# Effective Mie scattering of a spherical fractal aggregate and its application in turbid media

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An effective Mie-scattering model is developed to deal with the scattering property of a spherical fractal aggregate consisting of scattering particles. In this model the scattered field of a scattering particle is given by the classical Mie-scattering theory. On the basis of the Monte Carlo simulation method, we determine the physical parameters of a scattering aggregate, the scattering efficiency $Q$, and the anisotropy value $g$, as well as their dependence on the size and the effective mean-free-path length of a scattering aggregate. Accordingly, photon migration through a microscope objective focused into a turbid medium including scattering aggregates is simulated to understand the effect of complex tissue on image quality. 

*OCIS codes:* 290.7050, 290.4020, 290.4210, 290.0290.

Mie-scattering theory provides rigorous solutions on the basis of electromagnetic theory for light scattering by an isotropic sphere embedded in a homogeneous medium.[1,2] According to this theory, the scattering property of a spherical particle can be described by two important physical parameters, the scattering efficiency $Q$ and the anisotropy value $g$. The former gives the strength of the scattered field and the latter represents the averaged angle of the scattered field. The Mie-scattering theory provides an important physical foundation of the Monte Carlo simulation for optical microscopic imaging through a tissuelike turbid medium consisting of scattering particles such as cells and nuclei.[3–8]

However, these small scattering particles are sometimes aggregated because of their biological and chemical functions.[9,10] A fractal aggregate is a medium with an ensemble of small scattering particles that, because of the physical mechanisms of aggregation, lead to a fractal structure, i.e., a scale-invariant structure.[11] Optical excitations in fractal aggregates are substantially different from those in other media.[12] Scattering by a single fractal aggregate cannot be described by the Mie-scattering theory.[1,2] Instead, electromagnetic and Monte Carlo analyses have been developed to study the light-scattering behavior through a fractal aggregate.[13,14] However, the electromagnetic method is complicated even when one aggregate is considered.[13] Therefore, for a complex turbid tissue medium composed of many aggregates distributed at different sites,[9,10] the electromagnetic method is not practically suited for large-scale simulation, whereas in principle it is applicable. In addition, the electromagnetic method has its limitation in the treatment of only aggregates of small scatterers. For a complex aggregate model, e.g., a cell, that consists of multiple size scatterers, the electromagnetic method is not applicable and the Monte Carlo simulation model can treat such a problem appropriately. The existing Monte Carlo analysis also deals only with the backscattering features of a turbid medium consisting of one single aggregate.[14] To deal with scattering in a turbid medium made up of multiple-scattering aggregates, it is necessary to establish a new physical model that gives rise to the scattering parameters of one aggregate under plane-wave illumination.

Our aim in this paper is to present a model of light scattering by a spherical fractal aggregate. Using Monte Carlo simulation, we calculate the angular distribution of photons scattered by a spherical fractal aggregate consisting of small particles that satisfy the Mie-scattering theory. On this basis we derive the dependence of the scattering parameters of the

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Received 22 July 2003; revised manuscript received 23 February 2004; accepted 23 February 2004.

0003-6935/04/142925-05$15.00/0

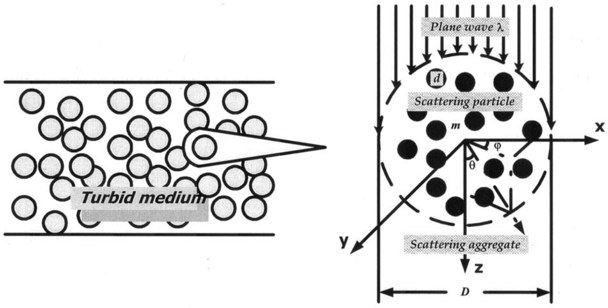


Fig. 1. Schematic diagram of the EMS model for an aggregate consisting of spherical particles.

aggregate, the scattering efficiency $Q$, and the anisotropy value $g$ (the average cosine of the scattering angle) on its size and the effective mean-free-path length. This method is termed the effective Mie-scattering (EMS) model with which we predict the focal spot in the tissuelike turbid medium made up of scattering aggregates (Fig. 1).

Figure 1 shows the schematic diagram of the EMS model for a fractal aggregate. A plane wave of wavelength $\lambda$ is illuminated on an aggregate for excitation. To avoid confusion, we clearly defined the terms of a scattering aggregate and a scattering particle. The scattering aggregate has an imaginary spherical shape of diameter $D$ (radius $R$) and a fractal dimension of $m$ and consists of spherical scattering particles of diameter $d$ (radius $a$) (in Fig. 1 as the dark circles). Here $2 < m < 3$ gives the fractal degree description of a fractal aggregate in three-dimensional space and $m = 3$ represents a homogeneously random medium.[14]

Because of the structural feature of a fractal medium, the effective mean-free-path length ($l_m$) for an aggregate is not simply related to the scattering cross section ($\sigma_p$) and the volume concentration ($K_p$) of scattering particles as that in a homogeneously random medium ($m = 3$), which is well known as $l = 1/K_p\sigma_p$. Instead, the effective mean-free-path length ($l_m$) for an aggregate as a medium with fractal structure has the following expression[14]:

$$l_m = a\left[\frac{4(m-2)}{K_m m Q_p}\right]^{1/(m-2)}, \tag{1}$$

where $K_m = [N_3(r_i)]/[(r_i/a)^m]$ and $Q_p = \sigma_p/\pi a^2$ are, respectively, the volume fraction of the fractal medium and the scattering efficiency of a scattering particle determined by the Mie-scattering theory.[2] $N_3(r_i)$ denotes the number of scattering particles in the homogeneous random medium within a certain radius $r_i$ of an imaginary sphere that is assumed to be centered at a particle of interest. In addition, the number of particles included in an aggregate has a certain relationship by the fractal dimension $m$ with the size (radius $R$) of the aggregate that centers at the particle of interest, which satisfies the equation $N_m(R) = (R/r_i)^m N_3(r_i)$. This equation can be used to determine the size of an aggregate in simulation.[14]

As with any scattering spherical particle, to understand the scattering properties of a spherical aggregate, one needs three physical parameters: the phase function $\rho(\theta)$, the scattering cross section $\sigma_s$ (or the scattering efficiency $Q$), and the anisotropy value $g$. A phase function $\rho(\theta)$ specifies the angular dependence of the photons scattered into a unit solid angle $d\Omega$ oriented at a scattering angle $\theta$ relative to the original light trajectory. To this end, we first calculate the angular distributions of scattered photons $N_s(\theta)$ and total photons $N_t(\theta)$. Because of the cylindrical symmetry, these two distributions are dependent only on the angle $\theta$. Therefore the normalized phase function $\rho(\theta)$ of an aggregate can be calculated by

$$\rho(\theta) = \frac{[N_s(\theta)/\sin\theta]}{\int_0^{2\pi} d\phi \int_0^{\pi} [N_s(\theta)/\sin\theta] d\theta}. \tag{2}$$

According to the original definition of the scattering efficiency $Q$ of a scattering particle in the Mie-scattering theory, the scattering cross section $\sigma_s$ is the ratio of the power scattered at $\theta$ and $W_s$ to the incident irradiance $I_i$, i.e., $\sigma_s = W_s/I_i$, and the scattering efficiency $Q$ is the ratio of the scattering cross section $\sigma_s$ of the particle to its geometric cross section $\sigma_g$, i.e., $Q = \sigma_s/\sigma_g$. Therefore, for a spherical aggregate of radius $R$, the scattering efficiency $Q_a$ of a spherical aggregate can be obtained through $Q_a = \int_0^\pi N_s(\theta)d\theta/\int_0^\pi N_t(\theta)d\theta$, and the geometric cross section of an aggregate is $\sigma_a = \pi R^2$. The average cosine of the scattering angle $\theta$ of the scattered light is called the anisotropy value $g$ and can be calculated by use of the phase function $\rho(\theta)$. In our case, the anisotropy value $g_a$ of an aggregate is given by $g_a = \int_0^\pi N_s(\theta)\cos \times d\theta/\int_0^\pi N_s(\theta)d\theta$.

The scattering cross section $\sigma_p$ and the anisotropy $g_p$ value of a scattering particle within an aggregate are determined by Mie-scattering theory,[2] and the effective mean-free-path length $l_m$ of an aggregate can be calculated with Eq. (1). Therefore the three physical scattering parameters of a spherical aggregate can be calculated with the Monte Carlo simulation method.[14] The parameters used in this Monte Carlo simulation are as follows. We use $10^7$ illumination photons to ensure the accuracy of simulation results. It should be pointed out that the relationship between the number of photons needed and the level of accuracy depends on the ratio of the effective mean-free-path length $l_m$ to the imaginary size of the aggregate $R$. If $l_m/R$ becomes smaller, which means more scattering events happen inside an aggregate, then more photons are needed to guarantee the accuracy, and accordingly more computation time is required. It is assumed that the excitation wavelength $\lambda$ is 0.4 $\mu$m throughout the paper. The diameter of the aggregate $D$ is 5 $\mu$m, and the diameter of the scattering particles that constitute the aggregate with a fractal dimension of $m = 2.5$ is $d = 0.2$ $\mu$m. The scattering particles have no absorption and are

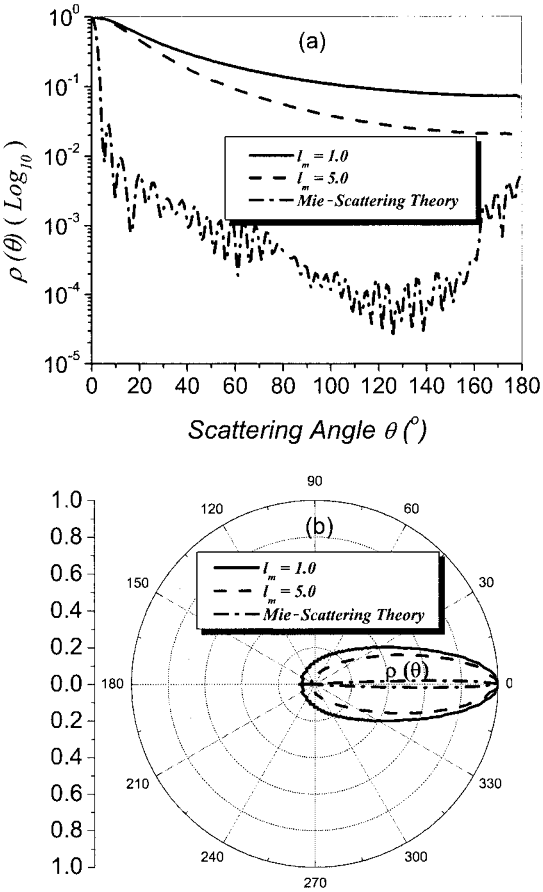


Fig. 2. Phase functions $\rho(\theta)$ of an aggregate based on the effective Mie-scattering model ($l_m = 1.0$ and $l_m = 5.0$ μm) and the phase function $\rho(\theta)$ based on Mie scattering: (a) logarithmic scale, (b) polar coordinate system.

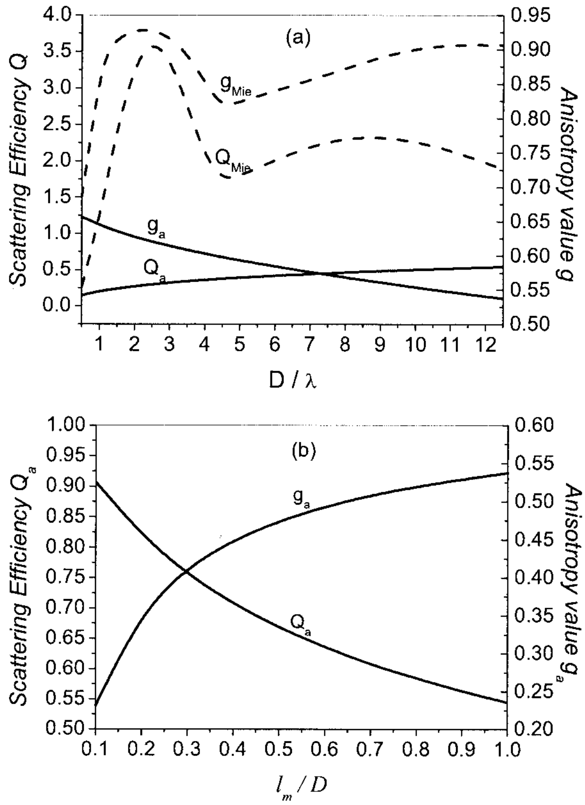


Fig. 3. Scattering efficiency $Q_a$ (left axes) and anisotropy $g_a$ value (right axes) of an aggregate as a function of its size (a) $D/\lambda$ and (b) mean-free-path length $l_m/D$.

suspended in air. The refractive index $n$ of the scattering particles is 1.59. For the demonstration of our methodology, the choice of the suspended medium of the scattering particles in this paper is air rather than water, which is close to the refractive index of tissue. However, use of the refractive index of water instead of air will induce only the change of the scattering properties of the scattering particles within an aggregate, and such an induced change of the described parameters of the scattering features of a scattering aggregate is not significant.

The phase function $\rho(\theta)$ of the EMS model for a fractal aggregate is demonstrated in Fig. 2 for two cases of $l_m = 1.0$ and $l_m = 5.0$. As expected, when the effective mean-free-path length $l_m$ becomes larger [the dashed curves in Figs. 2(a) and 2(b)], the angular distribution of the phase function becomes narrower because the longer $l_m$ means that there are less-effective scattering events through the aggregate.

For comparison, the phase function $\rho(\theta)$ from the conventional Mie-scattering theory[2] for a solid spherical particle of the same size as the aggregate is also depicted in Fig. 2. A comparison of Mie scattering and EMS shows that Mie scattering leads to a modulating dependence of the phase function [Fig. 2(a)], which does not exist in EMS. This difference results from the different physical mechanisms involved in Mie scattering and EMS. In the former case, the phase function is that of the intensity originating from the sum of complex amplitudes (waves), and thus such a superposition gives rise to the interference (modulating) feature. However, in the EMS model the phase function is given by the superposition of photons [see Eq. (2)]. Another feature of the comparison is that the solid particle results in a stronger forward-scattering characteristic than that from the fractal aggregate of the same size. This feature is caused by the fact that, within the aggregate, photons are multiply scattered, which gives rise to a broader angular distribution and stronger backscattering [Fig. 2(b)].

The dependence of the scattering efficiency $Q_a$ and the anisotropy value $g_a$ of an aggregate on the normalized aggregate size $D/\lambda$ is demonstrated in Fig. 3(a). It can be seen that as $D/\lambda$ becomes larger, the scattering efficiency $Q_a$ and the anisotropy value $g_a$ become large and small, respectively. This behavior is different from that predicted from the Mie-scattering theory [see the dashed curves in Fig. 3(a)] but understood because the number of the scattering events increases as the aggregate size becomes large. In addition, the dependence of the scattering efficiency $Q_a$ and the anisotropy value $g_a$ in EMS does not show the modulating nature, which is consistent

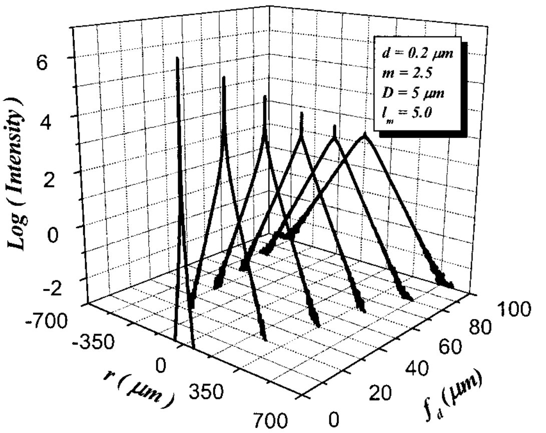


Fig. 4. Logarithmic representation of the excitation profiles (i.e., the focal spots) of an objective (numerical aperture of 0.25) in a homogeneously random medium consisting of fractal aggregates with a concentration of $0.002/\mu m^3$. The incident photon number is $10^7$.

with the superposition principle of photons shown in Fig. 2.

The effect of the normalized mean-free-path-length $l_m/D$ on the scattering efficiency $Q_a$ and the anisotropy value $g_a$ is demonstrated in Fig. 3(b). As expected, when $l_m/D$ increases, i.e., when either $l_m$ increases or $D$ decreases, the scattering efficiency $Q_a$ and the anisotropy value $g_a$ decreases and increases, respectively, because of the increased number of the scattering events within the aggregate.

The significance of the scattering efficiency $Q_a$ and the anisotropy value $g_a$ derived from the EMS model is that they allow for the Monte Carlo simulation[6–8] of photon migration through a complex turbid medium made up of a large number of aggregates. In this case, the aggregate with the known scattering efficiency $Q_a$ and the anisotropy value $g_a$ and the geometric size of radius $R$ can be treated as a normal scattering particle. Also, Monte Carlo simulation can be implemented in this medium consisting of such aggregates is those considered in our previous study[6–8] as long as the aggregates are distributed in the medium randomly and the volume concentration is known, which means that the simple mean-free-path length $l$ rather than $l_m$ is used. To demonstrate this, we simulate the focusing feature of an objective through such a complex turbid medium using these two parameters. Figure 4 shows the logarithmic representation of the focal spot of an objective as a function of the focal depth $f_d$ in a homogeneous turbid medium of fractal aggregates. Here $f_d$ is the distance between the surface of the turbid medium to the focal plane of the objective within the medium and $r$ is the radial distance in the focal plane. It can be seen from Fig. 4 that, as the focal depth $f_d$ increases, the narrow central peak disappears and the focal spot becomes broad, which means that the ballistic or snake photons around the focus decrease and that the scattering photons that deviate from the center path increase. Figure 4 implies that image quality, such as image resolution and signal level,[6–8] of an object embedded in an aggregate-distributed turbid medium can be studied in the future.

In conclusion, an EMS model has been established for the investigation into a fractal aggregate as a single scatterer. According to the Monte Carlo simulation method, the scattering parameters of a spherical aggregate, the scattering efficiency $Q_a$, and the anisotropy $g_a$ value have been derived to reveal their dependence on the physical size $D$ and the effective mean-free-path length $l_m$ of the aggregate. The model established here can be extended to analyze aggregates composed of particles of different sizes.[15] Consequently the mechanism for microscopic imaging through complex tissue media of aggregates[9,10] can be explored.

We thank the Australian Research Council for its support and Lu Qiang for valuable discussions.

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