IMPACTS OF ORIENTATION AND MORPHOLOGY OF SMALL ATMOSPHERIC ICE CRYSTALS ON *IN-SITU* AIRCRAFT MEASUREMENTS: SCATTERING CALCULATIONS

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EXECUTIVE SUMMARY

The single-scattering properties of ice crystals with maximum dimensions smaller than 50 µm were calculated at a wavelength of 0.55 µm using a numerically exact method (i.e., the discrete dipole approximation) and Mie theory. For these calculations, hexagonal columns and spheres were used to represent the shapes of the small ice crystals in natural clouds. Further, because the morphological features of nonspherical ice crystal are closely related to their single-scattering properties, varying aspect ratios were used to characterize the hexagonal column shapes in the scattering calculations. The results show the impacts of orientation, shape, and aspect ratio on the directional intensity of scattered light. Based on these calculations, potential errors due to shape and orientation on the sizing of particles by current forward scattering probes that measure ice crystals with maximum dimensions smaller than 50 µm are quantified in an inverse problem.

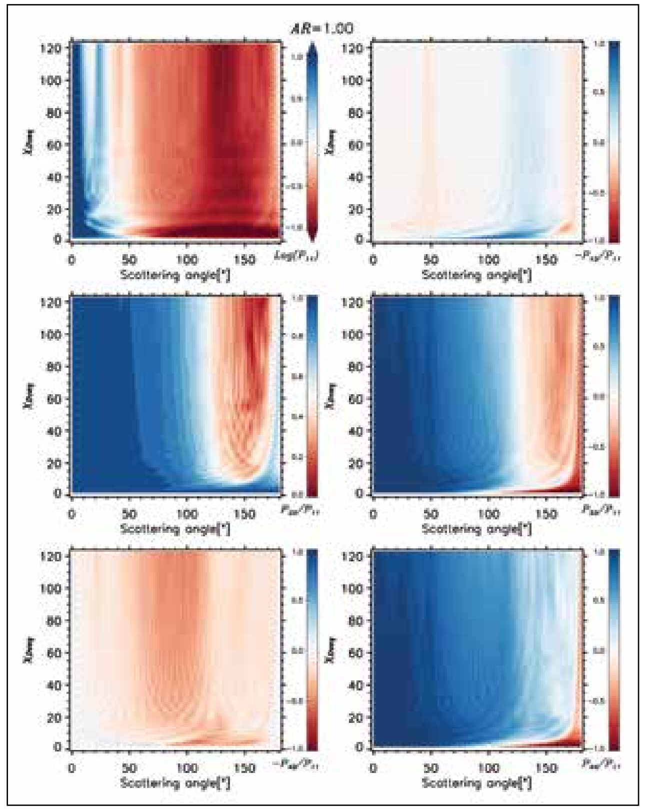

Figure 1: Non-zero scattering phase matric elements of hexagonal ice crystals with aspect ratio of 1.0 at wavelength of 0.55 µm as functions of scattering angle and volume equivalent size parameter.

RESEARCH CHALLENGE

Current *in situ* airborne probes (e.g., forward scattering spectrometer probes) that measure the sizes of ice crystals with maximum dimensions Dmax less than 50 µm are based on the concept that the measured intensity of light scattered by a particle in the forward and sometimes backward direction can be converted to particle size. The retrieval of ice crystal size from satellites also relies on relationships between light scattering and particle size, as do parameterization schemes for numerical models. The relationship between particle size and scattered light used to process data from current forward scattering probes is based on Mie theory, which assumes the refractive index of a particle is known and that all particles are spherical. Not only are small crystals not spherical, there are also a wide variety of nonspherical shapes that have been used to represent them based on images of actual observed ice crystals.

Although it is well known that the scattering properties of nonspherical ice crystals differ from those of spherical shapes, the impacts of this nonsphericity on derived *in situ* particle size distributions (PSDs), upon which satellite retrievals and parameterizations for large-scale numerical models depend, are unknown. To improve *in situ* airborne measurements of small crystals and PSDs, precise relationships among the intensity of light scattered in multiple directions by a particle and its size and shape are required and should be based on accurate calculations of single-scattering properties. Such calculations demand large computing time and memory that rapidly increase with particle size. Large computing resources such as Blue Waters are necessary for these calculations.

METHODS & CODES

The discrete dipole approximation (DDA), is a flexible technique that can calculate the scattering properties of irregularly shaped particles. In DDA, a particle is discretized into a number N of elementary polarizable units called dipoles. Specifying the location and polarizability of these dipoles allows calculations of the scattering and absorption of light. The number of dipoles N into which a particle is divided can be assigned to N CPUs (or cores) with the single-scattering properties then calculated within a parallel environment (e.g., message passing interface). In our study, a numerical code, the Amsterdam DDA (ADDA [1]) was used to calculate the scattering and absorption of electromagnetic waves by ice crystals.

RESULTS & IMPACT

We calculated the single-scattering properties (i.e., phase matrix, asymmetry parameter, and extinction efficiency) of hexagonal crystals with Dmax < 50 µm at a nonabsorbing wavelength (i.e., λ=0.55 µm) using Blue Waters. Because molecules in ice crystals form a hexagonal lattice structure, the most common crystal habits are hexagonal prisms [2]. To represent natural variations of hexagonal ice crystals [3], six different aspect ratios (AR=0.1, 0.25, 0.5, 1.0, 2.0, and 4.0) were used. The single-scattering properties of hexagonal columns with a width of up to 36 µm and a length of up to 48 µm were determined.

Fig. 1 shows the calculated nonzero phase matrix of hexagonal crystals with AR=1.0. Based on these calculations, a new conversion table (i.e., differential scattering cross sections) was generated (Fig. 2). The differential scattering cross sections of nonspherical crystals calculated using ADDA are significantly different from those of spherical particles (the brown and black lines in Fig. 2) determined using Mie theory. Errors in the sizing of ice crystals used in current forward scattering probes due to nonsphericity of atmospheric ice crystals were quantified for the first time using the newly developed conversion table. Differences in sizing particles were larger for those with Dmax<10 µm (due to interference structures) and with Dmax>10 µm (due to nonsphericity) than for those with Dmax=~10 µm. The differences were up to 112% (170%) in the forward (backward) direction depending on the degree of nonsphericity assumed in the orientation-averaged calculations. However, a measurement is made by a forward scattering probe within 1.0 µsec, which implies that a particle has a certain orientation. The differences became larger and were up to 515% (790%) when orientations were considered in scattering calculations.

Most research aircraft have at least one forward scattering probe to measure small cloud particles. Thus, developing a new probe that can measure sizes and shapes of small crystals and also distinguish them from liquid cloud droplets is important. However, improving the processing algorithms of current forward scattering probes that allow use of previous measurements acquired using the current model of forward scattering probes is also important.

WHY BLUE WATERS

Although numerically exact methods are typically used to calculate single-scattering properties of particles with small size parameters, approximations are often used for larger size parameters. Although exact methods can be used for particles with larger size parameters and provide more accurate results, they require more computing time and memory that rapidly increases with particle size, preventing their use in many circumstances. The accuracy of radiative transfer models and satellite retrieval algorithms depends heavily on accurate calculations of single-scattering properties of ice crystals. Blue Waters is an important resource in completing these calculations by allowing more exact calculations for larger particles.

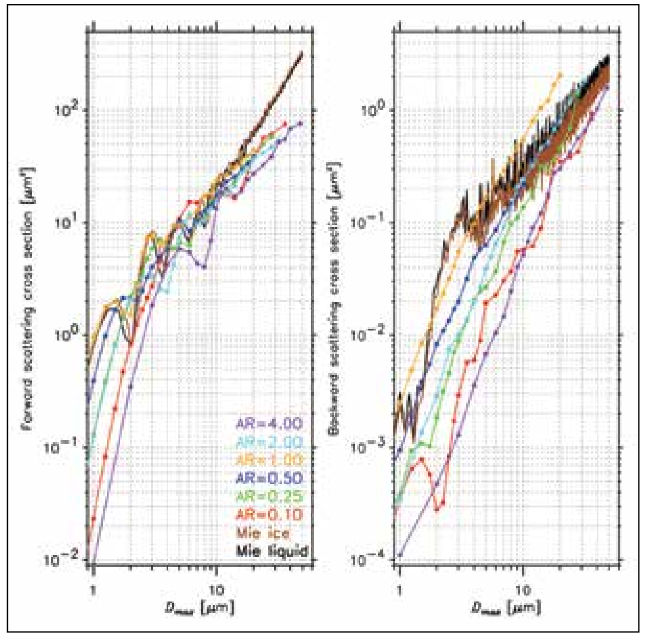

Figure 2: Calculated differential scattering cross sections of hexagonal ice crystals and spheres in forward (left) and backward (right) directions.

PUBLICATIONS AND DATA SETS

Baumgardner, D., et al., Chapter 9: Cloud Ice Properties - In Situ Measurement Challenges. in *Meteor. Monogr.*, 58 (2017), pp. 9.1–9.23, DOI: 10.1175/AMSMONOGRAPHS-D-16-0011.1.

Um, J., and G. M. McFarquhar, Quantifying uncertainty in forward scattering probes due to non-sphericity of atmospheric ice crystals. *17th International Conference on Clouds and Precipitations*, Manchester, UK, July 25–29, 2016.

Um, J., and G. M. McFarquhar, Accurate calculations of single-scattering properties of small ice crystals: Scattering database and application to in-situ forward scattering probes. *1st International Summer Snowfall Workshop*, Cologne, Germany, June 28–30, 2017.