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Radiative characteristics of a particle using a bump and pit sphere model

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ABSTRACT

Using the particle superposition method, we constructed a bump and pit sphere model that randomly distributes bumps and pits onto the surface of a wavelength-sized host sphere to simulate a rough particle. We studied both the influence of the imaginary part of the refractive index and the number of dusted grains on the particle's radiative properties and found that the linear polarization and phase function of the particle were sensitive to these two parameters. Changes in the imaginary part of the refractive index caused a regular change in the linear polarization, which was reflected in the number of positive peaks and negative troughs. In addition, the number of dusted grains on the surface of the particle changed the absolute value of the linear polarization, because the linear polarization of a particle with many grains on its surface has a smaller absolute value than a particle with few grains. The backward-scattering region of the phase function became significantly smoother for non-dielectric particles than for dielectric particles. Finally, we analyzed the radiative characteristics of polydisperse compound particles. We found that the optical effects of the ratio of pit number to bump number on the polydisperse compound particles are rather weak, if not negligible.

1. Introduction

Solid-phase particles with untreated surfaces, such as mineral dust in a planetary atmospheres or ice cloud particles, frequently possess rough surfaces [1]. Many studies have investigated the radiative properties of particles, and the effects of overall non-sphericity on a particle's radiative properties has been demonstrated to be highly significant [2–4].

Researchers have studied the effects of microscopic surface irregularities on the radiative properties of particles with sizes that are greater than the incident wavelength by using a geometric optics method [5–9]. However, this method is not suitable for wavelength-sized particles. For these particles, the general method is to solve Maxwell's equations to obtain numerically exact computer solutions. In this study, we present a study of the radiative characteristics of rough wavelength-sized particles using this method.

There are several methods available with which to construct a wavelength-sized rough particle model. One method uses random parameters to define the shape of a particle [10–12]. This model constructs particles that have variable shapes; therefore, it is difficult to tell whether the impact on the particle's radiative characteristics comes from its overall shape or from its rough surface. Another method uses a surface function to simulate the roughness of a particle's surface. One of the first model geometries generated by this method is the Chebyshev model. The non-convex geometries in light scattering studies were previously modeled by Chebyshev particles of low orders [13–16]. The article [17] created the Chebyshev of high orders and found that the optical properties no longer change with any further increase in the values of the order of the Chebyshev polynomial. Next, a Gaussian random sphere model [18] was implemented to create a more complex situation on the basis of Chebyshev particles. This method is convenient for constructing various rough particle models by changing the surface parameters, but there are several computational challenges. In the T-matrix method, the perturbation amplitude can only take on small values. In the DDA method, the microscopic surface irregularities require a large number of dipoles, greatly reducing the speed of the calculation [1].

Another method with which to construct a wavelength-sized rough particle is to dust grains onto the surface of the host sphere to simulate a rough particle. This [19] "dusted" model was introduced to simulate the effect of a rough surface on the radiative properties of wavelength-sized rough particles. These studies found that the effects of microscopic surface irregularities on

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the radiative properties of wavelength-sized particles are relatively weak. In [20], the researchers increased the number of dusted grains and found that the effect of small soot particles adhering to large mineral particles can be dramatic. In [21], the researchers increased the number of dusted grains and changed the complex refractive index, which showed that increasing the real part of the refractive index could make the effects more pronounced. Huang et al. [22] introduced a particle superposition model in which the dusted grains could overlapped either with each other or with the host sphere. These grains could be either bumps or pits in the surface of the model particle. This particle superposition method is a general method by which one can construct different models by changing the size and position of the spheres. In [23], sintering aggregates based on the particle superposition model were constructed. Huang et al. [22] developed four different models: the full sphere bump model; the half sphere bump model; the full sphere pit model; and the half sphere pit model. Huang et al. [22] concluded that the effects of microscopic surface irregularities on wavelength-sized particles cannot be neglected.

The bumps and pits on the surface of particles [24–26] can be observed by viewing the micrographs of particles with small-scale surface roughness. Huang et al. [22] showed that bumps have a different effect than pits on radiative properties. Thus, a model with only bumps or only pits may not fully simulate the radiative properties of wavelength-sized particles. To mimic the realistic small-scale rough particle and provide greater flexibility, we introduced a model that has both bumps and pits. We were not only able to change the number of dusted grains but were also able to control the pit to bump ratio to simulate different rough-surfaced particles. Since the superposition model containing overlapping spheres cannot be calculated by T-matrix code [27], we used the discrete-dipole approximation(DDA) method to calculate this model. In the DDA method, complex models require a long computation time. In many applications, such as satellite retrievals and climate models, simple non-spherical particle models are used to calculate the radiative characteristics quickly. Using bump and pit sphere models for these applications requires a high speed of computation. One of the feasible method is to use graphics processing units (GPUs) to speed the calculation when employing the DDA program. In [28], the authors rewrote their DDA program to include GPUs. These researchers' results illustrated that the GPU version is approximately four times faster than the CPU version.

In this study, we used the CPU version of the DDA program to calculate our model. We changed the value of the imaginary part of the refractive index to analyze the influences of these parameters on the particle's radiative properties.

2. Model and methods

We placed small grains onto the surface of a host sphere to construct the model. These grains included pits and bumps. Pits and bumps had different properties. The properties of pits were identical to those of the circumstance, and the properties of the bumps matched those of the host sphere. The positions of the dusted pits and bumps followed a uniform, random distribution on the surface of the host sphere. The centers of the grains were positioned randomly in the range $[R-r,\ R+r]$ measured from the center of the host sphere (Fig. 1). R and r are the radii of the host sphere and the grain, respectively. The value of R was 1 µm, and R/r was kept constant at 10.

The model was calculated by the DDScat code [29–30]. It was assumed that the model was illuminated by parallel monochromatic light and that all radiative properties were averaged over the uniform orientation distribution of the configuration of the model. For the computations, we used approximately 430 thousand dipoles in the target files describing the model shapes. We can get

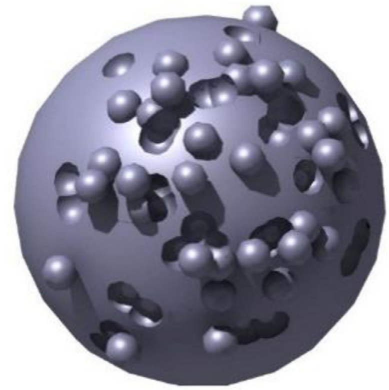

Fig. 1. Bump and pit sphere model.

accurate calculations of the scattering phase function if $d|m|k_0 < 0.5$, where k_0 is the wave number in free space and d is the dipole space [31]. In this article, the accuracy criterion $d|m|k_0 \approx 0.33$ was ensured in each realization. The Stokes parameters were used to measure the scattering and absorption characteristics of the model. The transformation of the Stokes parameters based on the incident and scattered Stokes vectors were written in matrix form [3] as:

$$\begin{bmatrix} I^{sca} \\ Q^{sca} \\ U^{sca} \\ V^{sca} \end{bmatrix} = \begin{bmatrix} S_{11}(\theta) & S_{12}(\theta) & 0 & 0 \\ S_{21}(\theta) & S_{22}(\theta) & 0 & 0 \\ 0 & 0 & S_{33}(\theta) & S_{34}(\theta) \\ 0 & 0 & S_{43}(\theta) & S_{44}(\theta) \end{bmatrix} \begin{bmatrix} I^{inc} \\ Q^{inc} \\ U^{inc} \\ V^{inc} \end{bmatrix} \tag{1}$$

where I,Q,U and V are Stokes parameters, and $\theta \in [0°,\ 180°]$ is the angle between the incidence and scattering directions. The elements filled with zeros were negligibly small (in the absolute-value sense) in comparison with the other elements [21]. The $S_{11}(\theta)$ that appears in the matrix is called the phase function.

We changed the number of dusted grains N_g and the ratio of pit number to bump number ε to analyze the effects of different dusted gains on the radiative properties. The values of N_g were 49, 249 and 549, and the values of ε were 0.2, 0.5 and 0.8. The refractive index was set constant at 1.55 and the imaginary part of the refractive index $\mathrm{Im}(m)$ was variable to analyze the effects of $\mathrm{Im}(m)$ on the particle's radiative properties. The wavelength was kept at 0.628 µm.

To analyze the radiative characteristics of polydisperse compound particles, the scattering and absorption characteristics were averaged over the standard power law distribution [3] with an effective radius $R_{eff} = 1$µm and effective variance $\nu_{eff} = 0.05$[21]:

$$n(R) = \begin{cases} const \times R^{-3}, R_{\min} \le R \le R_{\max} \\ 0 \qquad otherwise \end{cases} \tag{2}$$

Considering the computation time of DDA and the effects to eliminate resonance, we used 30 division points and computed the average using the Gauss-Legendre quadrature formula. The corresponding host radii were in the range of 0.661-1.439µm.

3. Results and discussion

3.1. Impact on the degree of linear polarization for incident unpolarized light

Fig. 2 presents the degree of linear polarization P (corresponding to the $-S_{21}/S_{11}$) as a function of phase angle θ and $\mathrm{Im}(m)$. $\mathrm{Im}(m)$ is 0.0003, 0.003, 0.03, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7 and 0.8. One can see that the graphs have similar features: eight red blocks in a "candle flame" shape appear in the places where $\mathrm{Im}(m)$ is small, and the blocks are uniformly distributed throughout the