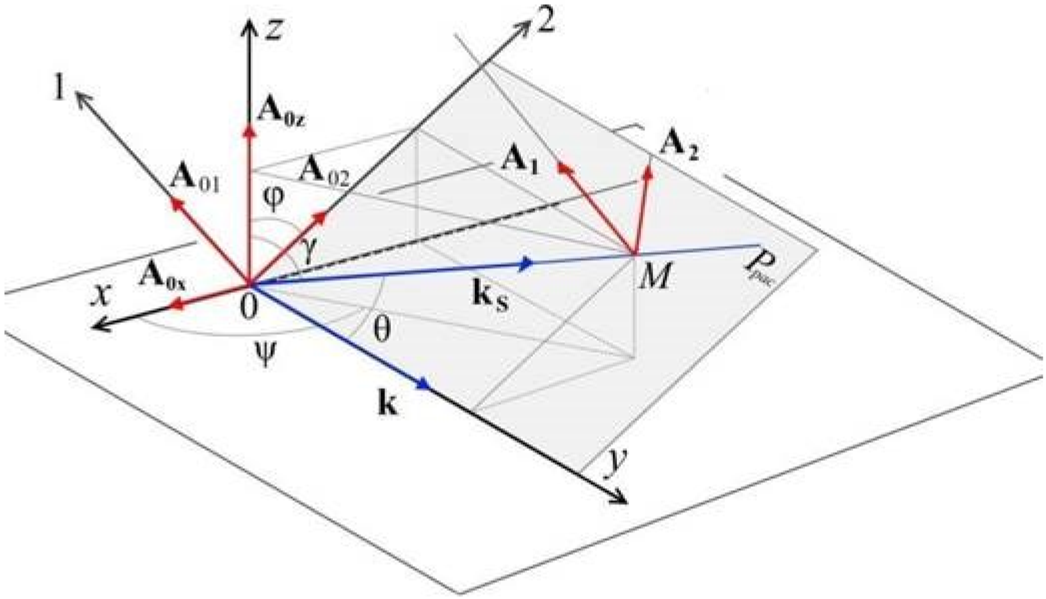

Fig. 1. Scattering scheme of a linearly polarized plane wave

The scattering indicatrix ξ(ψ, γ) is a function of the scattered radiation intensity distribution in all possible directions in space. To determine the intensity of radiation in a unit of solid angle in a given direction, a vector of the Stokes parameters of this radiation is used.

The elementary act of scattering of an arbitrarily polarized monochromatic plane wave can be mathematically described using the Stokes vector and the Muller matrix of the scattering volume (1).

$$\mathbf{I}(\boldsymbol{\theta})\Delta\omega = \boldsymbol{\sigma}(\boldsymbol{\theta})\mathbf{I}_0\Delta\omega_0\Delta\omega, \tag{1}$$

where $\mathbf{I_0}$ and $\mathbf{I}(\boldsymbol{\theta})$ –vector columns of the form $\begin{pmatrix} I_1 \\ I_2 \\ U \\ V \end{pmatrix}$, $\Delta\omega_0$ – the element of a spatial angle in the direction of the source in which the incident radiation propagates, $\Delta\omega$ – the element of a spatial angle in the direction of the source in which the scattered radiation propagates, a $\boldsymbol{\sigma}(\boldsymbol{\theta})$ – the Muller matrix of the scattering volume. The elements $\sigma_i(\theta)$ of the matrix have measurement units of the differential scattering cross section in a single solid angle.

In the case of radiation scattering on a spherical homogeneous isotropic optically inactive particle with a complex refractive index different from the refractive index of the environment, two complex quantities characterizing the amplitudes of the field strength in directions perpendicular and parallel to the scattering plane are sufficient to calculate the elements of the scattering volume matrix of particles and describe the complete transformation of the Stokes parameters. These values are the complex amplitude scattering functions of Mie S_1 and S_2.

To describe the scattering of light on a system of particles, it is convenient to carry out two normalizations, firstly, to normalize the intensity of incident radiation by one, and secondly, the intensity of scattered radiation in a solid angle unit by the intensity of incident radiation in a solid angle unit.

To calculate the Stokes vector of radiation scattered in a certain direction, it is necessary to form the Stokes vector of incident radiation in the coordinate system associated with the scattering plane, the position of which is determined by the selected scattering direction, to form the Muller matrix of the scattering volume of particles, and then use the expression (1).

The initial parameters of the incident radiation when modeling scattering indicators are the wavelength λ, the polarization degree P, the intensity of the incident radiation I_0, the ratio between the real amplitudes a_{0x} and a_{0z} of the component E_{0x} and E_{0z} of the intensity of the incident radiation polarized part, the phase difference between these components $\delta_{xz} = \varphi_{0x} - \varphi_{0z}$, while the initial phase of the component E_z is assumed to be zero $\varphi_{0z} = 0$.

The initial parameters of scattering centers are their complex refractive index m, the minimum and maximum radius of particles r_1 and r_2, the size distribution function of particles of volume $n(r)$.

To calculate the scattering, the polarized and unpolarized parts of the incident radiation are considered separately. For the polarized part of the radiation, the Jones vector is formed in the coordinate system (x, y, z), then the coordinates are rotated by the angle φ, where φ is the angle between the scattering plane and the $0z$ axis, in order to write the Jones vector of the incident radiation in the coordinate system associated with the scattering plane. The angle and position of the scattering plane are determined by the scattering direction under consideration, which is given by the angles ψ and γ (Fig. 1).

Using the values of the complex amplitudes A_{01p} and A_{02p} it is easy to find the amplitudes a_{01p} and a_{02p}, the initial phases φ_{01p} and φ_{02p} of the components E_{01p} and E_{02p} of the intensity vector of the incident radiation field polarized part in the coordinate system associated with the scattering plane, and then calculate the parameters of the basic model for describing polarization: the large and small semi-axes a_e and b_e of the polarizing ellipse, the azimuth angle α_e and the ellipticity angle ε. Using the found parameters of the basic polarization description model, it is possible to write down the Stokes parameters of the polarized part of the incident radiation.

Since the incident radiation unpolarized part can be represented by an incoherent superposition of two orthogonal components of the field strength vector, the type of the Stokes parameter vector for this part of the radiation will not depend on the position of the scattering plane.

The Muller matrix of the scattering volume is derived from the complex amplitude scattering functions of Mie S_1 and S_2, which are calculated within the theory of Mie. At the same time, if the particle system is polydisperse, then the volume scattering coefficient, the particle concentration and the elements of the scattering matrix are calculated by integrating the corresponding values over the range of particle sizes (r_1, r_2), present in the system.

After the vectors of the Stokes parameters of the incident radiation polarized and unpolarized parts are obtained , as well as the matrix of the scattering volume of particles, the vector of the Stokes parameters of the scattered radiation is calculated, containing information about the relative intensity in the unit of solid angle, taking into account the normalizations described above. The scattering indicatrix is determined by calculating the relative scattered intensity in a finite set of directions determined by a discrete grid of angular coordinates ψ and γ.

3. Visualization of radiation scattering indicatrix models on polydisperse spherical particles system

Based on the above algorithm, we describe a program for modeling the scattering indicatrix on a polydisperse system of particles. A modified gamma distribution was chosen as a model of the particle size distribution function $n(r)$ [5]

$$n(r) = a_d \cdot r^{\alpha} \cdot \exp\left(-b_d \cdot r^{\kappa}\right). \quad (2)$$

The peculiarity of this distribution is that n(0) = 0 and n(∞) → 0, which corresponds to reality, since there are no particles of infinitely small and infinitely large size. With the growth of the argument r from zero, the function $n(r)$ increases as a polynomial of the order α, then reaches its maximum value at the value of the argument $r = r_{max}$, which corresponds to the most probable particle size. With further growth of the argument r, the function $n(r)$ decreases, and the decay rate of the function is determined by the exponent κ. If the values α and κ are constant, the constant b_d is determined by the most probable particle size r_{max} in accordance with expression (3), and the constant a_d is determined by the concentration of particles N in accordance with expression (4)

$$b_d = \frac{\alpha}{\kappa \cdot r_{max}^{\kappa}}, \tag{3}$$

$$a_d = \frac{N}{\kappa^{-1} \cdot b_d^{-\frac{\alpha+1}{\kappa}} \cdot \Gamma\left(\frac{\alpha+1}{\kappa}\right)}, \tag{4}$$

where $\Gamma\left(\frac{\alpha+1}{\kappa}\right)$ – gamma function.

The change nature of particles SDF $n(r)$ (1) with a change of the parameter α from 0.75 to 24 ($\alpha_1 = 3, \alpha_2 = 7, \alpha_3 = 17, \alpha_4 = 27, \alpha_5 = 37$) at values of other parameters κ = 3, r_{max} = 40 nm, $N = 10^{14}$ м$^{-3}$ is represented in Fig. 2. To demonstrate the results of the program, Fig. 2 shows the dynamics of light scattering indicatrix models when the parameter α of the function $n(r)$ changes from 3 to 37.

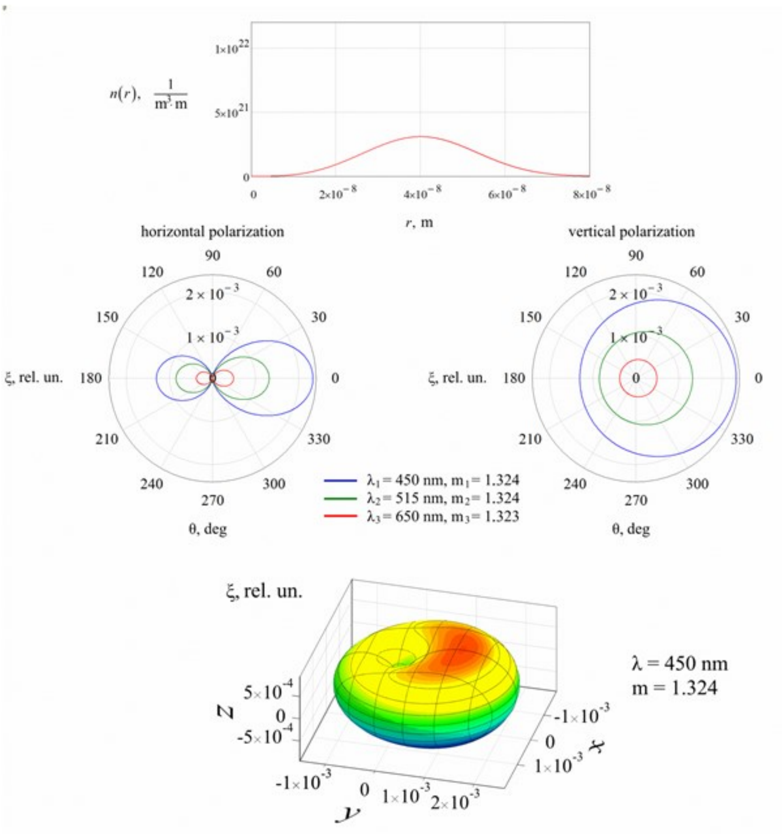

Fig. 2. Dynamics of particles SDF $n(r)$ and light scattering indicatrix on particle system when changing the particles SDF parameter α from 3 to 37 ($\alpha_1 = 3, \alpha_2 = 7, \alpha_3 = 17, \alpha_4 = 27, \alpha_5 = 37$), κ = 3, r_{max} = 40 nm, $N = 10^{14}$ м$^{-3}$

The change nature of particles SDF $n(r)$ (1) with a change of the parameter κ from 0.75 to 24 ($\kappa_1 = 0{,}75, \kappa_2 = 1{,}5, \kappa_3 = 3, \kappa_4 = 6, \kappa_5 = 12, \kappa_6 = 24$) at values of other parameters α = 3, r_{max}

= 40 nm, $N = 10^{14}$ m^{-3} is represented in Fig. 3. The modeling results of the light scattering indicatrix models dynamics with a change in the parameter κ of the function $n(r)$ from 0.75 to 24 are presented in Fig. 3.

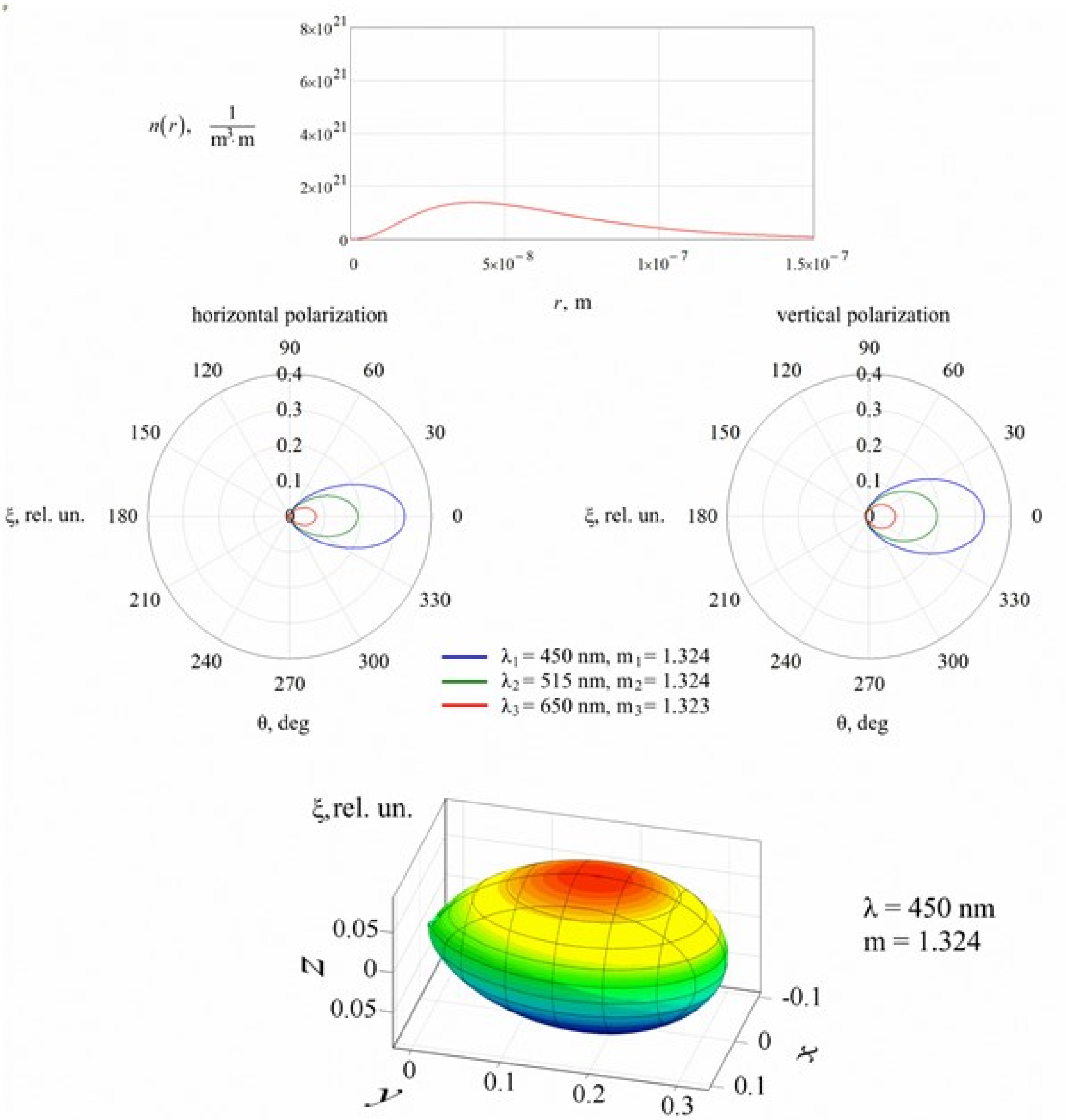

Fig. 3. Dynamics of particles SDF $n(r)$ and light scattering indicatrix on particle system when changing the particles SDF parameter κ from 0,75 to 24 ($\kappa_1 = 0{,}75$, $\kappa_2 = 1{,}5$, $\kappa_3 = 3$, $\kappa_4 = 6$, $\kappa_5 = 12$, $\kappa_6 = 24$), $\alpha = 3$, $r_{max} = 40$ nm, $N = 10^{14}$ m^{-3}

The change nature of the particles SDF $n(r)$ (1) when the r_{max} parameter is changed from 50 nm to 100 nm in 10 nm increments ($r_{max1} = 50$ nm, $r_{max2} = 60$ nm, $r_{max3} = 70$ nm, $r_{max4} = 80$ nm, $r_{max5} = 90$ nm, $r_{max6} = 100$ nm) is shown in Fig. 4 with values of other parameters $\alpha = 3$, $\kappa = 3$, $N = 10^{14}$ m^{-3}. Fig. 4 shows the results of modeling the dynamics of light scattering indicatrix models when the r_{max} parameter changes from 50 nm to 100 nm with the step 10 nm.

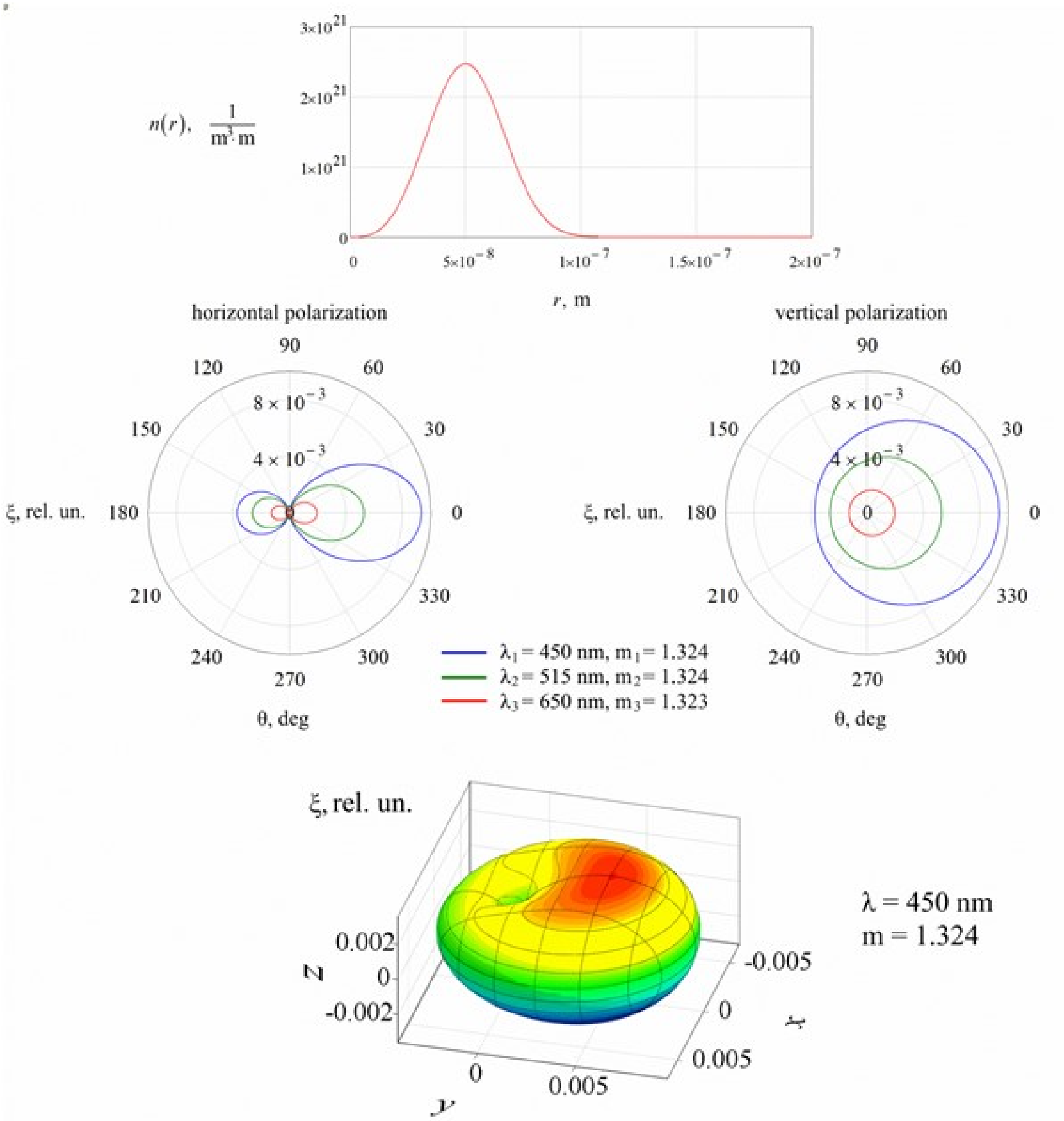

Fig. 4. Dynamics of particles SDF $n(r)$ and light scattering indicatrix on particle system when changing the particles SDF parameter r_{max} from 50 nm to 100 nm with the step 10 nm, $\alpha = 3$, $\kappa = 3$, $N = 10^{14}$ m^{-3}

4. Conclusion

The program algorithm has been developed that allows for calculating models of scattering indicatrix on homogeneous and isotropic spherical particles. The shape of the scattering centers is the only limiting factor of its application for calculating the scattered radiation intensity on real particle systems, despite this, the results of the program can be directly used to estimate the intensity that should be expected, for example, as a result of an experimental study of light scattering.

Light scattering on an ensemble of particles is simulated. The simulation program of experimental results allows varying the input parameters of the incident radiation, scattering centers and the receiving optical system, thereby providing the possibility of optimal selection of installation parameters and conditions for the experiment on registration of scattered radiation. It also makes it possible to restore the parameters of the scattering medium by selecting them based on a comparison of models and experimental data.

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