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The effects of surface roughness on the scattering properties of hexagonal columns with sizes from the Rayleigh to the geometric optics regimes

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ABSTRACT

Effects of surface roughness on the optical scattering properties of ice crystals are investigated using a random wave superposition model of roughness that is a simplification of models used in studies of scattering by surface water waves. Unlike previous work with models of rough surfaces applicable only in limited size ranges, such as surface perturbation methods in the small particle regime or the tilted-facet (TF) method in the large particle regime, ours uses a single roughness model to cover a range in sizes extending from the Rayleigh to the geometric optics regimes. The basic crystal shape we examine is the hexagonal column but our roughening model can be used for a wide variety of particle geometries. To compute scattering properties over the range of sizes we use the pseudo-spectral time domain method (PSTD) for small to moderate sized particles and the improved geometric optics method (IGOM) for large ones. Use of the PSTD with our roughness model is straightforward. By discretizing the roughened surface with triangular sub-elements, we adapt the IGOM to give full consideration of shadow effects, multiple reflections/refractions at the surface, and possible reentrance of the scattered beams.

We measure the degree of roughness of a surface by the variance (σ^2) of surface slopes occurring on the surfaces. For moderately roughened surfaces ($\sigma^2 \leq 0.1$) in the large particle regime, the scattering properties given by the TF and IGOM agree well, but differences in results obtained with the two methods become noticeable as the surface becomes increasingly roughened. Having a definite, albeit idealized, roughness model we are able to use the combination of the PSTD and IGOM to examine how a fixed degree of surface roughness affects the scattering properties of a particle as the size parameter of the particle changes. We find that for moderately rough surfaces in our model, as particle size parameter increases beyond about 20 the influence of surface roughness on the scattering properties of randomly oriented hexagonal particles starts to become evident. Somewhat surprisingly, in calculations using the IGOM certain qualitatively clear differences in patterns of roughness that have the same σ^2 result in negligible difference in scattering effects. The phase matrix elements given by the IGOM for smooth and roughened hexagonal columns with the "large" size parameter 100 agree very well with the PSTD results, and the integral scattering properties given by the PSTD for small-to-moderate sized particles are shown to merge smoothly with those given by the IGOM for moderate-to-large sizes.

1. Introduction

The scattering and absorption of solar radiation and terrestrial thermal emission by atmospheric particles play

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central roles in atmospheric radiative transfer [1–3] and remote sensing applications [4–7], and have a profound impact upon weather and climate processes [8–10]. Laboratory and aircraft-based observations [11–15] indicate that many atmospheric ice crystals and dust particles have some degree of surface roughness. Numerical studies indicate the surface roughness to be important in determining the single-scattering properties of the particles [15–18], and to have significant impact in radiative transfer models and remote sensing.

The effect of surface roughness on light scattering depends on the particle size, refractive index, and surface structure [18–21]. Small-scale surface roughness has significant influence on the backward scattering and single-scattering albedo of small spheres [20], and for large non-spherical ice crystals, surface roughness smooths out maxima in the scattering phase function as well as other elements of the phase matrix [16,22]. In ice cloud retrievals, Yang et al. [23] found the surface roughness to decrease the retrieved optical thickness and to increase the retrieved effective particle size in comparison with smooth particle counterparts. A number of studies have found that simulations of the polarized reflectance using scattering properties of regular smooth particles produce a poor fit with the satellite measurements, while simulations based on particles with inhomogeneity, distortions, or rough surfaces give much better agreement [24–26].

Substantial effort has been devoted to improving our understanding of the single-scattering properties of particles [27–29,10], and to accounting for the influence of such forms of particle complexity as non-sphericity [30–32], inhomogeneity [33], and surface roughness [16,34]. Both in situ and laboratory experimental measurements have been taken to obtain the scattering properties, e.g. extinction and absorption coefficients, phase function and full phase matrix, of ice crystals and mineral dust [12,13,35,36]. A number of numerical methods have been developed to calculate light scattering and absorption properties of non-spherical particles. Commonly used examples are the T-matrix method [37–39], the discrete-dipole approximation method (DDA) [40–42], the finite-difference time domain method (FDTD) [43,44], the pseudo-spectral time domain method (PSTD) [45–48], and such geometric optics methods (GOMs) [49], as the conventional GOM (CGOM) [50] and the improved GOM (IGOM) [51,52].

In distinguishing between various computational methods the potentially confusing terminology "numerically exact" is sometimes used in electromagnetic scattering studies. We will use this terminology, and for clarity explain here what we understand by it. Underlying any computational method is a physical model and a numerical model. The physical model has mathematical expression in differential or integro-differential equations that have "exact" solutions; the numerical models are also expressed as equations, usually in algebraic form, and have "numerical" solutions. The numerical model is designed so that its numerical solution is an approximation of the exact solution of the corresponding physical model, and the closeness of this approximation is controlled by one or more key numerical parameters. In principle (that is, ignoring computational cost and machine-specific issues of round-off error) the numerical parameters can be adjusted to achieve any desired level of accuracy. In the terminology of numerical analysis this property of a numerical scheme is called "convergence." The term "numerically exact" has come to be reserved in electromagnetic scattering studies for a computational method in which the numerical scheme is convergent *and* the exact model is some form of Maxwell's equations.

The T-matrix, DDA, FDTD, and PSTD methods, all solve Maxwell's equations in this "numerically exact" sense, with the parameter controlling some form of spatial resolution. The methods can, aside from considerations of the computational cost that grows with particle size, be applied throughout the entire range of sizes of atmospheric aerosols. In Practice there is an upper limit on size that is determined by the state of the computational hardware available. The various GOMs, on the other hand, are not numerically exact because they involve approximations whose physical justification limits use to "large" particles. While the smallest size for which a GOM can be used depends on particle shape and criteria for acceptability of results, it is uncommon to find these methods useful for size parameters smaller than 20. It is more common, especially in the case of non-spherical particles, to find them the method of choice for size parameters above 100 because they are accurate in this range and are significantly less demanding of computational time than numerically exact methods.

Hence studies of scattering properties that aim to consider the full range of sizes from the Rayleigh to the geometric optics regimes typically use some combination of a numerically exact method and a GOM [30–32]. This is the approach taken in our study: the numerically exact method is the PSTD method and the geometric optics method is the IGOM. In many previous studies of roughened particles the use of the IGOM has not taken much advantage of its full power [53], while our study makes much more use of this power.

In spite of considerable research effort, our knowledge of the microphysical properties and related optical effects of surface roughness remains limited. Previous studies have considered the effect of surface roughness by using either the numerically exact methods, e.g. the FDTD [17], DDA [18], or T-matrix methods [19] for relatively small particles, or the GOMs for particles much larger than the incident wavelength. In the GOM studies no attempts were made to construct a single particle geometry for the scattering calculations: as will be explained in more detail below, each individual ray reaching a point on the particle surface has an interaction with a surface element with orientation that is chosen at random and hence is unique to that *ray*. While the GOM methods have had some successes, the fact that they involve no well-defined surface of the particle makes it challenging to relate results, especially ones using the more sophisticated versions, to any particular kind of surface roughness observed in naturally occurring atmospheric particles, or to any completely defined particle in a numerically exact method. In this study we will employ a model of surface roughness that considers roughness to be "essentially random