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Note

Scattering properties of heterogeneous mineral particles with absorbing inclusions

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ABSTRACT

We analyze the results of numerically exact computer modeling of scattering and absorption properties of randomly oriented polydisperse heterogeneous particles obtained by placing microscopic absorbing grains randomly on the surfaces of much larger spherical mineral hosts or by imbedding them randomly inside the hosts. These computations are paralleled by those for heterogeneous particles obtained by fully encapsulating fractal-like absorbing clusters in the mineral hosts. All computations are performed using the superposition *T*-matrix method. In the case of randomly distributed inclusions, the results are compared with the outcome of Lorenz–Mie computations for an external mixture of the mineral hosts and absorbing grains. We conclude that internal aggregation can affect strongly both the integral radiometric and differential scattering characteristics of the heterogeneous particle mixtures.

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1. Introduction

Mineral particles are abundant in various natural and artificial environments and are often characterized using non-invasive optical techniques (see, e.g., Refs. [1–4] and references therein). Therefore, accurate numerical modeling of their scattering and absorption properties (such as the optical cross sections, single-scattering albedo, and scattering matrix) can be important in various fields of science and engineering. Quite often mineral particles have attached or imbedded absorbing impurities, which can make the calculation of their scattering and absorption properties rather involved. Whether the scattering and absorption characteristics of an external mixture of "independently scattering" mineral hosts and absorbing contaminants change upon aggregation depends on the strength of the resulting electromagnetic interaction between the mineral and absorbing components, which are now in direct physical contact instead of being widely separated. This interaction and the accompanying optical effects are still poorly studied and so warrant a special analysis.

Previously, in Ref. [5], we discussed potential effects caused by the adherence of small strongly absorbing grains to the surfaces of larger mineral hosts (so-called semi-external mixing [6]), as opposed to the scenario when the hosts and the grains are all widely separated (i.e., externally mixed [6]), and these effects were shown to be quite substantial. In this Note, we consider the case of internal mixing [6], wherein the absorbing grains are imbedded randomly in a larger silicate host, and compare the traits of light scattering characteristics of such heterogeneous particles with those studied in Ref. [5]. Also, we analyze the results of computations performed for a compound particle obtained by arranging the absorbing inclusions into a fractal-like cluster fully imbedded in a silicate host.

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2. Modeling methodology

We consider three models of compound particles, each consisting of a relatively large spherical mineral host which:

(i) is dusted by identical, small, non-overlapping, absorbing spherical grains (Model A);
(ii) is randomly filled with identical, small, non-overlapping, absorbing spherical grains (Model B); or
(iii) encapsulates a fractal-like cluster composed of identical, small, touching, absorbing spherical grains (Model C).

The attraction of these models consisting of only spherical components is that they allow one to isolate unequivocally the scattering effects of the host shape from the effects of the host being mixed with grains of another size and refractive index. In order to generate such scattering targets, we use random-number subroutines that create fixed quasi-random and quasi-uniform configurations of small grains while ensuring that the grains do not overlap and lie on the surface of the host or are imbedded inside the host without crossing its boundary. Fig. 1 illustrates these models of compound particles.

It is assumed that a small polydisperse group of such heterogeneous particles is illuminated by a parallel quasi-monochromatic beam of light and that the observation point is located sufficiently far from the group (e.g., Chapter 14 of Ref. [7]). It is also assumed that all scattering and absorption characteristics are averaged over the uniform orientation distribution of the resulting host–grains configurations with respect to the laboratory reference frame. The transformation of the Stokes parameters I, Q, U, and V caused by electromagnetic scattering by the polydisperse group of compound particles is then written in terms of the normalized Stokes scattering matrix [7,8]:

$$\begin{bmatrix} I^{\text{sca}} \\ Q^{\text{sca}} \\ U^{\text{sca}} \\ V^{\text{sca}} \end{bmatrix} \propto \begin{bmatrix} a_1(\theta) & b_1(\theta) & 0 & 0 \\ b_1(\theta) & a_2(\theta) & 0 & 0 \\ 0 & 0 & a_3(\theta) & b_2(\theta) \\ 0 & 0 & -b_2(\theta) & a_4(\theta) \end{bmatrix} \begin{bmatrix} I^{\text{inc}} \\ Q^{\text{inc}} \\ U^{\text{inc}} \\ V^{\text{inc}} \end{bmatrix}, \tag{1}$$

where $\theta \in [0^\circ, \ 180^\circ]$ is the angle between the incidence ("inc") and scattering ("sca") directions, while both Stokes column vectors are defined with respect to the scattering plane. In our notation, the zeros denote the scattering matrix elements negligibly small (in the absolute-value sense) relative to the nonzero elements at the same scattering angles. The (1,1) element, $a_1(\Theta)$, is called the phase function and satisfies the integral normalization condition

$$\frac{1}{2}\int_0^\pi a_1(\theta) \sin\,\theta \, d\theta = 1. \tag{2}$$

The elements of the scattering matrix (1) can be used to identify specific optical observables corresponding to different types of polarization state of the incident radiation. For example, if the incident beam is unpolarized then the phase function characterizes the angular distribution of the scattered intensity, while the ratio $-b_1/a_1$ gives the degree of linear polarization of the scattered light. In the case of linearly polarized incident light, the ratio a_2/a_1 can serve as an indicator of nonsphericity of the scattering particles (e.g., [7,8]).

The specific morphologies of the three models of compound aerosols allow us to compute all their scattering and absorption characteristics using the highly efficient and numerically exact superposition T-matrix method [9,10] implemented in the form of the public-domain parallelized FORTRAN program MSTM Version 3.0 [11]. To eliminate oscillations typical of monodisperse particles [7,8], we average all scattering and absorption characteristics over a standard power-law size distribution

$$n(R) = \begin{cases} \text{constant} \times R^{-3}, & R_1 \le R \le R_2, \\ 0, & \text{otherwise.} \end{cases} \tag{3}$$

Another benefit of size averaging is that it yields a better quantitative representation of polydisperse particle ensembles typically encountered in natural and artificial environments.

3. Numerical modeling and discussion

3.1. Mixtures of host particles with randomly distributed small grains

In order to identify distinct optical effects of absorbing grains randomly imbedded in mineral hosts, all computations were performed for the same parameter values as in Ref. [5]. Specifically, the ratio of the radius of a mineral host to that of small absorbing grains was kept constant at $R/r \equiv 10$. The numerical size averaging according to

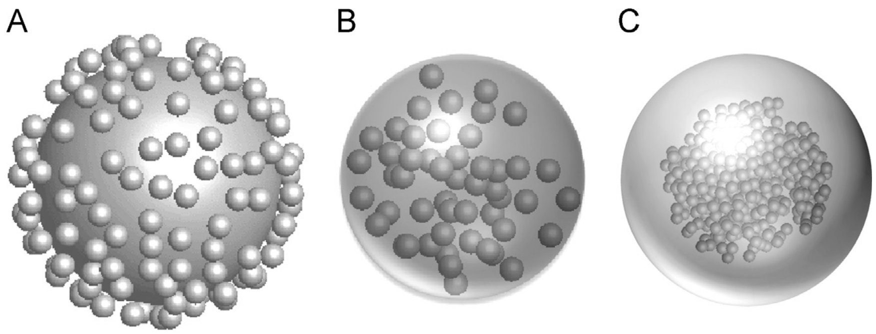

Fig. 1. Three models of compound particles.