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Application of corpuscular and wave Monte-Carlo methods in optics of dispersive media

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***Abstract*.** **Two ways of simulating statistically the propagation of laser radiation in dispersive media by the Monte-Carlo method are compared. The first approach can be called corpuscular because it is based on the calculation of random photon trajectories, while the second one can be referred to as the wave approach because it is based on the calculation of characteristics of random wave fields. It is shown that, although these approaches are based on different physical concepts of radiation scattering by particles, they yield almost equivalent results for the intensity of a restricted beam in a dispersive medium. However, there exist some differences. The corpuscular Monte-Carlo method does not reproduce the diffraction divergence of the beam, which can be taken into account by introducing the diffraction factor. The wave method does not consider backscattering, which corresponds to the quasi-optical approximation.**

Keywords: *Monte-Carlo method, dispersive medium, corpuscular approach, wave approach, light scattering, light diffraction, stratified model.*

1. Introduction

The Monte-Carlo method (MCM) is used in the optics of scattering media, as a rule, for obtaining and statistical processing of the trajectories of many photons interacting with optical inhomogeneities (particles) of a medium. Such an approach, which had been first developed in neutron physics in calculations of reactors and then applied to problems of atmospheric optics (see, for example, [1]), was later used in the optics of biological tissues (see, for example, [2]). At the same time, the MCM involves in a broad sense a set of procedures for constructing ensembles of random numbers and functions whose statistic moments are the required quantities [3]. In the optics of random and dispersive media, the statistic characteristics of a light field can be determined both for ensembles of photon trajectories and random waves (Fig. 1). Accordingly, the approach considering radiation as a photon flux can be conventionally called the corpuscular MCM, whereas the approach based on wave concepts can be called the wave MCM [4].

The corpuscular MCM allows one to study the propagation of light both in weakly and strongly scattering media, where the diffusion component of the light field dominates.

The wave MCM can be applied to analyse the unidirectional propagation of radiation, which can be described by the Markovian process [5] by using the model of a stratified

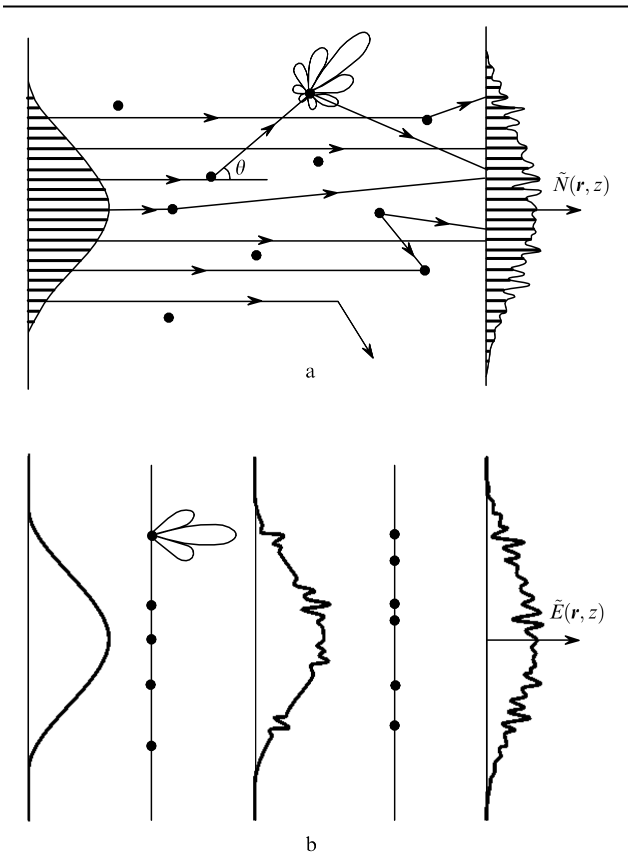

Figure 1. Schematic illustration of the corpuscular (a) and wave (b) MCMs used for solving the problem of scattering of a restricted beam in a dispersive medium. The scattering function $\sigma(\theta)$ is shown schematically in the form of a multilobe indicatrix in the polar coordinate system.

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medium. In the optics of random media, the stratified model forms the basis of the local method of small perturbations [6]. A random light field is formed in the wave MCM upon its diffraction propagation through the sequence of screens imitating perturbations of the light field caused by fluctuations in the refractive index and scattering in the medium. The wave model assumes that the wave passes successively through the screens in the absence of backscattering from particles.

In this paper, we perform a comparative analysis of the corpuscular and wave Monte-Carlo methods by the example of a linear problem of scattering of a restricted laser beam in a dispersive medium. The similarity and difference of these methods and regions of their applicability are discussed. The analysis is performed in the scalar approximation.

2. Corpuscular and wave models of light scattering in a dispersive medium

2.1 Scattering function

Monte-Carlo methods in the optics of dispersive media are based on the unified concept of scattering and absorption of radiation by an individual particle. The function $\sigma(\theta,\varphi)$ of light scattering by a particle (where θ is the angle in the scattering plane and φ is the azimuthal angle), which is also called the scattering indicatrix or phase function, depends on the size parameter $\rho = 2\pi R/\lambda$, where R is the particle radius and λ is the radiation wavelength. In many cases, scattering in mutually perpendicular planes is statistically independent, so that $\sigma(\theta,\varphi) = \sigma(\theta)\sigma(\varphi)$. If scattering is symmetric with respect to the wave vector of the incident wave, the scattering function depends only on the angle θ, while $\sigma(\varphi) = 1/(2\pi)$. For $\rho \gg 1$, the scattering function $\sigma(\theta)$ is strongly forward-elongated and scattered radiation is localised within a narrow cone with the cone angle $\theta \approx \lambda/R$ [7]. In this case, the radiation scattered during propagation along restricted paths does not come out outside the laser beam and the contribution of multiple scattering in the propagation direction of the beam becomes significant.

The scattering indicatrix is also often characterised by the mean cosine of the scattering angle or the anisotropy factor $g = \langle\cos\theta\rangle$ taking values from zero (completely isotropic scattering by particles of radius much smaller than the wavelength) to $+1$ (only forward scattering by particles of radius greatly exceeding the wavelength). As the size parameter ρ and anisotropy factor g decrease, the intensity of the component scattered at large angles increases and scattering becomes isotropic. In particular, for $\rho \leqslant 0.3$ and $g \approx 0$, the scattering function $\sigma(\theta)$ can be described in the Rayleigh approximation in which the intensities of forward and backward scattered radiation coincide [8].

2.2 Corpuscular Monte-Carlo method

The trajectory of a photon in the corpuscular method is a sequence of random events of its free path between particles and interaction events with the particles (Fig. 1a). In a dispersive medium with the known concentration n of particles, the attenuation coefficient $\alpha_0 = \mu_s + \mu_a$ determines the distribution function $F(l)$ for the random free path $\tilde{l}$ of the photon between particles and the particle albedo $A = \mu_s/(\mu_s + \mu_a)$ – the probability of photon scattering by a particle, while the function $\sigma(\theta,\varphi)$ of scattering by a particle determines the probability density for random deviation angles $\tilde{\theta}$ and $\tilde{\varphi}$ of the photon trajectory after its interaction with the particle. Here, μ_s and μ_a are the scattering and absorption coefficients of the medium. The angle of scattering $\tilde{\theta}$ by a spherical particle can take values in the interval $0 - \pi$, so that the corpuscular model permits the study of backward scattering.

The random trajectory of a photon in a scattering medium is calculated as follows. By using a random number generator, the realisation of the random free path $\tilde{l}$ and new coordinates of the interaction point with a particle are determined from the known distribution function $F(l)$. Then, a random event of interaction with the particle is considered, which can be elastic and quasi-elastic scattering or absorption. The scattering probability is equal to the albedo A, and the absorption probability is $1 - A$. If the photon was not absorbed, the random scattering angles $\tilde{\theta}$ and $\tilde{\varphi}$ are calculated whose probability density is proportional to the scattering function $\sigma(\theta,\varphi)$. Then, the photon free path $\tilde{l}$ is determined again, the event of the photon interaction with particles is considered, and so on until the photon is either incident on a photodetector or goes away to remote regions of the medium from which the probability of its return to the detector is negligibly small.

In the corpuscular MCM, an ensemble of photons $\{\boldsymbol{r}_j, \tilde{N}_j(\boldsymbol{r})\}$ is statistically processed (where $j = 1, 2, ..., M$ is the realisation number of a photon trajectory, M is the total number of photons, $\boldsymbol{r}_j$ are photon coordinates, and $\tilde{N}_j(\boldsymbol{r})$ are the distributions of their number depending on the coordinate $\boldsymbol{r}$ in the fixed plane z), which allows one to determine the parameters of radiation in a dispersive medium. Thus, the mean number of photons $\langle\tilde{N}_j(\boldsymbol{r}, z)\rangle$ is proportional to the intensity distribution $I(\boldsymbol{r}, z)$ in the plane z. The propagation of a restricted beam in a dispersive medium is studied by specifying the photon distribution $N_0(\boldsymbol{r}, z = 0)$ in their start plane $z = 0$, which is proportional to the initial intensity profile $I(\boldsymbol{r}, z = 0)$ of the beam (Fig. 1a). In [9], the photon distribution $N_0(\boldsymbol{r}, z = 0)$ was assumed proportional to the beam intensity $I(\boldsymbol{r}, z = 0)$ measured at the laser system output, which made it possible to reproduce laboratory experimental conditions by using the MCM. The authors of [9] obtained good agreement between calculated and experimental object images in a dispersive medium.

The corpuscular model operating with the number of photons determining the radiation intensity neglects phase relations for a propagating wave. As a result, this model does not describe the diffraction divergence of the beam as a whole but reproduces the diffraction of light from an individual particle. At the same time, the phase shift for the scattered component was determined in a number of papers (see, for example, [10]) where each photon was related to a hypothetic plane wave propagating between particles. Such an approach allows one to use the corpuscular MCM for simulating the formation of heterodyne and Doppler signals in coherent measurement systems, for example, in systems of optical coherent tomography of dispersive media and its Doppler variant [11, 12]. To obtain statistically reliable results for scattering media in the corpuscular MCM, an ensemble is needed containing, as a rule, $M = \int N_0(\boldsymbol{r}, z = 0)\mathrm{d}^2 r = 10^6 - 10^8$ photon trajectories. To accelerate the divergence of the method, photons are used with the 'weight' multiplied by A ($A \leqslant 1$) during each collision with a particle [13]. The initial 'weight' of each photon is unity, and a photon whose 'weight' achieves a certain threshold value, for example, 0.0001 is assumed absorbed. It is assumed that the contribution of photons with a lower 'weight' is insignificant.

2.3 Wave Monte-Carlo method

The wave model describes multiple scattering of the light field by particles. In this model of a dispersive medium, a light wave propagates successively through a chain of screens in which particles are located (Fig. 1b). The wave is scattered by particles on screens and diffracts freely between the screens in the absence of particles [14]. Particles are distributed randomly with the uniform density in the screen plane, their number being proportional to the concentration n, the screen area S, and the distance Δz between the screens. In this case, the number of particles with a radius R in a polydisperse medium is specified by the size distribution function $\Gamma(R)$. The amplitude and phase of a wave scattered by a particle at angles θ and φ are determined and can be calculated based on the scattering function $\sigma(\theta, \varphi)$. Due to the interference of the unperturbed component and component scattered by a set of randomly distributed particles, the wave scattered from the screen becomes stochastic with random variations in the amplitude and phase. Thus, the screen reproduces the diffraction of the wave by a set of randomly distributed particles on the screen.

Free diffraction between screens is considered in the Fresnel approximation [8]. The calculation of the wave propagation through a chain of scattering screens gives the complex amplitude of the random light field $\tilde{E}_j(\boldsymbol{r}, z)$ in a fixed plane z. The ensemble of such fields $\{\tilde{E}_j(\boldsymbol{r}, z)\}$ (where $j = 1, 2, \ldots, M$) found for statistically independent screen chains allows one to determine the statistical characteristics of the light field upon multiple scattering in a dispersive medium.

An individual field realisation $\tilde{E}_j(\boldsymbol{r}, z)$ obtained for a chain of scattering screens has a simple physical analogy. The field $\tilde{E}_j(\boldsymbol{r}, z)$ is formed after multiple scattering from a chain of many screens and is calculated by averaging statistically the contribution of scattering by many randomly distributed particles. The physical realisation of the field $\tilde{E}_j(\boldsymbol{r}, z)$ is similar to the detection of the amplitude and phase of the light field in the detection plane at a low exposure. In this case, the dispersive medium can be considered stationary during the detection time. For a dynamic dispersive medium with known microphysical parameters, the concentration n, and the size distribution function $\Gamma(R)$ of particles, the determination of the ensemble of particles $\{\tilde{E}_j(\boldsymbol{r}, z)\}$ on statistically independent screen chains is equivalent to the detection at a long exposure during which a random distribution of particles in the medium frequently changes. The ensemble of fields corresponds to a finite sampling, for example, during prolonged measurements of the light field in the atmospheric aerosol, aqueous hydrosols or in measurements in many stationary media with identical microphysical parameters.

The stratified model of wave scattering in a dispersive medium is the development of models of phase screens describing the propagation of radiation in a continuous random medium [15–17]. The wave MCM developed in [14] was used in the optics of atmospheric aerosols for numerical studies of the influence of coherent scattering in an aerosol on the formation of filaments in a high-power laser pulse propagating in atmospheric clouds and drizzle [18, 19].

3. Propagation of a light beam in a dispersive medium

3.1 Approximation of the scattering function

We compared the corpuscular and wave MCMs by the example of a linear problem of propagation of a light beam in a monodisperse aqueous aerosol.

A collimated axially symmetric beam at a wavelength of 0.8 μm with the Gaussian intensity profile

$$I(r, z = 0) = I_0 \exp\left(-\frac{r^2}{a_0^2}\right) \tag{1}$$

was considered, where I_0 is the axial intensity of the beam and a_0 is the beam radius at the e^{-1} level.

The absorption coefficient of an aqueous aerosol at 0.8 μm is negligibly small [20], and a change in the beam intensity in the aerosol is determined by scattering by particles and diffraction. The scattering function is obtained by the method of anomalous diffraction, which takes into account only the phase shift upon propagation of the wave through a particle without refraction on its boundaries [21, 22]. This method, proposed for 'soft' particles with the relative refractive index n_p/n_0 (where n_0 is the refractive index of the environment) close to unity, can be also applied for aqueous particles with $n_\mathrm{p}/n_0 = 1.33$ [23].

Figure 2 shows scattering functions $\sigma(\theta)$ for a spherical particle of radius $R = 15$ and 2 μm calculated by the method of anomalous diffraction and using the Mie theory [8, 21]. One can see that although the method of anomalous diffraction is approximate, the scattering functions $\sigma(\theta)$ obtained by this method are close to those calculated by using the exact Mie theory. For particles of a greater radius (15 μm), the angular width of the central lobe of the scattering diagram is smaller, while the relative intensity of radiation scattered at the angle $\sigma(\theta)$ is greater than these quantities for particles of a smaller radius (2 μm). In this case, radiation is scattered by particles mainly to the front hemisphere, while the intensity of radiation scattered into

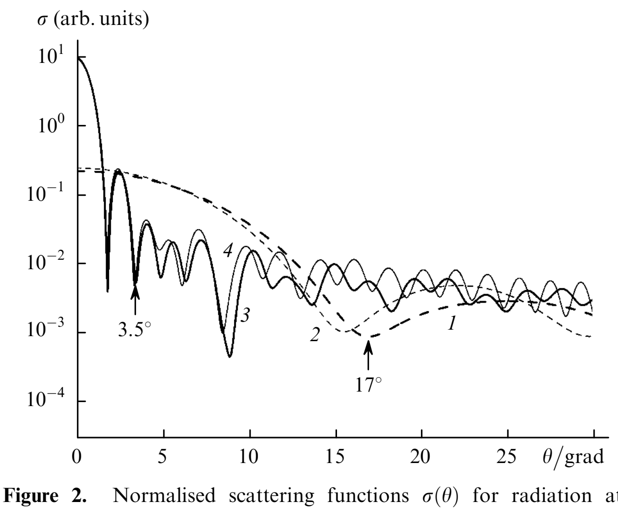

Figure 2. Normalised scattering functions $\sigma(\theta)$ for radiation at a wavelength of 0.8 μm for spherical aqueous particles of radius $R = 2$ (*1, 2*) and 15 μm (*3, 4*) calculated by the method of anomalous diffraction (*1, 3*) and using the Mie theory (*2, 4*). The arrows indicate maximal angles used in calculations of the intensity distribution in the wave MCM.

the side lobes of the scattering diagram is much lower than that scattered to the central lobe for $\theta = 0$. The radiation power scattered into the central and first side lobes of the function $\sigma(\theta)$ for a particle of radius $R = 15$ μm, i.e. at scattering angles $\theta \leqslant 3.5^\circ$ amounts to 46% of the total scattered radiation. For a particle of radius $R = 2$ μm, the relative radiation power scattered into the central lobe for $\theta \leqslant 17^\circ$ is 67 %.

The corpuscular and wave MCMs simulate the propagation of a light beam in a dispersive medium in the anomalous diffraction approximation taking into account only the contribution of radiation scattered at angles $\theta \leqslant 3.5^\circ$ for particles of radius 15 μm and angles $\theta \leqslant 17^\circ$ for particles of radius $R = 2$ μm. Radiation scattered at greater angles was interpreted as attenuation and its power was equated to losses of the beam power upon scattering by particles. In the corpuscular method, this corresponded to the albedo $A = 0.46$ and 0.67 for particles of radius 15 and 2 μm, respectively.

3.2 Statistical ensembles in Monte-Carlo methods

In the corpuscular MCM, the trajectories of 'weighted' photons were calculated, the total number of photons in a beam being 10^7. To reproduce the intensity profile (1) of the incident beam, the distance from its centre to a random entrance point of each photon to a medium was determined by the corresponding Gaussian distribution. The azimuthal distribution of photons with respect to the beam centre was assumed uniform. The average number of photons per circular region of area $2\pi r h_r$ (where h_r is the ring width) decreased according to (1) and was 10^2, in particular, for $r = 3a_0$ at the beam periphery. For such a number of photons, the relative deviation of the results of statistical averaging in the MCM from the mathematical expectation for the beam intensity did not exceed 2 %.

In the wave MCM, the stratified model of a dispersive medium with a chain of aerosol screens separated by a distance of 20 cm was used. For the concentration $n = 50$ cm^{-3}, more than 3000 particles were contained within a circle of radius $r = 3a_0$ on an aerosol screen, which mainly determined the scattering of a beam. More than 50 aerosol screens with statistically independent distributions of particles were located on paths under study. This provided the statistical averaging of realisations of the light field during propagation of the beam to the detection plane. The beam intensity profile was determined for an ensemble of $M = 50$ realisations, each of them being obtained for statistically independent chains of aerosol screens.

3.3 Beam profile in monodisperse aerosol

We considered the propagation of a beam of radius $a_0 = 3$ mm in monodisperse aerosol with particles of radii 15 and 2 μm and concentrations $n = 50$ and 2010 cm^{-3}, respectively. These values of concentrations were selected to provide the same attenuation coefficients for particles with these radii. For these parameters of the medium, the scattering coefficient μ_s was 0.0724 m^{-1}, which corresponds to the photon mean free path $l = 13.8$ mm. The photon transport path l^* is 94 and 70 m for a medium containing particles of radius 15 and 2 μm, respectively. The length l^* determines the distance at which the propagation direction of a photon is completely randomised (the photon 'forgets' its initial direction) and can be calculated from the expression $l^* = [\mu_s(1 - g) + \mu_a]^{-1}$. The intensity profiles $I(r)$ obtained by the MCM for a beam in an aerosol with particles of radius 15 μm at distances $z = 10$ and 30 m are presented in Fig. 3. The root-mean-square deviation for this ensemble is ~ 1 % for the wave MCM and varies from 0.5 % in the axial region to 2 % at the beam periphery for the corpuscular MCM. One can see that for $z = 10$ m the intensity profiles $I(r)$ obtained by both these methods virtually coincide. However, the intensity $I(r)$ at a distance of 30 m calculated by the corpuscular method exceeds that calculated by the wave method. This is explained by the fact that the corpuscular method does not reproduce the diffraction divergence of a restricted beam. The intensity $I(r, z)$ of a collimated Gaussian beam changes upon diffraction as [24]

$$I(r, z) = \frac{I_0}{1 + (z/L_d)^2} \exp\left\{ -\frac{r^2}{a_0^2[1 + (z/L_d)^2]} \right\}. \qquad (2)$$

The diffraction length $L_d = 2\pi a_0^2/\lambda$ for such a beam of radius $a_0 = 3$ mm is 70.68 m. The diffraction decrease in the beam intensity at a distance of $z = 10$ m does not exceed 2 %. At a distance of $z = 30$ m, this decrease is 15 %, which coincides with the relative deviation of results obtained by the corpuscular and wave methods.

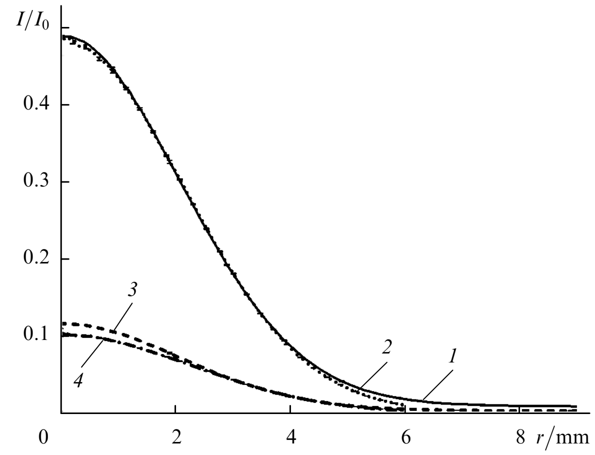

Figure 3. Intensity profiles $I(r)$ of a collimated radiation beam of radius $a_0 = 3$ mm at a wavelength of 0.8 μm propagating in monodisperse aerosol with particles of radius $R = 15$ μm and concentration $n = 50$ cm^{-3} at distances $z = 10$ (*1*, *2*) and 30 m (*3*, *4*) calculated by the corpuscular (*1*, *3*) and wave (*2*, *4*) methods.

The systematic error of the corpuscular MCM in the analysis of the beam scattering under diffraction conditions is clearly illustrated in Fig. 4 where the intensity profiles are presented for beams of radius $a_0 = 3$ and 1.5 mm. In corpuscular MCM calculations, the beam radius remains constant during the beam propagation $[a(z) = a_0]$ and the change in the axial intensity $I(0, z)$ of the beam with the propagation distance is independent of the initial radius a_0 of the beam. At the same time, for $a_0 = 1.5$ mm, diffraction causes a considerable redistribution of the radiation intensity in the beam cross section, resulting in a decrease in the axial intensity and an increase in the beam radius. The systematic error of the corpuscular method in the analysis of the propagation of a restricted beam in a dispersive medium can be excluded by multiplying the beam profile obtained by

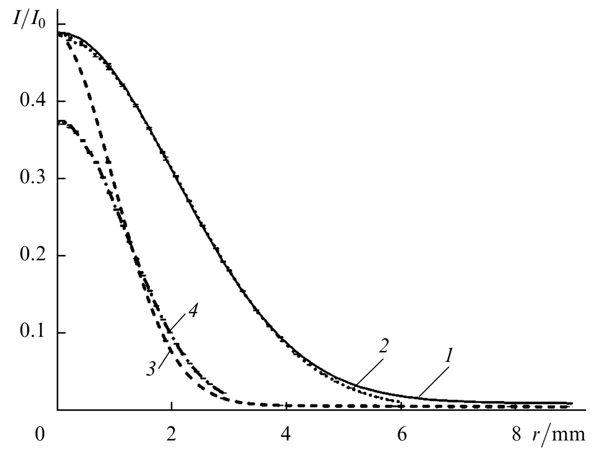

Figure 4. Intensity profiles at a distance of $z = 10$ m in a monodisperse aqueous aerosol with particles of radius $R = 15$ μm and concentration $n = 50$ cm^{-3} for a collimated beam of radius $a_0 = 3$ (*1, 2*) and 1.5 mm (*3, 4*) calculated by the corpuscular (*1, 3*) and wave (*2, 4*) methods.

this method by the diffraction factor $I(r, z)/I_0$ determining the relative change in the intensity caused by diffraction [see expression (2)]. This is possible due to the multiplicativity of scattering and diffraction processes in a dispersive medium. Note that the stratified model used in the wave MCM is based on the multiplicativity of radiation scattering and diffraction.

It is interesting to compare the MCM results with the dependence determined by the Bouguer law describing the attenuation of a plane wave in a dispersive medium [23]:

$$I_{\mathrm{B}}(z) = I(0)\exp(-\tau), \tag{3}$$

where $\tau = \alpha_0 z$ is the optical thickness of the dispersive medium at a distance of z. The attenuation (α_0) and scattering (μ_{s}) coefficients in a medium with absorbing particles coincide and are equal to

$$\mu_{\mathrm{s}} = \alpha_0 = K_{\mathrm{p}}\pi R^2 n \tag{4}$$

for a monodisperse aerosol [21], where K_{p} is the scattering factor for an aqueous spherical particle depending on its radius and the radiation wavelength [25]. The intensity profiles $I(r, z)$ of a collimated beam with the initial Gaussian profile (1) calculated by the Bouguer law (3) coincide with the profile obtained by the corpuscular MCM but differ from profiles obtained by the wave MCM because expression (3) neglects diffraction.

3.4 Influence of the particle size and scattering function on the beam profile

The angular width of the scattering function increases with decreasing the particle size [21, 22]. However, upon propagation of a restricted light beam in a dispersive medium with particles of radius much smaller than the wavelength, the scattering function weakly affects the beam intensity profile. The wave MCM calculations of the beam propagation in a monodisperse medium containing particles of radii 15 and 2 μm have shown that the intensity profile for the same optical thickness τ of the medium is independent of the particle radius.

The influence of different approximations of the scattering function of particles on the beam profile was studied only by the corpuscular MCM describing multiple scattering at large angles and, in particular, scattering into a rear hemisphere. Analysis performed for a medium with particles of radii 15 and 2 μm showed that the consideration of scattering into the rear hemisphere by using the Mie scattering function did not change the beam intensity profile obtained in the anomalous diffraction approximation taking into account all the lobes of the scattering diagram despite the fact that in the latter case only scattering into the front hemisphere was considered. The error of measuring the beam intensity by neglecting the side lobes of the scattering diagram does not exceed 2 %. It was also shown by using the corpuscular MCM that due to a smaller width of the scattering function of large particles, the beam intensity in a medium with particles of radius 15 μm was higher by 2 % than that for particles of radius 2 μm. The influence of different approximations for the scattering function of particles in a polydisperse medium was studied in [26].

4. Conclusions

The corpuscular and wave MCMs are identical methods for statistical studies of the propagation of radiation multiply scattered in dispersive media. Despite different physical concepts of radiation scattering by a set of particles, both these methods give equivalent results by analysing the intensity of a beam propagating in a dispersive medium. The corpuscular MCM does not describe the diffraction divergence of a restricted beam, which can be taken into account by introducing the diffraction factor. The wave MCM does not describe backscattering, which for the size parameter $\rho > 1$ does not result in considerable errors in the description of directional radiation and corresponds to the approximation of slowly varying amplitudes. The wave MCM is intended for solving the problems of nonlinear statistical optics, while the corpuscular MCM can be used for studying the propagation of low-intense radiation in random media.

We have presented in this paper the results of analysis performed in the scalar approximation. To take into account the depolarisation of radiation upon multiple scattering by particles in a dispersive medium, it is necessary to substantiate additionally the models used above.

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