FINAL REPORT

Project Title: Modeling Single Scattering and Radiative Properties of Cirrus Clouds

Dates Covered: 23 September 1996 – 30 September 1998

Sponsoring Organization: Department of the Navy
Naval Research Laboratory
4555 Overlook Avenue, SW
Washington, CD 20375-5326

Grant No. N00014-96-1-G020

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ABSTRACT

The specific objective of this research has been the development and improvement of theoretical models to simulate the effect of nonsphericity on single-scattering properties of cirrus cloud particles in the visible and infrared spectral regions. First, we have shown that using a matrix inversion scheme based on a special LU factorization rather than on the standard Gaussian elimination significantly improves the numerical stability of T-matrix computations for nonabsorbing and weakly absorbing nonspherical particles. Second, we use exact T-matrix computations and the Kirchhoff approximation to show that the δ-function transmission peak predicted by the GO approximation for hexagonal ice crystals is an artifact of GO completely ignoring physical optics effects and must be convolved with the Fraunhofer pattern, thereby producing a phase function component with an angular profile similar to the standard diffraction component. Third, we have used the improved *T*-matrix method to compute the linear depolarization ratio for polydispersions of randomly oriented ice spheroids, circular cylinders, and Chebyshev particles with sizes typical of young contrails. We have shown that ice crystals with effective radii as small as several tenths of a micron can already produce δ exceeding 0.5 at visible wavelengths.

INTRODUCTION

This research project was intended to deliver crucial modeling products for use in the project headed by Dr. B.-C. Gao and called "Cirrus Cloud Characterization and Correction." It is well known that the accuracy of determining the cirrus cloud optical thickness and correcting the effect of cirrus on the retrieved aerosol and lower-cloud optical thicknesses and surface reflectance critically depends on the accuracy of modeling the cirrus cloud particle single-scattering properties, first of all the scattering phase function. The knowledge of the phase function is also crucially important in an accurate evaluation of the radiative effect of cirrus on climate. Cirrus clouds consist of ice particles having an wide variety of shapes. For typical cirrus environments ice crystals exist both in single and aggregated forms, and the surface of the ice particles can be highly irregular. Because of ignorance about the distribution of cirrus particles over shapes, knowledge of cirrus scattering phase function has progressed very slowly. Theoretical phase function calculations have mostly assumed that cirrus ice particles are spheres or randomly-oriented, infinitely-long circular cylinders; this remains a common assumption both in global climate models and in satellite retrieval algorithms. The geometric-optics hexagonal-crystal phase functions of Takano and Liou have become quite popular, but do not seem to fit the known facts very well. Phase function calculations for small ice particles have been difficult and computationally intensive.

Because of these factors, the focus of this research during the period 23 September 1996 – 30 September 1998 was on further development and use state-of-the-art numerical techniques for computing scattering properties of nonspherical ice crystals. The specific objective has been the development and improvement of theoretical models to simulate the effect of nonsphericity on single-scattering properties of cirrus cloud particles in the visible and infrared spectral regions.

IMPROVEMENTS OF THE T-MATRIX METHOD

The Waterman's T-matrix approach is one of the most powerful exact techniques for computing light scattering by nonspherical particles based on solving Maxwell's equations. However, even this method can exhibit convergence problems when any of the variables defining the scattering particle (size parameter, deviation from sphericity, refractive index) becomes too extreme. Standard T-matrix computations become especially ill-conditioned for particles with a small or zero imaginary part of the refractive index because of the strong effect of the ripple structure. For example, the maximum convergent equivalent-sphere size parameter (i.e., the ratio of particle circumference to wavelength of scattered light for the surface-equivalent sphere) in double-precision FORTRAN computations for oblate spheroids with refractive index 1.53 and aspect ratio 2 is only 8, whereas the maximum convergent size parameter for the same particles but with a moderately absorbing refractive index of 1.53 + 0.001i is 33.

The origin of the numerical instability of the standard T-matrix procedure for extreme values of particle characteristics can be explained as follows. Calculations based on the extended boundary condition method (EBCM) assume the representation of the T-matrix in the form $\boldsymbol{T} = -\boldsymbol{Q}^{-1}\,\mathrm{Rg}\boldsymbol{Q}$, where the elements of the matrices $\boldsymbol{Q}$ and Rg$\boldsymbol{Q}$ are integrals over the particle surface. The numerical inversion of the matrix $\boldsymbol{Q}$ is usually performed using the standard Gaussian elimination (GE). Unfortunately, the calculation of the inverse matrix $\boldsymbol{Q}^{-1}$ is an ill-conditioned procedure strongly affected by round-off errors and by the fact that different elements of the $\boldsymbol{Q}$ matrix can differ by many orders of magnitude. As a result, T-matrix computations for extreme particle parameters can be poorly convergent and even divergent.

This sensitivity of the standard T-matrix procedure to weak or zero absorption has been a serious limiting factor since many commonly encountered substances are weakly absorbing in some spectral ranges. The example of water ice in the visible is particularly important because quite often a significant fraction of cirrus and contrail ice particles are not much larger than a visible wavelength, thus potentially precluding the use of the geometric optics approximation (GO) in light scattering computations.

During the course of this research, we have significantly improved the T-matrix technique for computing light scattering by nonspherical ice crystals. Specifically, we have shown that using a matrix inversion scheme based on a special LU factorization rather than on the standard Gaussian elimination significantly improves the numerical stability of T-matrix computations for nonabsorbing and weakly absorbing nonspherical particles. We have also developed an improved scheme for evaluating Clebsch-Gordon coefficients with large quantum numbers which allowed us to extend the analytical orientational averaging method developed by Mishchenko [J. Opt. Soc. Am. A **8**, 871 (1991)] to larger size parameters. As a result, the maximum convergent size parameter for particles with small or zero absorption can increase by a factor of several and can exceed 100. The ability of the new T-matrix scheme to treat such large size parameters is accompanied by an extremely high numerical efficiency which makes our code orders of magnitude faster than any alternative technique for exactly computing light scattering by nonspherical particles in random orientation. The unique capabilities of the T-matrix code make it very useful in practice, but also make difficult checks of its numerical accuracy since independent results for the largest size parameters cannot be obtained with any other currently available method. Therefore, we have paid special attention to making sure that our calculations fully satisfy such fundamental physical constraints as symmetry, reciprocity, and energy conservation. Also, we have computed benchmark results for a challenging test case that can be used for checking the accuracy of the most advanced nonspherical scattering codes at higher frequencies.

Using the present version of the T-matrix code, we have extended comparisons of exact T-matrix and approximate ray tracing calculations to much larger size parameters and to all elements of the scattering matrix. Our results suggest that equivalent-sphere size parameters larger than about 80 are already big enough to ensure acceptable accuracy of GO phase function computations (except, perhaps, at exactly the backscattering direction). However, GO calculations of the other elements of the scattering matrix are stronger affected by wave effects and become reasonably accurate only at significantly larger size parameters. GO calculations of lidar depolarization can be expected to be especially inaccurate unless the equivalent-sphere size parameter exceeds several hundred.

An interesting result of our calculations is that the T-matrix method can be successfully applied to large sharp-edged particles such as finite circular cylinders with equivalent-sphere size parameters exceeding 100. It has been often claimed that the presence of sharp edges can be difficult to handle with a method that uses "smooth" spherical functions in the internal and scattered field decompositions. We have found, however, that the use of a special numerical integration scheme for computing the surface integrals needed to calculate the T matrix ameliorates the problem of sharp edges and makes T-matrix computations for cylinders almost as accurate as those for surface- and aspect-ratio-equivalent smooth-shaped spheroids. Much more difficult problems are encountered when the T-matrix method is applied to particles with large aspect ratios. In this case a single spherical function expansion of the internal and scattered fields can fail, and the use of several overlapping subdomain spherical function expansions may become necessary.

We published a user guide describing in detail a software implementation of the current version of the *T*-matrix method for computing light scattering by polydisperse, randomly oriented, rotationally symmetric particles. The FORTRAN *T*-matrix codes are publicly available on the World Wide Web at http://www.giss.nasa.gov/~crmim. We provided all necessary formulas, described input and output parameters, discussed numerical aspects of *T*-matrix computations, demonstrated the capabilities and limitations of the codes, and discussed the performance of the codes in comparison with other available numerical approaches.

This research was published in Refs. 1 and 2 below.

INCORPORATION OF PHYSICAL OPTICS EFFECTS INTO RAY-TRACING PHASE FUNCTIONS COMPUTED FOR HEXAGONAL ICE CRYSTALS

It is well known that a convenient way of representing the scattering phase function $P(\Theta)$ for aerosol and cloud particles is expanding it in Legendre polynomials as

where Θ is the scattering angle, $P_n(\cos\Theta)$ are Legendre polynomials, and the value of the upper summation limit n_{max} depends on the desired numerical accuracy of the expansion.

$$P(\Theta) = \sum_{n=0}^{n_{max}} x_n \, P_n(\cos\Theta), \tag{1}$$

Since the number of numerically significant terms in the Legendre expansion is finite and often relatively small, this expansion can be used for efficiently computing the phase function for essentially any number of scattering angles with a small consumption of CPU time. Furthermore, the Legendre expansion coefficients x_n can be used to directly compute the Fourier components of the phase function via simple and exact analytical formulas, which is the first step in radiative transfer computations using different numerical techniques.

The Legendre expansion coefficients for the widely used Henyey-Greenstein phase function are given by the simple analytical formula

$$x_n = (2n+1) g^n, \tag{2}$$

where g is the asymmetry parameter. Efficient analytical methods based on solving Maxwell's equations exist for computing the expansion coefficients for spherical particles and randomly oriented, rotationally symmetric nonspherical particles. For irregular particles with sizes much larger than the wavelength of the incident radiation, such as cirrus cloud particles in the visible, direct numerical solutions of Maxwell's equations do not currently exist. Therefore the expansion coefficients have to be computed using an approximate technique such as the geometric optics approximation (GO). Using the orthogonality property of Legendre polynomials, we easily derive from equation (1)

$$x_n = \frac{2n+1}{2} \int_0^{\pi} d\Theta \, P(\Theta) \, P_n(\cos\Theta) \sin\Theta . \tag{3}$$

The integral in equation (3) can be calculated numerically by using a quadrature formula provided that the phase function values at the division points are known. This numerical approach works well if the phase function is rather smooth but becomes problematic for particles having parallel planes such as hexagonal columns and plates or finite circular cylinders. In this case, the standard GO predicts a strong, infinitesimally narrow peak in the exact forward-scattering direction which is caused by rays that undergo two refractions through parallel plane facets and is superimposed on the diffraction component of the phase function. This effect was called by Takano and Liou the δ-function transmission.

It is obvious, however, that GO predicts the infinitesimally narrow δ-function transmission peak only because it completely ignores physical optics effects. Simple physical optics considerations cause us to conclude that although a strong non-diffraction forward-scattering peak does exist and can be qualitatively explained in GO terms as a manifestation of the δ-function transmission, it nonetheless has an appreciable angular width comparable to that of the Fraunhofer diffraction peak and a diffraction-like angular profile. It is clear that however large a particle is compared to the wavelength, physical optics effects will preclude the appearance of perfect singularities in the scattering pattern like the δ-function transmission peak in the phase function. Instead, a wave front emerging from a flat crystal facet should spread and produce an angular intensity distribution in the far-field zone similar to the well known Fraunhofer diffraction pattern. Of course, in the theoretical limit of an infinite size parameter the δ-function transmission peak becomes a true δ-function. However, the angular width of the δ-function transmission peak is always comparable to that of the Kirchhoff diffraction component, and as long as the latter is computed explicitly, so should be the δ-function transmission component.

We used exact T-matrix computations for rather large nonspherical particles to demonstrate that the effect that can be interpreted in geometric optics terms as δ-function transmission through parallel planes indeed results in a quasi-Fraunhofer forward-scattering peak rather than in a true δ-function peak. We then developed a very simple numerical procedure which incorporates this physical optics effect in the standard ray tracing procedure for computing the phase function for large particles having parallel plane facets. This procedure not only makes ray tracing computations more physically relevant, but also simplifies and makes more accurate the computation of the phase function and its Legendre expansion. Although the accuracy of our procedure cannot be assessed directly due to the lack of exact theoretical methods based on solving Maxwell's equations and applicable to size parameters exceeding several hundred, our approach is physically-based and appears to be simple and well justified since it consists of directly computing the amount of energy contained in the δ-function transmission peak and convolving it with the Fraunhofer angular pattern.

This research was summarized in Ref. 3 below.

Depolarization of lidar returns by small ice crystals

Because of intensifying air traffic, there has been increasing interest in the potential impact of aircraft condensation trails (contrails) on climate through a direct radiative forcing. The estimation of the climatic effect of contrails requires knowledge of their radiative properties, which can be substantially different from those of ambient cirrus clouds. The latter, in turn, necessitates the determination of the size and shape distribution of contrail particles and their time evolution using in situ and/or remote sensing techniques.

Measurements of the lidar linear depolarization ratio δ can be a powerful remote sensing technique for characterizing the microphysics of contrail particles. Since young contrails often consist of relatively small ice crystals, the quantitative interpretation of lidar measurements requires accurate theoretical computations of δ for polydisperse, randomly oriented nonspherical particles with size parameters ranging from zero to at least several tens, thus ruling out most of the currently available numerical techniques. We used the recently improved T-matrix method and computed δ for polydispersions of randomly oriented ice spheroids, circular cylinders, and Chebyshev particles with sizes typical of young contrails. We showed that ice crystals with effective radii as small as several tenths of a micron can already produce δ exceeding 0.5 at visible wavelengths. This may explain the frequent occurrence of large δ values for very young contrails. We also showed that observed increases of δ with the contrail's age can be explained either by a rapid increase of the particle size parameter from essentially zero to about 5 or by assuming that the contrail particles originate as perfect spheres and then acquire a certain degree of asphericity.

This research was summarized in Ref. 4.

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REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY *(Leave blank)*	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
		Final Report: 23/09/96-30/09/98

4. TITLE AND SUBTITLE
Modeling Single Scattering and Radiative Properties of Cirrus Clouds

5. FUNDING NUMBERS
N00014-96-1-G020

6. AUTHORS
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7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
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8. PERFORMING ORGANIZATION REPORT NUMBER

8. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
Department of the Navy
Naval Research Laboratory
4ok Avenue. SW
Washington, DC 20375-5326

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION/AVAILABILITY STATEMENT

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*

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14. SUBJECT TERMS

15. NUMBER OF PAGES
10

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT