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Comparison of measured and computed phase functions of individual tropospheric ice crystals

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ABSTRACT

Airplanes passing the incuda (lat. *anvils*) regions of tropical cumulonimbi-clouds are at risk of suffering an engine power-loss event and engine damage due to ice ingestion (Mason et al., 2006 [1]). Research in this field relies on optical measurement methods to characterize ice crystals; however the design and implementation of such methods presently suffer from the lack of reliable and efficient means of predicting the light scattering from ice crystals. The nascent discipline of direct measurement of phase functions of ice crystals in conjunction with particle imaging and forward modelling through geometrical optics derivative- and Transition matrix-codes for the first time allow us to obtain a deeper understanding of the optical properties of real tropospheric ice crystals. In this manuscript, a sample phase function obtained via the Particle Habit Imaging and Polar Scattering (PHIPS) probe during a measurement campaign in flight over Brazil will be compared to three different light scattering codes. This includes a newly developed first order geometrical optics code taking into account the influence of the Gaussian beam illumination used in the PHIPS device, as well as the reference ray tracing code of Macke and the T-matrix code of Kahnert.

1. Introduction

It has been known since the mid-90s that the incus region of tropical cumulonimbus clouds poses a certain threat to commercial jet-powered aircraft [2]. The dominant types of particles under these atmospheric conditions are ice crystals and ice crystal aggregates [1]. Thus, measurement devices capable of acquiring specific data about the ice particles in flight, which are robust and compact enough for use in commercial airliners, are highly desirable. As a prerequisite for the use of optical measurement devices, similar to those already employed for monitoring liquid water droplets in aerodynamic flows [3], a numerical forward model of the laser-light scattering by a single ice crystal is required and has been developed. From the perspective of atmospheric physics, it is likewise desirable to acquire an understanding of real atmospheric ice crystals that is as complete as possible, for instance in order to accurately predict the terrestrial radiation budget, as explained in the books by Chandrasekhar and Yang et al. [35,4]. To this end, the Particle Habit Imaging and Polar Scattering probe was developed at the Karlsruhe Institute of Technology, which is capable of simultaneously measuring the polar phase function and capturing the generating particle shape via stereoscopic imaging. A comprehensive description of the construction and working principle of the probe is given in the article [5]. While the basic idea is not new, the practical realization of phase function measurements has only recently come to fruition. First efforts include e.g. the work of Ulanowski in 2005 [6], who has worked with sodium fluorosilicate ice crystal analogues. The most recent and carefully

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conducted laboratory measurements of water ice crystal phase functions generated in the Manchester ice cloud chamber have been published by Smith et al. [7]. The work described in the present manuscript goes beyond previous publications, as for the first time phase functions of individual *real* tropospheric ice crystals obtained during a measurement campaign over Brazil are considered. The PHIPS probe correlates the phase function to the precise shape of the particle generating it, which is in contrast to the study [7] of Smith, who had to rely on size and shape averaged distributions of ice crystals generated in the laboratory under idealized thermodynamical conditions. In order to predict the measurement outcome, three different calculation approaches are considered. First of all, the ray tracing code [8,10] of Macke is used as a reference method. This code may treat arbitrary concave particles, but only considers perfectly incoherent incident radiation in the form of a plane wave. As a theoretically exact method, the T-matrix code [9] of Michael Kahnert was considered for the problem at hand. Unique amongst other T-matrix formulations, Kahnert's code exploits the fact that the transition operator $\hat{\mathbf{T}}$ does commute with representations of the discrete symmetries of the scattering particle, in order to speed up the calculations. Nevertheless it has been found that the size of the measured particles as discussed in Section 7 is beyond the range of applicability of the code. Consequently, the computed T-matrix phase function has been discarded. Further possible light scattering codes which have not been considered in this study include the Improved Geometrical Optics code [11] by Yang and Liou, as well as the Invariant Imbedding T-matrix code by Bi and Yang [12]. Finally, as none of the above mentioned codes takes shaped beam incidence such as the laser used in the PHIPS probe into account, a separate first-order geometrical optics code has been developed and will be presented in this manuscript. In the following, Sections 2–4 of the manuscript explain how first-order geometrical optics is applied to prismatic ice crystals. Section 5 explains the description of the Gaussian beam, while Sections 6 and 7 provide the validation of the new code and the final comparison between all three codes and the measurement data, respectively.

2. Algorithm overview

This second section gives an overview of the workflow of the Geometrical Optics code which essentially relies on Ray Tracing to compute the scattered electromagnetic field. The following list enumerates all calculation steps in the same order as they are executed in the code.

1. Both laser beam and scattering particle as physical entities are initialized as computational objects, given their relevant properties, such as the frequency ω of the incident monochromatic light.
2. The user defines a *transition plane* between the two models of the laser beam as an electromagnetic field and as a bundle of straight rays. All geometric rays involved in the calculation will be emanating from this surface. In all calculations, this surface was chosen to be identical with the illuminated surface of the scattering particle.
3. On this surface, a starting point $\mathbf{x}_0$ is chosen, from which a light ray starts in the direction $\hat{\mathbf{k}}$. For reasons explained in Section 5, this point will be chosen at random.
4. All other initial properties necessary for the definition of a Geometrical Optics light ray, such as initial electric field vector $\mathbf{E}_0$, initial phase φ_0, initial wave front curvature matrix Q and initial wave vector $\hat{\mathbf{k}}$ are calculated from the given electromagnetic field of the laser beam at the chosen starting point $\mathbf{x}_0$. The necessary formulae for this calculation are also explained in Section 5.
5. An intersection check between the ray and the surfaces of the scattering particle is performed. The properties of the ray at the intersection point are calculated.
6. At the intersection point, a reflected and a refracted sub-ray or ray segment are created. The new direction, electric field and wavefront curvature matrix of the reflected and refracted ray are calculated using Descartes' law, the Fresnel equations for the electromagnetic amplitudes and a transfer equation for the curvature matrix. These new ray segments are connected to a *binary tree* together with the incident ray segment. The very first ray segment of a ray tree which depends on the properties of the shaped beam is called the *root* segment. This is illustrated schematically in Fig. 1 below.
7. If the reflected or refracted sub-ray does not interact with the scatterer again, its outgoing direction and electric field vector are stored in an array.
8. If the sub-ray does not leave the scatterer, a new intersection check with the scatterer surface is performed and the Ray Tracing procedure starts again at point 5. The process will be repeated recursively, until a given scattering order has been reached. The tracing of the ray segments is illustrated in Fig. 2.
9. When the Ray Tracing for a single ray-tree has been completed, the process starts again at point 3 for another ray-tree, until a large number ($\mathcal{O}(10^3)$) of ray-trees have been calculated.
10. After the Ray Tracing has been completed, the distribution of the scattered electric field over a spherical coordinate system enclosing the scatterer will be calculated. Given the direction of each outgoing ray, its corresponding electric field vector will be added to an angular bin in the spherical coordinate system. It is understood that this approach does not create a continuous distribution of the scattered electric field, but rather a histogram that approaches a continuous distribution for decreasing angular bin size.

If not only results for a single orientation in space of the scattering particle are desired, the algorithm above can be repeated for a large number of random particle orientations. The proper results of each individual orientation will then be sampled to obtain a statistical result.

The Geometrical Optics code also has several limitations depending on its application case. It only allows monochromatic light and thus cannot consider a moving scatterer or a pulse of incident radiation. It also does not include diffraction, as the Mie parameter of the scattering problem is assumed to be very high.