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OPTICAL PROPERTIES OF NONSPHERICAL ATMOSPHERIC PARTICLES AND RELEVANT APPLICATIONS

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(Invited paper)

ABSTRACT. Recent progress in the study of the single-scattering properties of nonspherical ice crystals within cirrus clouds and nonspherical dust particles is reviewed. We have been using the finite-difference time domain (FDTD) method, the discrete dipole approximation (DDA), and an improved geometric optics method (IGOM) to compute the singlescattering properties of nonspherical particles. We have incorporated the so-called edge effect associated with the surface wave into the IGOM extinction and absorption efficiencies. The simulation results in the solar and thermal infrared spectral regimes are presented. Furthermore, the impacts of particle nonsphericity on downstream remote sensing implementations and radiative transfer simulations involving ice clouds and dust aerosols are also summarized.

1. Introduction

Steady progress has been made in the simulation of the single-scattering properties of nonspherical particles. Specifically, significant improvements have been made on the computational methods and the definitions of more realistic particle morphologies for ice crystals and mineral dust aerosols. In this paper, we review some recent progress in the computational methods, and present typical numerical examples for hexagonal ice crystals.

2. Methods

The finite-difference time-domain (FDTD) [1, 2] and the discrete-dipole-approximation (DDA) [3, 4] are two widely used methods for the solution of light scattering by arbitrarily shaped particles. The two methods are usually employed for the simulation of light scattering by particles of small size parameters. By using advanced computational resources (e.g., supercomputers), the optical properties of moderate-to-large sized particles can be obtained. Our understanding of the accuracy and efficiency of the two methods has been substantially improved in the past several years.

Because of the inefficiency/inapplicability of the FDTD and DDA methods to particles of moderate and large size parameters, we have been developing an approximate method, namely, an improved geometric optics method (IGOM), so that the optical properties of the particles in a wide range of size parameters can be obtained [5, 6]. To validate the IGOM

and understand its range of applicability, a case study regarding the comparison between the IGOM and the FDTD/DDA is carried out for some typical nonspherical morphologies (e.g., hexagonal ice crystals, triaxial ellipsoids, and nonsymmetric hexahedra) defined for ice crystals and mineral dust aerosols. In the computation of the extinction and absorption efficiency factors, the IGOM results are found to be smaller than their counterparts computed from the FDTD/DDA. The differences are interpreted as the edge-effect contribution [7]. The edge-effect contribution has been incorporated into the IGOM solution so that the FDTD/DDA results merge with the IGOM counterparts "smoothly" [8, 9].

3. Results

Figure 1 shows a comparison of the six elements of the phase matrix for a hexagonal ice crystal simulated from the FDTD and DDA methods. The aspect ratio (i.e., the width divided by the length) is 0.7. The particle is assumed to be randomly oriented in space. After consideration of 6-fold rotational symmetry and mirror symmetry with respect to top and bottom, 51 orientations are used in the simulation. 18 dipoles per wavelength are set in the DDA simulation, and 25 cells per wavelength are set in the FDTD simulations. As shown in the figure, the results from the two methods are essentially the same with largest differences in the side-scattering directions.



Figure 1. Comparison of six non-zero elements of a randomly oriented hexagonal ice crystal simulated from the FDTD and DDA methods. D is the length of the particle, λ is the wavelength, and $k = 2\pi/\lambda$.

Figure 2 shows a comparison of the phase functions of a hexagonal particle simulated from FDTD and IGOM for two selected refractive indices at the wavelengths of 0.66 and 12 μ m as indicated in the figure. The orientations and the aspect ratio of the particle are the same as those shown in Fig. 1. The scattering patterns simulated from FDTD and the IGOM are similar, although some differences are still noticed in side-scattering directions.

Figure 3 shows the extinction efficiency factor, the single-scattering albedo for hexagonal ice crystals simulated from the DDA, the FDTD, and the IGOM. The results simulated



Figure 2. Comparison of the phase functions of hexagonal ice crystal simulated from from the FDTD and IGOM. D is the length of the particle. k is the wave number.

from DDA agree with the results from the FDTD. After the consideration of the edge effect contribution to the extinction efficiency and absorption efficiency, the extinction efficiency and the single-scattering albedo simulated from the DDA and FDTD methods smoothly merge with the IGOM results in the geometric-optics regimes.



Figure 3. The extinction efficiency and single-scattering albedo for a randomly oriented hexagonal ice crystal simulated from the DDA, FDTD, and IGOM for a complete range of size parameters.

The effect of ice crystal nonsphericity on the optical properties and downstream applications have been extensively investigated, for example, by Yang et al. [10], which has been found to be significant. The optical properties of nonspherical particles have been employed to assess the effect of the nonsphericity of mineral dust aerosols on remote sensing [11]. It is found that neglecting the nonsphericity of dust particles usually leads to an underestimate of retrieved dust aerosol optical depth although an overestimate may be noted in some cases, depending on the scattering angles.

Atti Accad. Pelorit. Pericol. Cl. Sci. Fis. Mat. Nat., Vol. 89, Suppl. No. 1, C1V89S1P012 (2011) [4 pages]

4. Conclusions

We have presented some typical single-scattering properties of hexagonal ice crystals simulated from the DDA, FDTD and IGOM to illustrate the applicability of the three methods to the study of radiative properties of ice crystals and dust aerosols.

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