LIGHT SCATTERING BY LARGE HEXAGONAL COLUMN WITH MULTIPLE DENSELY PACKED INCLUSIONS

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Abstract—The scattering of visible light by hexagonal-shaped column containing densely packed inclusions is simulated by a combination of ray-tracing and Monte Carlo techniques. While the ray tracing program takes care of the individual reflection and refraction events at the outer boundary of the particle, the Monte Carlo routine simulates internal scattering processes. A dense-medium light-scattering theory based on the introduction of the static structure factor is used to calculate the phase function for densely packed inclusions. Numerical results of the phase function for a randomly oriented hexagonal-shaped ice crystal with multiple densely packed inclusions are evaluated.

1. INTRODUCTION

Understanding the radiation budget of Earth and the atmosphere system, and hence its climate, must begin with an understanding of the scattering and absorption properties of clouds particles [1– 7]. A large number of clouds particles are nonspherical ice crystal. The study of light scattering by atmospheric ice crystals is basically motivated by large variability of ice particle shapes. In many study, the shape of the ice crystals is usually regard as hexagonal-shaped column [8]. While the shape problem is obvious from numerous in situ aircraft measurements, little is know about the internal structure of the ice particles. In recent years, many possible increase of the concentration of aerosol particles, for example, volcanic eruptions [9], industrial combustions [10], sand and dust storms [11], may well lead to a large number of particles inside an ice crystal. Many of these particles have long been recognized as an important atmospheric pollutant. They play a significant role in the absorption of solar radiation. So, particles imbedded in ice crystals could potentially reduce the cloud albedo, thereby causing a significant indirect forcing of climate. Some researchers [12] even think it can be used to interpret the cloud absorption anomaly.

Macke [13] has studied light scattering by ice particles with multiple distinct inclusions. He assumed that the inclusions are randomly and sparsely distributed, so the multiple scattering of the inclusions is based on the independently scattering theory. However, when the density of the internal scatterers reach a limit, the spatial correlation among densely packed inclusions can substantially change their single scattering properties (such as optical cross sections and phase function [14]), thus making questionable the applicability of the independent scattering approximation in calculation of light scattering by multiple inclusions.

In this paper, we studied how the phase function is changed with the compaction state of scattering particles at first. In our calculations, we use a dense-medium light-scattering theory based on introducing the so-called static structure factor. The main formula and

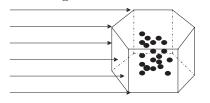


Figure 1. Sketch map of light scattering by a hexagonal-shaped ice column with multiple densely packed inclusions. numerical results of this theory are given in the following section. Then, we present the theoretical procedure for the determination of the single scattering properties by combining ray-tracing and Monte Carlo techniques, and numerical results for the light scattering by a hexagonal-shaped ice column with multiple densely packed inclusions (Fig. 1) are given. The results of the paper are summarized in the concluding section.

2. SINGLE SCATTERING CHARACTERISTICS OF DENSELY PACKED INCLUSIONS

For sparsely distributed, independently scattering particles, the phase function is given by [15]

$$P(\theta) = \frac{4\pi}{C_{sca}} \frac{dC_{sca}}{d\Omega} \tag{1}$$

where θ is the scattering angle and $dC_{sca}/d\Omega$ is the differential scattering cross section [15] and

$$C_{sca} = \int_{4\pi} d\Omega \frac{dC_{sca}}{d\Omega} \tag{2}$$

is the total scattering cross section.

Densely packed particles are not independent scatterers. Therefore, the concept of the single-scattering phase function can not be used in the same sense as it is used in computations of light scattering by sparsely distributed particles. However, the concept of the singlescattering phase function can still be used with some modification to calculate the intensity of light singly scattered by a layer densely packed particles [14, 16]. The differential scattering cross section is equal to the product of the independent-scattering differential cross section and so-called static structure factor $S(\theta)$. Thus, instead of Eqs. (1)–(2), we have for densely packed particles

$$P(\theta) = \frac{4\pi}{C_{sca}} \frac{dC_{sca}}{d\Omega} S(\theta)$$
(3)

$$C_{sca} = \int_{4\pi} d\Omega \frac{dC_{sca}}{d\Omega} S(\theta) \tag{4}$$

Note that the theory based on the introduction of the static structure factor has a rather strong physical background and is based on solving Maxwell's equations for calculating light scattering and on statistical mechanics for describing the statistics of mutual positions of densely packed particles [16, 17]. The problem of computing the static structure factor for arbitrary particle size distribution and shape is extremely difficult, so we used two usual approximations which have been used by Mishchenko [14]. From the approximation, we assume scattering particles to be nearly spherically shaped and nearly monodisperse (the range of sizes is narrow compared with the mean particles size). The structure factor in the Percus-Yevick approximation is given by [18]

$$S(\theta) = \frac{1}{1 - nC(p)} \tag{5}$$

where

$$p = [4\pi \sin(\theta/2)]/\lambda \tag{6}$$

n is the number density of scattering particles, λ is wavelength of light, and C(p) is given by

$$C(p) = 24 \frac{f}{n} \left[\frac{\alpha + \beta + \delta}{u^2} \cos u - \frac{\alpha + \beta + 4\delta}{u^3} \sin u - \frac{2(\beta + 6\delta)}{u^4} + \frac{2\beta}{u^4} + \frac{24\delta}{u^5} \sin u + \frac{24\delta}{u^6} (\cos u - 1) \right] \quad p \neq 0$$
(7)

and

$$C(0) = -24\frac{f}{n}\left(\frac{\alpha}{3} + \frac{\beta}{4} + \frac{\delta}{6}\right) \tag{8}$$

where

$$u = 2pr_0 \tag{9}$$

$$\alpha = \frac{(1+2f)^2}{(1-f)^4} \tag{10}$$

$$\beta = -6f \frac{(1+f/2)^2}{(1-f)^4} \tag{11}$$

$$\delta = \alpha f/2 \tag{12}$$

where $f = 4/3\pi n r_0^3$ is the filling factor (i.e., the fraction of a volume occupied by he particles). Note that for sparsely distributed particles (n = 0), the structure factor is identically equal to unity [14].

An interesting question is whether the modified dense-medium phase function given by Eq. (3) can be used to calculate the multiplescattering contribution to the reflected intensity of densely packed particles. It has been shown in [14] that it can be used to compute the full intensity for nonabsorbing or moderately absorbing particles. So the phase function can be used in our Monte Carlo simulations of the light scattering by inclusions.

In our study, the internal scatterers are considered to be ammonium sulfate aerosols $((NH_4)_2SO_4)$, which is a naturally occurring aerosol type. The shape of the particles is assumed to be spherical, and the mean radius of the inclusions is assumed to be $0.5 \,\mu$ m. Mie theory is used to obtain the optical properties of the internal scatterers. It is well known that monodisperse Mie quantities as a function of size parameter contain a high frequency ripple which is usually suppressed in practice because, in nature, there is always

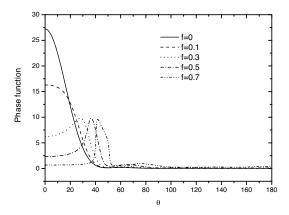


Figure 2. Scattering phase functions of spherical inclusions made of ammonium sulfate.

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a dispersion of grain sizes [15]. Therefore, following Wiscombe and Warren [19], we reduced the ripple by averaging the phase function over a range of sizes which was small relative to the mean grain size. The relative refractive indices of $(NH_4)_2SO_4$ to ice is taken to be 1.15 [14].

Our calculations were performed at a wavelength of $\lambda = 0.55 \,\mu\text{m}$, i.e. at the maximum of the solar irradiation. We compared the phase functions of densely packed internal scatterers and sparsely distributed ones in Fig. 2. The phase function is shown as a function of the scattering angle θ for five values of the filling factor. It is seen that increasing packing densely results in an angular redistribution of the scattered intensity. The influence of packing density is especially significant at scattering angles $\theta < 50^{\circ}$. This agrees well with the conclusion of Mishchenko's [14].

3. TOTAL SCATTERING SIMULATIONS WITH THE RAY-TRACING AND MONTE CARLO MODEL

The total scattering of light ray by a hexagonal ice column containing densely packed spherical inclusions is calculated by a combination of ray tracing and Monte Carlo techniques [13]. The ray tracing programs takes care of the reflection and refraction events, and the Monte Carlo methods do with the internal scattering processes.

After an incident photon is refracted into the crystal, it travels a free path length l given by

$$l = -\langle l \rangle \log[R(0,1)] \tag{13}$$

where $\langle l \rangle$ is the mean free path length between two subsequent scattering events and R(0, 1) is an equally distributed random number within the interval (0, 1). The number density of the inclusion n is described by the mean free path length $\langle l \rangle$ or by the volume extinction coefficient $\beta_x = 1/\langle l \rangle$. For an ensemble of N particles per volume element whose size obey a standard gamma distribution, β_x is given by

$$\beta_x = n \int_{r_1}^{r_2} \beta_x(r) n(r) dr \tag{14}$$

where n(r) is the normalized particle size distribution function. In this paper, we choose n(r) to be equally distributed.

If the photon has not reached one of the boundaries of the medium, its previous direction is changed along the scattering angle and azimuth angle according to

$$\int_0^\theta P^{(i)} \sin \theta d\theta = R(0,1) \int_0^\pi P^{(i)}(\theta) \sin \theta d\theta$$
(15)

$$\phi = R(0, 2\pi) \tag{16}$$

where $P^{(i)}(\theta)$ denotes the scattering phase function of the internal inclusions. The processes stated in (14) and (15) are repeated until the photon enters one of the crystal facets, where it is again subject to reflection and refraction events. The whole procedure is again repeated for internally reflected component until the photon energy falls below 10^{-15} times the incident energy.

The effects of internal inclusions are studied for one hexagonalshaped ice column, defined by a length to diameter ratio of $100 \,\mu m/50 \,\mu m$. Fig. 3 present results of the total phase function for a random oriented ice crystal containing densely packed inclusions. Results are shown for the filling factor f = 0.1, 0.3, 0.5, for comparison, the phase function of pure ice crystal is also shown. It is seen from Fig. 3 that for pure ice crystal, dominant features of the phase function are enhanced scattering at angles of 22° and 46° , corresponding to the so-called halos. With increasing the filling factor f, the intensity of the halos and the backscattering maximum are reduced, and the phase functions tend to more and more homogeneous except the diffraction region. These results come from the effects of the internal impurities. A photon will suffer much more scattering by the inclusions, so the scattering intensity will be homogeneous distributed in the inner of the ice crystal. The difference of the total phase function is relatively small from 0° to 5° , this is because that this energy comes mostly from the contribution of diffraction.

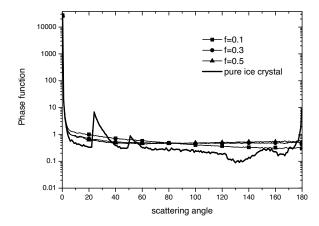


Figure 3. Total scattering phase function of a hexagonal column with internal sulfate. The filling factor is f = 0.1, 0.3, and 0.5. The scattering phase function of a pure ice crystal without inclusions is given for a comparison.

4. CONCLUSION

In this paper, we used a combination of ray-tracing and Monte Carlo techniques to compute the single scattering phase function for a randomly oriented hexagonal ice column containing densely packed ammonium sulfate inclusions. A dense-medium light scattering theory based on introducing the static structure factor was used to consider the spatial correlation among densely packed particles, and the single scattering properties of the inclusions were calculated. A ray tracing program takes care of the individual reflection and refraction events at the outer boundary of the particle. Our calculations show that the effects of the internal impurities on the total scattering phase function is great. The total scattering phase function was smoothed relative to the pure ice crystal. This is because that a photon will suffer much more scattering by the inclusions, the scattering intensity will be homogeneous distributed in the inner of the ice crystal.

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