



Scattering and absorption of light by ice particles: Solution by a new physical-geometric optics hybrid method

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ARTICLE INFO

Article history:

Received 9 December 2010

Received in revised form

19 February 2011

Accepted 21 February 2011

Available online 4 March 2011

Keywords:

Light scattering

Geometric optics

Physical optics

Hexagonal ice crystal

ABSTRACT

A new physical-geometric optics hybrid (PGOH) method is developed to compute the scattering and absorption properties of ice particles. This method is suitable for studying the optical properties of ice particles with arbitrary orientations, complex refractive indices (i.e., particles with significant absorption), and size parameters (proportional to the ratio of particle size to incident wavelength) larger than ~ 20 , and includes consideration of the edge effects necessary for accurate determination of the extinction and absorption efficiencies. Light beams with polygon-shaped cross sections propagate within a particle and are traced by using a beam-splitting technique. The electric field associated with a beam is calculated using a beam-tracing process in which the amplitude and phase variations over the wavefront of the localized wave associated with the beam are considered analytically. The geometric-optics near field for each ray is obtained, and the single-scattering properties of particles are calculated from electromagnetic integral equations. The present method does not assume additional physical simplifications and approximations, except for geometric optics principles, and may be regarded as a “benchmark” within the framework of the geometric optics approach. The computational time is on the order of seconds for a single-orientation simulation and is essentially independent of the size parameter. The single-scattering properties of oriented hexagonal ice particles (ice plates and hexagons) are presented. The numerical results are compared with those computed from the discrete-dipole-approximation (DDA) method.

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1. Introduction

The scattering and absorption of light by nonspherical ice particles has been of great interest in the atmospheric radiation research community. Over the past several decades, steady improvements have been made in the numerical modeling of the scattering and absorption of light by nonspherical particles [1–5]. Rigorous techniques developed for

various applications involving electromagnetic scattering by nonspherical particles include the T-matrix method [6–8], the finite-difference time-domain (FDTD) method [9–11], and the discrete-dipole-approximation (DDA) method [12–15]. Although these exact methods are efficient for the calculation of the optical properties of ice particles with small size parameters ($\kappa = 2\pi r/\lambda$, where r is radius and λ is wavelength), they are impractical and computationally inefficient for large size parameters ($\kappa > 20$). In practice, the most effective approach to deriving the solution to light scattering by ice particles over a large size parameter range is a combination of exact numerical techniques for small

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particles and other methods based on the geometric optics approximation for moderate-to-large sized particles [16,17].

The conventional geometric optics method (CGOM) is based on a straightforward combination of the ray-tracing technique and Fraunhofer diffraction to calculate the angular distribution of the far-field scattered energy and polarization state of the radiation field [18–21]. The advantages of the CGOM are its formalism simplicity and numerical simulation efficiency. However, there are some inherent limitations in the CGOM that limit its applicability to randomly oriented particles with large (> 100 – 200) size parameters. The CGOM is not well suited for calculations of oriented ice particles. Another limitation is that the ray spreading effect in the forward scattering angles is not considered. Additionally, the edge effects [22] are not properly considered in deriving extinction and absorption efficiencies. Research to improve the accuracy of the geometric optics method and to incorporate semi-classical scattering effects in the computation of the single-scattering properties of non-spherical particles has been reported in the literature [23–25].

To circumvent the limitations in the CGOM, several physical-geometric optics hybrid (PGOH) methods have been suggested [26–30]. The PGOH methods calculate the scattered or total near-field (i.e., the electromagnetic field in or near the particle) based on geometric optics principles. The near-field is mapped to the far-field to obtain the single-scattering properties of particles through electromagnetic integral equations. The PGOH methods have been demonstrated to have a better approximation than the CGOM and are applicable to moderate size parameters. However, the applicability of the PGOH methods has not been well quantified because of the lack of a rigorous and efficient numerical algorithm.

The present study employs a beam-splitting technique [28,30] to enhance the PGOH ice particle modeling capabilities. Instead of adopting a large number of straight-line rays (or numerical photons) assumed by most ray-tracing algorithms, the beams that propagate within the particle have well defined polygonal-shaped cross sections. In the beam-tracing process, several facets may intercept a beam, and subsequently the wavefront of the localized wave associated with the beam splits and undergoes Fresnel reflections and refractions on different facets. The advantage of tracing beams with well-defined cross sections is that the total number of beams in the numerical simulation is independent of the size parameter. A distinct advantage of this approach is that the computational time is significantly reduced for particles with large size parameters.

In the present PGOH formulation, the geometric-optics near-field is obtained analytically based on Snell's law and the Fresnel formulae. We further develop a theoretical formalism to calculate the scattered far-field based on an exact near-to-far field transformation. The extinction and absorption efficiency factors are derived based on the optical theorem and an electromagnetic volume integral equation. Note that the near-to-far field transformation is based on an exact electromagnetic integral equation more theoretically rigorous than the Fraun-

hofer diffraction approximation assumed in the previous studies [28,30]. In addition, the variation of the amplitude of the electric field [28] over a beam's cross section is considered. Therefore, the present PGOH algorithm is applicable to absorptive particles.

Briefly stated, the PGOH method herein is suitable for studying the optical properties of ice particles with arbitrary orientations, complex refractive indices, and size parameters larger than ~ 20 . To examine the accuracy of the present method, we compare results with those computed from the DDA method. From an application perspective, ice particle orientation and ice habit geometry are the two issues of the most concern to studies associated with ice cloud radiative properties [31–33]. To demonstrate the benefits of the present method for studying the two issues, we model the effect of preferentially oriented ice plates on the backscattering properties and the effect of hexagonal ice particle geometries on the angular distribution of scattered light.

This paper is organized into six sections. Section 2 outlines the theory of the present PGOH method including the beam-splitting algorithm, the representation of geometric-optics near-field, and the PGOH formalism for the single-scattering properties. Section 3 compares the representative results simulated from the PGOH and DDA methods, and discusses the accuracy of the PGOH simulations and the deviations from their DDA counterparts. In Section 4, the present PGOH algorithm is applied to model the effects of preferable orientations of hexagonal ice particles on their optical properties, and we focus on the two quantities, backscattering efficiency and color ratio. In Section 5, we discuss the approach to modeling imperfect hexagonal ice particles and how the lack of ice particle perfection affects the phase function. The concluding remarks are given in Section 6.

2. Theoretical basis

The three components of the present PGOH method include: (1) tracing beams within a particle based on the beam-splitting algorithm, (2) specifying the electric field and polarization state of each beam, and (3) calculating the optical properties of a particle (phase matrix, extinction efficiency, and absorption efficiency) based on electromagnetic integral equations. For algorithm simplicity, the particle is assumed to be dielectric, isotropic, and homogenous, and the geometry of a particle is assumed to be convex and faceted. Concave particles are not considered in this study. Moreover, the time dependence of a harmonic electromagnetic wave is assumed to be $\exp(-i\omega t)$, leading to a positive imaginary part of the refractive index in the case of absorptive particles.

2.1. Beam-splitting algorithm

When a plane wave of light is incident on a faceted particle, the portion of the wavefront of the incident electromagnetic wave that is intercepted by the projected geometric cross section of the particle subsequently splits into several parts. As a wavefront (or localized wave) impinges on a given facet, the subsequent electromagnetic interaction leads to outgoing reflected and inwardly

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