Database of scattering properties of small ice crystals: implications for satellite retrieval algorithms and numerical models

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2. Executive Summary

Ice clouds exhibit a cooling impact on Earth's climate by reflecting solar radiation and a warming impact through absorption of infrared radiation and thermal emission towards Earth's surface. Ice clouds consist of non-spherical ice crystals with various shapes and sizes. To determine the influence of ice clouds on Earth's radiation budget and hence climate, knowledge of how they scatter and absorb radiation, henceforth called their single-scattering properties, is required. A geometric optics method (GOM) has been widely used to calculate the single-scattering properties of ice crystals. A GOM is an asymptotic solution that is appropriate when a particle is much larger than the wavelength of incident light. However, the exact size range of applicability of GOM has not been well established and should be determined through comparison against numerically exact methods. In this study, single-scattering properties of ice crystals are calculated using both GOM and a numerically exact method to determine the range of applicability of GOM.

3. Description of Research Activities and Results

To calculate impacts of ice clouds on the Earth's radiation budget and hence climate system, knowledge of how they scatter and absorb radiation, henceforth called their single-scattering properties, is required across a large spectrum of wavelengths (i.e., ultraviolet to microwave). However, since ice clouds consist of wide variety of shapes and sizes of non-spherical ice crystals, a simple solution, such as Mie theory, cannot be applied to calculate such properties, so that more complex exact methods that solve Maxwell's equation are required. These numerically exact methods, such as the discrete dipole approximation (DDA) and T-matrix, are computationally very expensive and the required computing time and memory rapidly increases with the size of the ice crystal. Therefore large computing resources, such as Blue Waters, are required for such calculations. Because such large computing resources have not always been available and because such calculations need to be performed for many different shapes, a computationally cheap method with unknown errors, i.e., the geometric optics method (GOM), has been widely used to calculate the single-scattering properties of ice crystals. A GOM is an asymptotic solution that is appropriate when a particle is much larger than the wavelength of incident light. However, the exact size range of applicability of GOM has not been well established and should be determined through comparison against numerically exact methods. In this study, single-scattering properties of ice crystals were calculated using both GOM and a numerically exact method to determine the range of applicability of GOM.

The single-scattering properties (i.e., phase matrix, asymmetry parameter g, and extinction efficiency Q_{ext}) of randomly oriented hexagonal ice crystals were calculated using an exact method (i.e., the Amsterdam DDA (ADDA)) and an approximation (i.e., conventional GOM) at a wavelength λ=0.55 μm. For these calculations, a width (W) of up to 36 μm and a length (L) of up to 48 μm of hexagonal ice crystals with aspect ratios (AR=L/W) of 0.1, 0.25, 0.5, 1.0, 2.0, and 4.0 were used. These crystals correspond to volume-equivalent-sphere size parameters χ_{veq} of up to 124.

It was shown that the calculated phase matrixes of hexagonal ice crystals using ADDA approached those calculated using conventional GOM as the size of the crystal increased for all six *AR*s. The agreement between the phase matrixes calculated suing ADDA and those using conventional GOM was better for large hexagonal crystals with compact shapes (e.g., *AR*=1.0) compared to those with oblate (e.g., *AR*=0.1) and prolate (e.g., *AR*=4.0) shapes. Further, analysis of the generated scattering functions showed that the threshold sizes at which atmospheric halos begin to form varies with the *AR* of the hexagonal crystals. The estimated 22 degree halo forming χ_{veq} of hexagonal crystals with *AR*=0.1 (0.25; 0.5; 1.0; 2.0; 4.0) was ~52 (60; 58; 49; 61; 77), whereas it was ~58 (49; 92) for 46 degree halo. Figure 1 shows the calculated phase matrixes of hexagonal crystals with *AR*=1.0.

The differences between ADDA and GOM simulations of *g* and Q_{ext} became smaller as crystal size increased. The estimated errors of conventional GOM were ~1.2% (7.0%) for *g* (Q_{ext}) of hexagonal crystals with χ_{veq}=90 for all *AR*s, whereas they were ~0.8% (3.3%) for hexagonal crystals with χ_{veq}=100. Figure 2 shows calculated differences in *g* and Q_{ext} of hexagonal ice crystals using the ADDA and GOM as a function of χ_{veq}. Since methods that directly solve Maxell's equation, such as ADDA and T-matrix, are computationally expensive for large particles, while conventional GOM is a fast and flexible method to calculate scattering properties of non-spherical particles, inevitably conventional GOM will continue to be used for scattering calculations even in non-appropriate regions. The results quoted here provide guidance on the applicability of conventional GOM in such situations.

The calculations of the single-scattering properties of non-spherical, non-axial symmetric, and randomly oriented atmospheric ice crystals using an exact method on Blue Waters for crystals with χ_{veq} up to 124 include simulations of the largest crystals ever made so far. The previous largest simulation was for χ_{veq}=~100 made by Bi and Yang (2014). Although we have also used other supercomputers, such as the DOE NERSC Hopper and TACC Stampede, for similar computations, we have shown that **Blue Waters is the only suitable platform to calculate the single-scattering properties of non-spherical atmospheric ice crystals larger than ~16 μm at non-absorbing wavelengths using exact methods due to required large number of cores and memory.** Therefore, we need to continue to calculate the single-scattering properties of ice crystals using other plausible shape models (i.e., Gaussian random spheres, droxtal, and budding Bucky ball) using Blue Waters to improve our knowledge of small crystal single-scattering properties.

Previous Blue Waters allocations allowed us to publish peer-reviewed (Um and McFarquhar, 2013; 2015a) and non-peer reviewed papers and to give conference presentations as listed in next section. We are preparing two more papers (Um and McFarquhar, 2015b; 2015c) that will be completed with the anticipated new Blue Waters allocations. In addition to publications, the PI has also submitted a research proposal to the National Aeronautics and Space Administration (NASA) entitled "Use of CloudSat and CALIPSO data to evaluate consistent retrievals for microphysical and radiative properties of ice clouds", PI: Junshik Um, to support continued analysis of the calculated single-scattering properties of atmospheric ice crystals so that they can be ultimately used in NASA satellite retrieval algorithms.

4. List of Publications Associated with this Work

- Peer-Reviewed Publications

Um, J. and G. M. McFarquhar, 2013: Optimal numerical methods for determining the orientation averages of single-scattering properties of atmospheric ice crystals. *J. Quant. Spectrosc. Radiat. Transfer,* **127,** 207-223.

Um, J. and G. M. McFarquhar, 2015a: Formation of atmospheric halos and applicability of geometric optics for calculating single-scattering properties of hexagonal ice crystals: Impacts of aspect ratio and ice crystal size. *J. Quant. Spectrosc. Radiat. Transfer,* **165,** 134-152.

Um, J. and G. M. McFarquhar, 2015b: The impacts of shapes and concentrations of small ice crystals on bulk scattering properties of tropical cirrus. *J. Geophys. Res.,* in preparation.

Um, J. and G. M. McFarquhar, 2015c: Exact solutions of single-scattering properties of small atmospheric ice crystals: Impacts of area ratio and ice crystal size. *J. Quant. Spectrosc. Radiat. Transfer,* in preparation.

- Non-Peer-Reviewed Publications

Um J. and G. M. McFarquhar, 2014: Scattering calculations of atmospheric ice crystals: Studies on orientation average and atmospheric halo. *Blue Waters Symposium,* NSF, Champaign, IL, USA.

McFarquhar, G. M. and J. Um, 2014: Influence of orientation averaging scheme on the scattering properties of atmospheric ice crystals: Application to atmospheric halo formation. *Blue Waters Annual Report Book,* 28-29.

Um, J. and G. M. McFarquhar, 2014: Formation of atmospheric halos by hexagonal ice crystals. *14th Conference on Atmospheric Radiation,* AMS, Boston, MA, USA.

McFarquhar, G. M. and J. Um, 2014: The impact of natural variations of ice crystal aspect ratios on single-scattering radiative properties. *14th Conference on Atmospheric Radiation,* AMS, Boston, MA, USA.

Um, J., 2014: Calculations of microphysical and radiative properties of ice clouds. *National Institute of Meteorological Research,* KMA, Jeju, Republic of Korea.

Um, J. and G. M. McFarquhar, 2015: Applicability of geometric optics method for calculations of single-scattering properties of atmospheric ice crystals. *Blue Waters Symposium,* NSF, Sunriver, OR, USA.

Um, J. and G. M. McFarquhar, 2015: Applicability of geometric optics method for calculations of single-scattering properties of atmospheric ice crystals. *Blue Waters Annual Report Book,* in press.

Um, J. and G. M. McFarquhar, 2015: A lower limit of applicability of the conventional geometric optics method: A comparison with the discrete dipole approximation for the scattering properties of atmospheric ice crystals. *4th XSEDE Annual Conference,* NSF, St. Louis, MO, USA.

References

Bi, L. and P. Yang, 2014: Accurate simulation of the optical properties of atmospheric ice crystals with the invariant imbedding T-matrix method. *J. Quant. Spectrosc. Radiat. Transfer,* **138,** 17-35.

Um, J. and G. M. McFarquhar, 2013: Optimal numerical methods for determining the orientation averages of single-scattering properties of atmospheric ice crystals. *J. Quant. Spectrosc. Radiat. Transfer,* **127,** 207-223.

Um, J. and G. M. McFarquhar, 2015a: Formation of atmospheric halos and applicability of geometric optics for calculating single-scattering properties of hexagonal ice crystals: Impacts of aspect ratio and ice crystal size. *J. Quant. Spectrosc. Radiat. Transfer,* **165,** 134-152.

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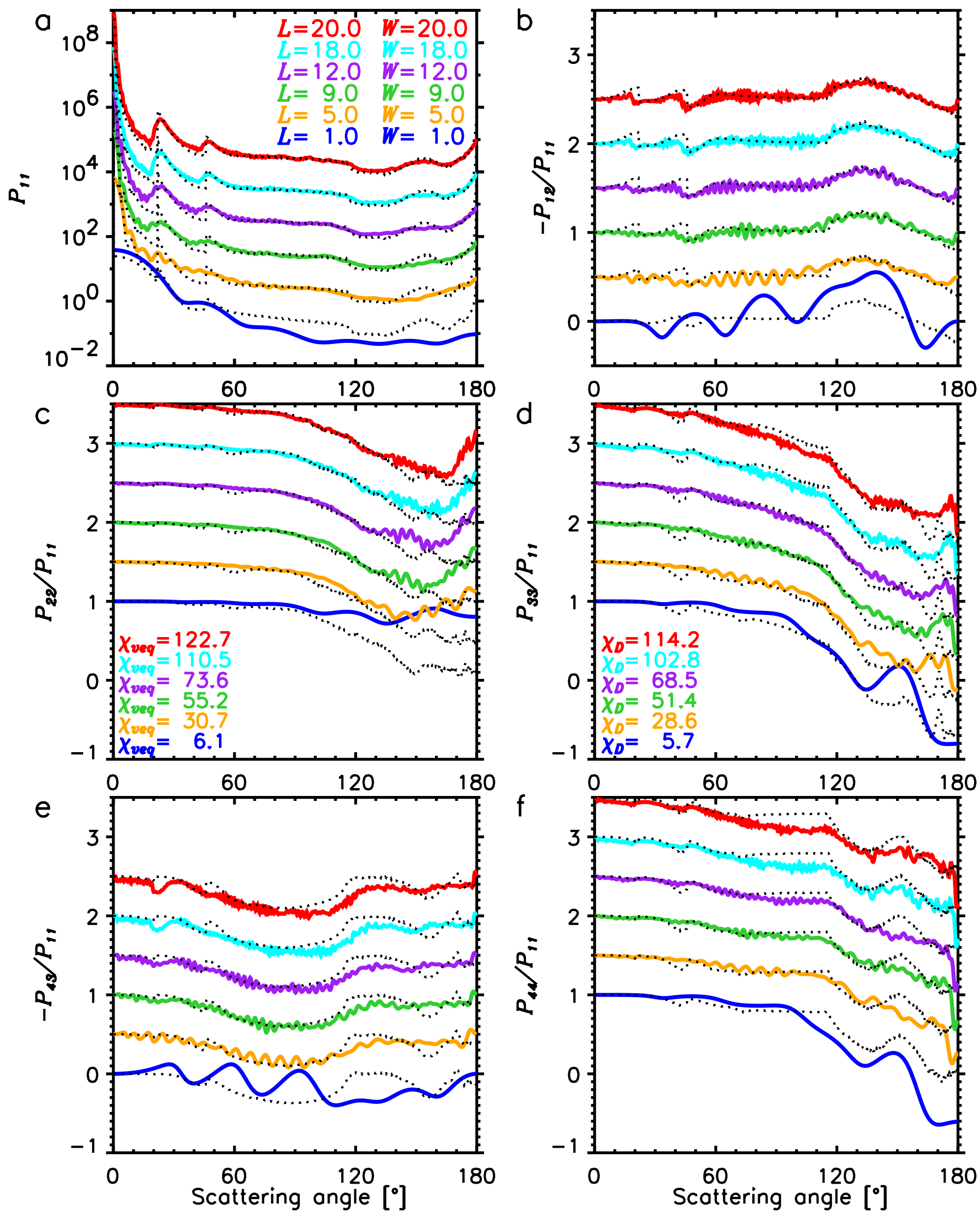

Figure 1. Calculated non-zero elements of phase matrix of hexagonal crystals with *AR*=1.0 using the ADDA (color solid lines) and GOM (black dotted lines): (a) P_{11}, (b) $-P_{12}/P_{11}$, (c) P_{22}/P_{11}, (d) P_{33}/P_{11}, (e) $-P_{43}/P_{11}$, and (f) P_{44}/P_{11}. Different colors indicate different crystal sizes with corresponding length (*L*), width (*W*), volume-equivalent-sphere size parameter (χ_{veq}), and conventional size parameter (χ_D) embedded in panels. In order to distinguish lines, 10^i is multiplied to each of the original values from small to large sizes in (a), whereas $0.5\times i$ is added to the original values in the other panels, where i=0, 1, 2, 3, 4, and 5.

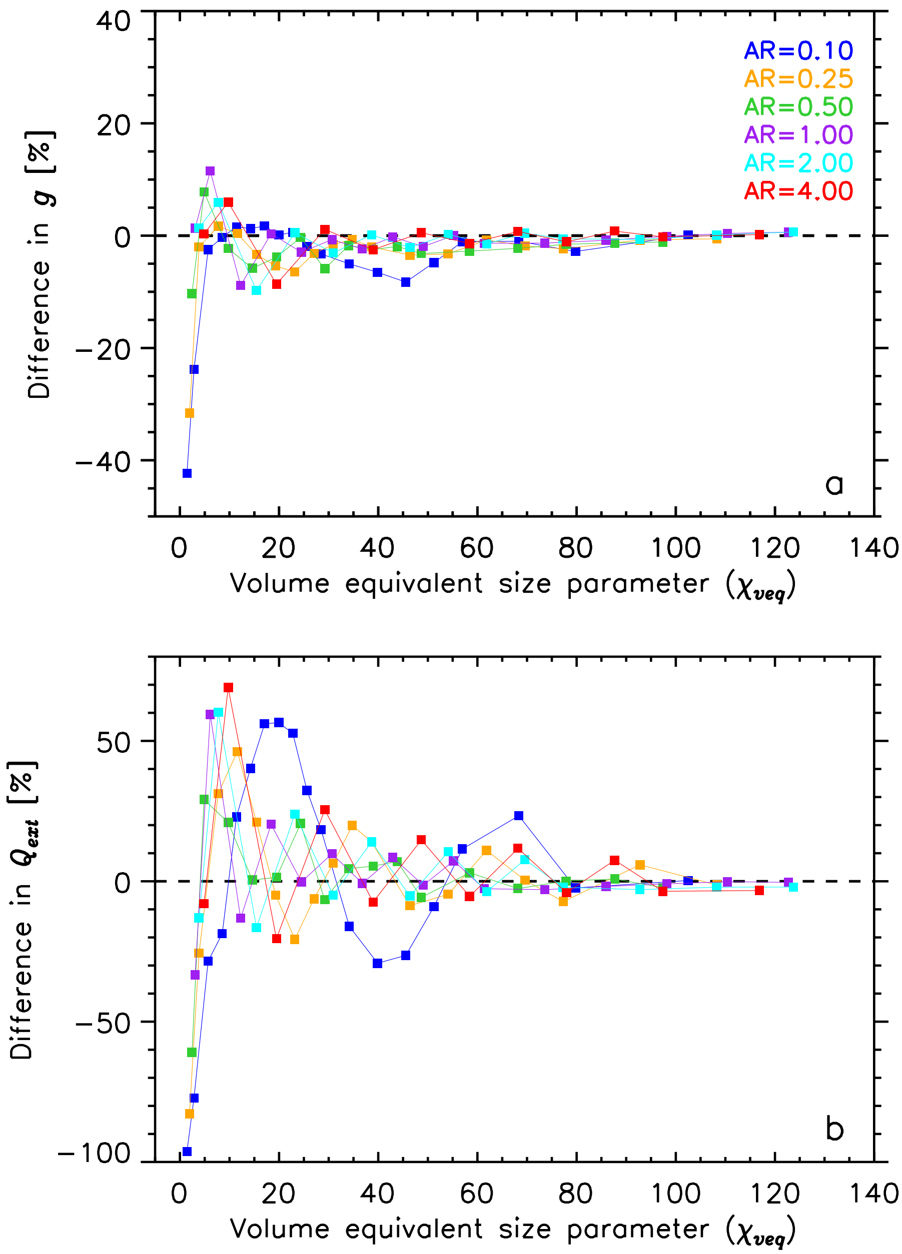

Figure 2. Differences (%) in (a) g and (b) Q_{ext} of hexagonal ice crystals using the ADDA and GOM as a function of volume-equivalent-sphere size parameter (χ_{veq}). Differences are calculated as 100×(ADDA-GOM)/GOM. Different colors correspond to different aspect ratio (AR).