Scattering of light by fluffy aggregates consisting of small and large particles

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Abstract

We study intensity and polarization of radiation scattered by fluffy aggregates. Model is porous pseudosphere with small size (Rayleigh) inclusions and inclusions of different sizes. The calculations are carried out using the discrete dipole approximation (DDA) code for several materials with complex refractive indices ranging from 1.20 + 0.00i to 1.75 + 0.58i. The results are compared with the predictions of the Lorenz-Mie theory with a refractive index found from the effective medium theory based on the Bruggeman rule and the extended Mie theory for *n*-layered spheres. It is found that the scattering characteristics of particles with small inclusions are described by the Bruggeman–Mie theory quite well (deviations usually do not exceed ~ 5 - 15%). For particles with inclusions of different sizes the satisfactory agreement between *n*-layered spheres and DDA computations is obtained for small and intermediate porosity.

1 Introduction

Finding the optical properties of fluffy aggregate particles is an important task for different fields of science and industry. Such particles are generally assumed to be constituents of interstellar clouds, circumstellar and protoplanetary disks, various suspensions, etc. Because the numerical methods developed for the aggregate optics calculations are rather computationally expensive, we develop "effective" models where complex particle is replaced by a simple model with similar optical properties. In papers [1] and [2] it was shown that the extinction efficiencies and other integral scattering characteristics of porous pseudospheres with small size (Rayleigh) inclusions can be well described using Lorenz-Mie theory and a refractive index found from the Bruggeman mixing rule of the effective medium theory (EMT). At the same time, the extinction of heterogeneous particles having inclusions of various sizes (Rayleigh and non-Rayleigh) are found to resemble those of spheres with a large number ($\geq 15 - 20$) of different layers [1].

Here, we study angular scattering properties of particles consisting of vacuum and some material. As earlier [2], five refractive indices of materials corresponding to biological, atmospheric and cosmic particles were selected. Previous analysis of applications of different mixing rules was mainly focused on extinction efficiencies (see Refs. [3], [4] and references therein). Only a couple times intensity and polarization of scattered radiation calculated using some EMT mixing rule compared with the results of microwave analog experiments [5] and the results of DDA calculations [6] and [7].

2 Models and calculations

We consider spherical particles consisting of some amount of a material and some amount of vacuum. The amount of vacuum characterizes the particle porosity \mathcal{P} ($0 \leq \mathcal{P} < 1$), which is introduced as

$$\mathcal{P} = V_{\text{vac}}/V_{\text{total}} = 1 - V_{\text{solid}}/V_{\text{total}}$$

where V_{vac} and V_{solid} are the volume fractions of vacuum and solid material, respectively. If $\mathcal{P} = 0$ the particle is homogeneous and compact. Fluffy particles also can be presented as homogeneous spheres of the

same material mass with radius r_{porous} and a refractive index found using an EMT. The size parameter of porous particles can be found as

$$x_{\text{porous}} = \frac{2\pi r_{\text{porous}}}{\lambda} = \frac{x_{\text{compact}}}{(1-\mathcal{P})^{1/3}} = \frac{x_{\text{compact}}}{(V_{\text{solid}}/V_{\text{total}})^{1/3}},$$

where λ is the wavelength of incident radiation.

The optical properties of particles with inclusions are evaluated using program DDSCAT (version 6.0) [8]. The particles ("targets" in the DDSCAT terminology) are reproduced by pseudospheres with inclusions of a fixed size or with a given distribution of inclusions over their sizes (see [1] for details). Targets with the values of d_{incl} ranging from 1 to 9 are considered. The inclusions of the size $d_{incl} = 1$ are dipoles, while the inclusions with $d_{incl} = 3, 5, 7$ and 9 consist of 27, 125, 343 and 729 dipoles, respectively. Contrary to previous calculations, the optical characteristics of pseudospheres with inclusions are averaged over 256 target orientations.

The effective models of aggregates includes the Lorenz-Mie calculations for homogeneous spheres with refractive index found from Bruggeman mixing rule and calculations for *n*-layered spheres.

We consider non-polarized incident radiation and analyse the angular dependence of the intensity (element S_{11} of the Müller scattering matrix) and linear polarization of scattered radiation ($P = -S_{12}/S_{11}$).

3 Results and discussion

Computations were performed for fluffy particles with size parameters $x_{compact} = 1, 3$, and 10 and porosity $\mathcal{P} = 0.33, 0.5$ and 0.9. The refractive indices of compact particles are chosen to be $m_{compact} = 1.20 + 0.00i$, $m_{compact} = 1.33 + 0.01i$, $m_{compact} = 1.68 + 0.03i$, $m_{compact} = 1.98 + 0.23i$, and $m_{compact} = 1.75 + 0.58i$. These values are typical of refractive indices of biological particles, dirty ice, silicate, amorphous carbon and soot in the visual part of the spectrum, respectively. The effective refractive indices calculated using Bruggeman mixing rule are given in Table 3 in [2].

Some results for aggregates with Rayleigh inclusions are shown in Figs. 1 and 2. It is seen that satisfactory agreement between the effective model and DDA computations is obtained for almost all scattering angles excluding deep minima. As usual, the agreement improves for particles with smaller size parameters, smaller values of refractive index and smaller porosity. If we are restricted to porosity $\mathcal{P} = 0.33$, the deviations in calculated intensity do not exceed ~ 5%, ~ 15% and ~ 25% for $x_{compact} = 1, 3$, and 10, respectively. For very porous particles (right panels in Figs. 1 and 2) the difference between the effective model and DDA computations becomes rather large for scattering angles $\Theta \ge 100^{\circ}$ (for $x_{compact} = 10$ this occurs for $\Theta \ge 60^{\circ}$) This is not unexpected, since diffraction plays a major role for small scattering angles, and this depends primarily on the external morphology of the particle. At larger scattering angles, the internal composition plays a larger role.

Figure 3 illustrates the behaviour of angular scattered characteristics for aggregates with Rayleigh and non-Rayleigh inclusions. More or less similar behaviour of intensity and polarization takes place for porosity $\mathcal{P} = 0.33$ only. For $\mathcal{P} = 0.9$ the model of *n*-layered spheres gives satisfactory agreement only in the case of forward intensity and backscattering polarization. However, we expect that the deviations decrease after the averaging over size distribution because in this case, the minima become washed out (see, for example, discussion in [9]).

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Figure 1: Intensity and polarization of the scattered radiation calculated for pseudospheres with small inclusions (DDA computations) and effective models (Bruggeman–Mie computations). The refractive indices of the inclusions are $m_{\text{compact}} = 1.33 + 0.01i$, the size parameter is $x_{\text{compact}} = 3$, the porosity of particles $\mathcal{P} = 0.33$ (left) and $\mathcal{P} = 0.9$ (right).



Figure 2: The same as in Fig. 1 but now for refractive index $m_{\text{compact}} = 1.75 + 0.58i$.



Figure 3: Intensity and polarization of the scattered radiation calculated for pseudospheres with small and large inclusions (DDA computations) and effective models (*n*-layered spheres). The refractive indices of the inclusions are $m_{\text{compact}} = 1.33 + 0.01i$, the size parameter is $x_{\text{compact}} = 3$, the porosity of particles $\mathcal{P} = 0.33$ (left) and $\mathcal{P} = 0.9$ (right).

References

- [1] N. V. Voshchinnikov, V. B. Il'in, and Th. Henning, "Modelling the optical properties of composite and porous interstellar grains", Astron. Astrophys., **429**, 371–381 (2005).
- [2] N. V. Voshchinnikov, G. Videen, and Th. Henning, "Effective medium theories for irregular fluffy structures: aggregation of small particles," Applied Optics, 46, 4065–4072 (2007).
- [3] N. V. Voshchinnikov, "Optics of Cosmic Dust. I", Astrophys. & Space Phys. Rev., 12, 1–182 (2004).
- [4] N. Maron and O. Maron, "Criteria for mixing rules application for inhomogeneous astrophysical grains", Monthly Notices Roy. Astron. Soc., in press ([arXiv:0712.3796]).
- [5] L. Kolokolova, and B. Å. S. Gustafson, "Scattering by inhomogeneous particles: microwave analog experiments and comparison to effective medium theory", J. Quant. Spectrosc. Rad. Transfer, 70, 611– 625 (2001).
- [6] M. J. Wolff, G. C. Clayton, and S. J. Gibson, "Modeling composite and fluffy grains. II. Porosity and phase function", Astrophys. J., 503, 815–830 (1998).
- [7] M. Kocifaj, and G. Videen, "Optical behavior of composite carbonaceous aerosols: DDA and EMT approaches", J. Quant. Spectrosc. Rad. Transfer, **109**, 1404–1416 (2008).
- [8] B. T. Draine, and P. J. Flatau, "User Guide for the Discrete Dipole Approximation Code DDSCAT.6.0," [astro-ph/0309069] (2003).
- [9] M. I. Mishchenko, L. D. Travis, and A. A. Lacis, "Scattering, Absorption, and Emission of Light by Small Particles," Cambridge University Press (2002).