Blue Waters Illinois Allocations Report

Exact solutions of light scattering by small atmospheric ice crystals to improve in-situ measurements, satellite retrieval algorithms, and numerical models

1. Name of Illinois PI and Co-PI

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2. Executive Summary

Accurate calculations of the single-scattering properties of ice crystals with realistic shape models are important to interpret in-situ aircraft observations. Some current in-situ airborne probes (e.g., forward scattering spectrometer probes) measure the sizes of ice crystals smaller than 50 μm using the intensity of a laser beam scattered by a particle in the forward and sometimes backward direction. The conversion between intensity and particle size is based on Mie theory, which assumes the refractive index of a particle is known and particles are spherical. Not only are ice crystals not spherical, but they also have a wide variety of nonspherical shapes. Such effects on current forward scattering probes have not been quantified. In this study, it was shown that errors in the sizing nonspherical ice crystals using current forward scattering probes was up to 40% based on hexagonal ice crystal simulations.

3. Description of Research Activities and Results

Large uncertainties on the influence of ice clouds on the climate system exist because of inadequate representations of both the concentrations and shapes of small ice crystals, hereafter ice crystals with maximum dimensions less than 50 μm, in radiative calculations. Recently, uncertainties in measurements of the concentrations of small ice crystals (Korolev et al. 2011; Jackson et al. 2014) and their impacts on radiative calculations have been emphasized (McFarquhar et al. 2007; Jackson and McFarquhar 2014). The assumed shapes can also impact the radiative transfer (Um and McFarquhar 2011).

Concentrations (i.e., size distributions) of small atmospheric ice crystals have been measured by cloud probes mounted on aircrafts. Current in-situ airborne probes (e.g., forward scattering spectrometer probes (FSSP)) that measure the sizes of ice crystals smaller than 50 μm are based on the concept that the measured intensity of a laser beam 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, and parameterization schemes for numerical models assume such relationships. The relationship between particle size and scattered light used in 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, but also there is a wide variety of non-spherical shapes that have been used to represent them. Although it is well known that the scattering properties of non-spherical ice crystals differ from those of spherical shapes, the impacts of non-sphericity on derived in-situ particle size distributions (PSDs) on which satellite retrievals and parameterizations for numerical models depend are unknown. Thus, to improve in-situ airborne measurements of small crystals and corresponding PSDs that are used for satellite retrieval algorithms and numerical models, precise relationships between 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 of crystals. **It is a challenging problem because such calculations require large computing resources, such as Blue Waters.** Global climate model (GCM) calculations have shown that these uncertainties in concentrations of small ice crystals can cause a 12% difference in cloud ice amount and a 5.5% difference in cirrus cloud coverage globally producing an uncertainty in the net cloud forcing in the Tropics of −5 Wm^{-2} and in the warming of the upper tropical troposphere of over 3°C (Mitchell et al. 2008). This is comparable to the radiative impacts of CO_2 doubling.

Thus, we calculated the single-scattering properties (i.e., phase matrix, asymmetry parameter, and extinction efficiency) of hexagonal ice crystals smaller than 50 μm at non-absorbing wavelengths (i.e., λ=0.55 μm) using Blue Waters. To represent natural variations of ice crystals, six different aspect ratios, defined as a ratio between dimension along the c-axis of crystal and dimension along the a-axis of crystal, (*AR*=0.1, 0.25, 0.5, 1.0, 2.0, and 4.0) were used. Based on these calculations, a new conversion table (i.e., differential scattering cross sections) was generated as shown in Fig. 1. The differential scattering cross sections of nonspherical ice crystals calculated using an exact method (i.e., Amsterdam Discrete Dipole Approximation (ADDA)) that solves Maxwell's equation are significantly different from those of spherical particles (i.e., brown and black lines in Fig. 1) using Mie theory with an assumption of a spherical shape. 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 (Fig. 2). It was shown that differences in sizing particles were larger for D_{max}<10 μm (due to interference structures, Fig. 1) and D_{max}>10 μm (due to nonsphericity) than those for D_{max}=~10 μm in the forward direction (Fig. 2). The differences were up to 112% (170%) in the forward (backward) direction. Oblate (*AR*=0.1) and prolate (*AR*=4.0) shapes caused larger errors than those of compact shapes (*AR*=1.0). To calculate other shapes of small ice crystals with varying orientations of ice crystals and polarization information, 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.

In summary, 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 a volume equivalent size parameter up to ~125 include simulations of the largest crystals ever made so far. Although we have also used other supercomputers, such as the DOE NERSC Edison and Cori, TACC Stampede, and SDSC Comet, 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 (Baumgardner et al. 2016; Um and McFarquhar 2016a) and non-peer reviewed papers and to give conference presentations including the 2016 Blue Waters Symposium as listed in next section. We are preparing two more papers (Um and McFarquhar, 2016b; 2016c) that will be completed with the anticipated new Blue Waters allocations. Preliminary results are shown in Figs. 3 and 4, respectively. In addition to publications, the PI has also submitted a research proposal to the National Science Foundation (NSF) entitled "Development of consistent model for realistic surface roughness and morphology of ice crystals to improve radiative properties of ice clouds based on laboratory experiments, in-situ aircraft and balloon observations, and theoretical calculations", PI: Junshik Um, to support continued analysis of the calculated single-scattering properties of realistically shaped atmospheric ice crystals.

4. List of Publications Associated with this Work

- Peer-Reviewed Publications

Baumgardner, D., S. Abel, D. Axisa, R. Cotton, J. Crosier, P. Field, C. Gurganus, A. Heymsfield, A. Korolev, M. Kramer, P. Lawson, G. McFarquhar, J. Z. Ulanowski, and J. Um, 2016: In situ measurement challenges. *AMS Meteorological Monographs,* in review.

Um, J. and G. M. McFarquhar, 2016a: Quantifying errors in sizing small ice crystals using forward scattering probes. *Atmos. Meas. Tech.,* will be submitted.

Um, J. and G. M. McFarquhar, 2016b: 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.

Um, J. and G. M. McFarquhar, 2016c: Linear depolarization ratios of atmospheric ice crystals: Impacts of orientation, shape, size, and aspect ratio of ice crystals. *J. Quant. Spectrosc. Radiat. Transfer,* in preparation.

- Non-Peer-Reviewed Publications

McFarquhar, G. M. and J. Um, 2016: Scattering by atmospheric hexagonal ice crystals for determination of applicability of geometric optics and formation of atmospheric circumscribed halos. *International Symposium on Radiation,* Auckland, New Zealand.

Um, J, 2016: Quantifying and reducing uncertainty in forward scattering probes, and results from in situ aircraft measurements. *9th Workshop on Cloud Physics and Aerosols,* NIMR, Daegu, Republic of Korea (Invited).

Um, J. and G. M. McFarquhar, 2016: Light scattering by atmospheric ice crystals: Applications to forward scattering probes. *International Symposium on Radiation,* Auckland, New Zealand.

Um, J. and G. M. McFarquhar, 2016: Dependence of directional intensity and polarization of light scattered by small ice crystals on microphysical properties: Application to forward-scattering probe, satellite retrieval, and numerical models. *2016 Blue Waters Symposium,* NSF, Sunriver, OR, USA.

Um, J. and G. M. McFarquhar, 2016: Dependence of the directional intensity and polarization of light scattered by small ice crystals on their shape and size: Application for airborne cloud probes. *Blue Waters Annual Report Book,* in press.

Um, J. and G. M. McFarquhar, 2016: Quantifying uncertainty in forward scattering probes due to non-sphericity of atmospheric ice crystals. *17th International Conference on Cloud Precipitation,* Manchester, UK.

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Jackson, R.C., and G.M. McFarquhar, 2014: An assessment of the impact of antishattering tips and artifact removal techniques on bulk cloud ice microphysical and optical properties measured by the 2D cloud probe. *J. Atmos. Ocean. Tech.*, **31,** 2131-2144.

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Korolev, A. V., E. F. Emery, J. W. Strapp, S. G. Cober, G. A. Isaac, M. Wasey, D. Marcotte, 2011: Small Ice Particles in Tropospheric Clouds: Fact or Artifact? Airborne Icing Instrumentation Evaluation Experiment. *Bull. Amer. Meteor. Soc.*, **92**, 967–973.

McFarquhar, G. M., J. Um, M. Freer, D. Baumgardner, G. L. Kok, and G. G. Mace, 2007: Importance of small ice crystals to cirrus properties: Observations from the Tropical Warm Pool International Cloud Experiment (TWP-ICE). *Geophys. Res. Lett.*, **34,** doi:10.1029/2007GL029865.

Mitchell, D. L., R. Phillip, D. Ivanova, G. M. McFarquhar, and T. Nousiainen, 2008: Impacts of small ice crystal assumption on ice sedimentation rates in cirrus clouds and GCM simulations. *Geophys. Res. Lett.*, **35,** doi: 10.1029/2008GL033552.

Um, J. and G. M. McFarquhar, 2011: Dependence of the single-scattering properties of small ice crystals on idealized shape models. *Atmos. Chem. Phys.*, **11**, 3159-3171.

Um, J. and G. M. McFarquhar, 2016a: Quantifying errors in sizing small ice crystals using forward scattering probes. *Atmos. Meas. Tech.,* will be submitted.

Um, J. and G. M. McFarquhar, 2016b: 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.
Um, J. and G. M. McFarquhar, 2016c: Linear depolarization ratios of atmospheric ice crystals: Impacts of orientation, shape, size, and aspect ratio of ice crystals. *J. Quant. Spectrosc. Radiat. Transfer,* in preparation.

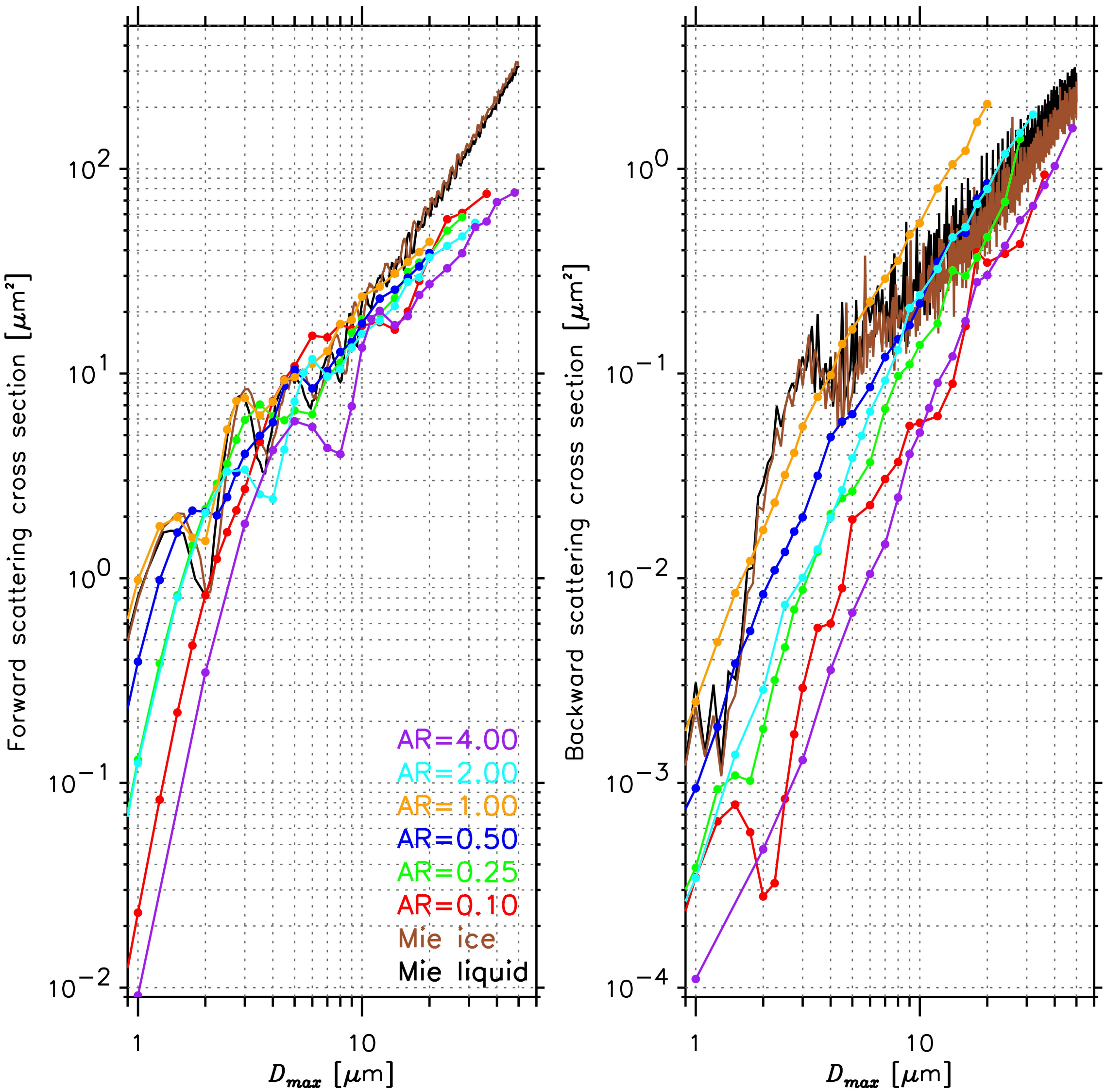

Figure 1. Calculated differential scattering cross sections of hexagonal ice crystals and spheres in forward (left) and backward (right) directions.

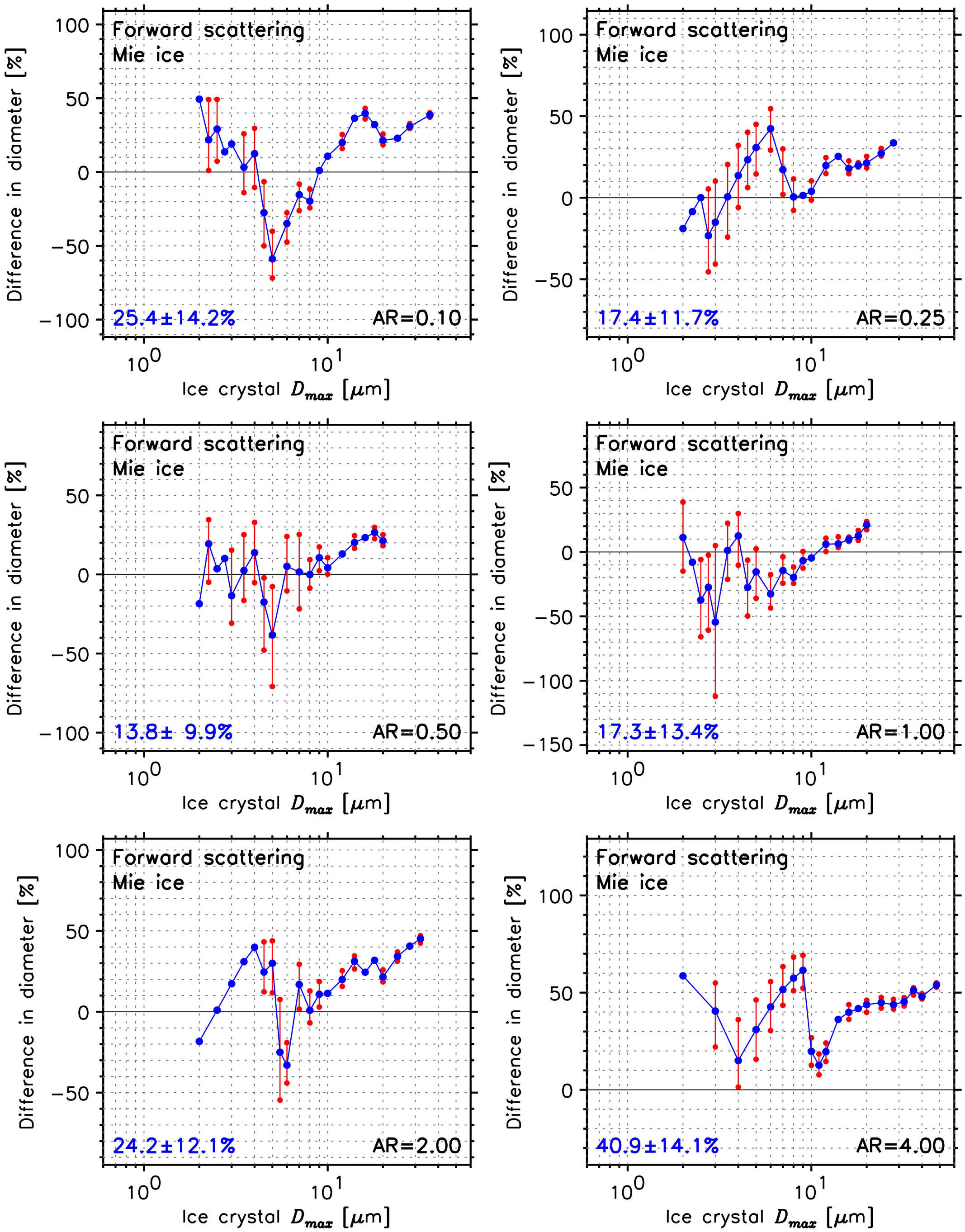

Figure 2. Differences (100% × (D_{max} - Mie D_{max})/D_{max}) between actual sizes of ice crystals and those determined based on Mie calculations in forward (left) and backward (right) directions as a function of *AR* of hexagonal ice crystals (each panel). Mean and standard deviation of absolute values of blue circles are embedded in each panel.

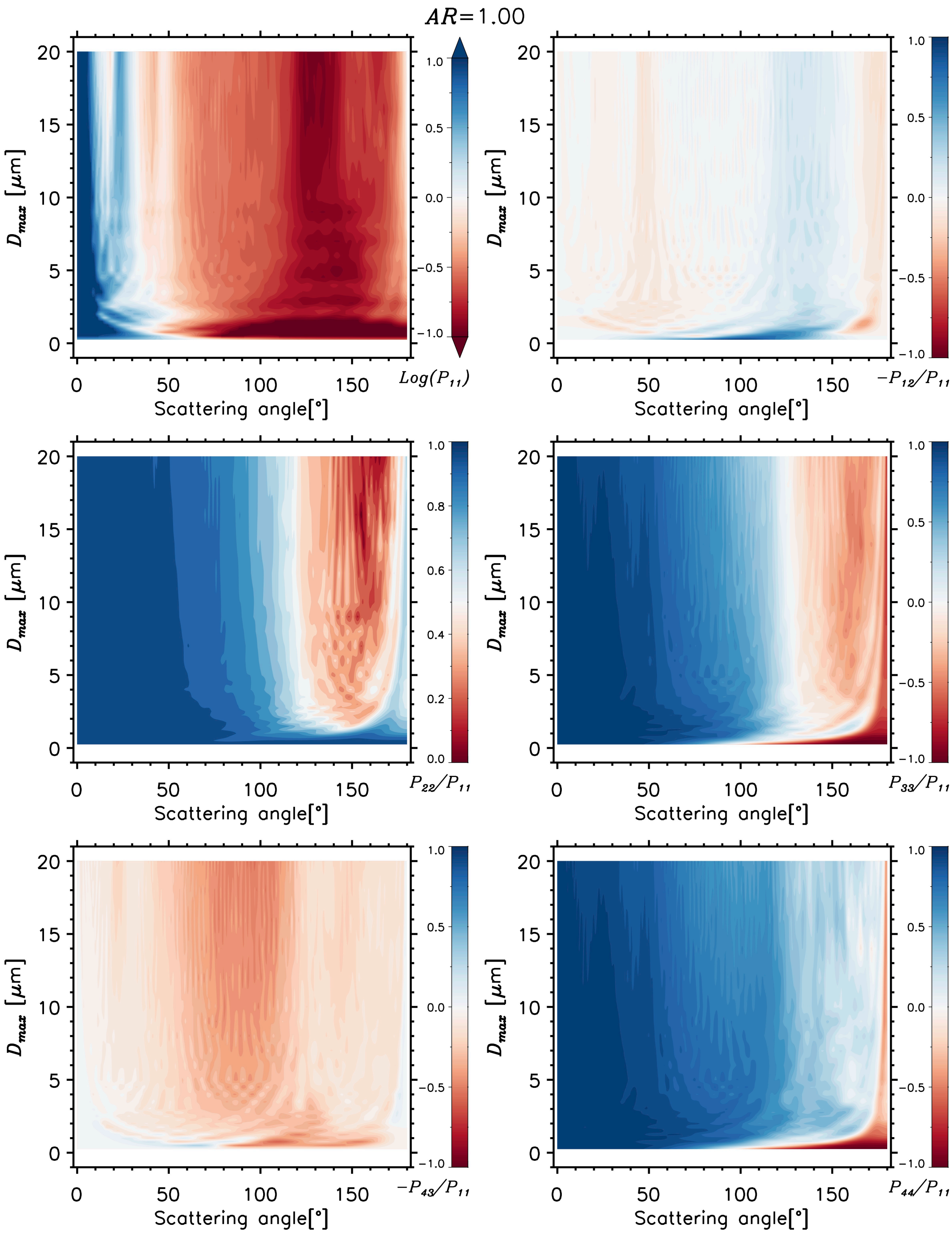

Figure 3. Non-zero scattering phase matrix elements of hexagonal ice crystals with aspect ratio (*AR*) of 1.0 at wavelength of 0.55 μm.

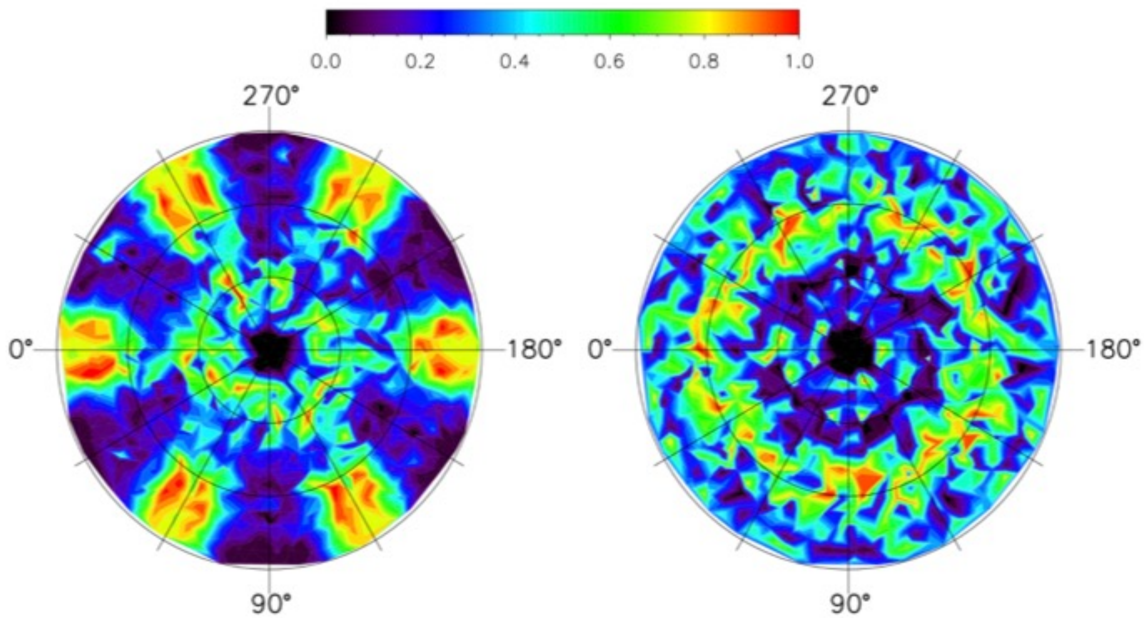

Figure 4. Linear depolarization ratio of hexagonal column (left) and spheroid (right) as a function of orientation of particle at λ=0.55 μm. Both the hexagonal column and spheroid have the same size (L=10 μm and W=2.5 μm) and aspect ratio of 4.0.