A Database of Microwave Single-Scattering Properties for Nonspherical Ice Particles

By Guosheng Liu

Department of Meteorology, Florida State University
Tallahassee, Florida

Capsule Summary

A database containing microwave single-scattering properties for 11 ice particle shapes have been produced using discrete dipole approximation and is now publicly available.

Corresponding Author:

Guosheng Liu
Department of Meteorology
Florida State University
Tallahassee, FL 32306-4520
(850) 644-6298
(850) 644-9642 (fax)
liug@met.fsu.edu
Abstract
As satellite observations at high microwave frequencies have recently become available, there is an increasing demand for methods that accurately evaluate the single-scattering properties of nonspherical ice particles at these frequencies. Algorithm developers can use the single-scattering data sets in the retrievals of cloud ice water content and snowfall rate. However, the methods that correctly handle the scattering of complex nonspherical particles are computationally inefficient and impractical for physical retrieval algorithms, in which scattering needs to be evaluated many times for particles with various sizes and shapes. As a remedy, during the past several years we have computed the scattering properties – scattering and absorption cross sections, phase functions, asymmetric parameters and backscattering cross sections – using an accurate discrete dipole approximation method and arranged the results into an easy-to-access database. The database contains the scattering properties at frequencies from 15 to 340 GHz, with temperatures from 0 to -40 °C, of particle sizes (maximum dimension) from 50 to 12,500 μm, and for 11 particle shapes. The database along with an easy-to-use reading program is now made available to interested investigators. This article explains how this database is derived and how it can be used.
Despite their great significance in modulating the Earth radiation budget and the global hydrological cycle (e.g., Liou 1986; Stephens et al. 1990, Lynch et al., 2002), cloud ice water and snow precipitation remain to be the most inadequately measured geophysical variables. For example, global climate models can hardly agree with each other on the order of magnitude of the global mean ice water path (Del Genio 1997, Stephens et al. 2002) in light of the lack of observational guidance. Clearly, global measurements of cloud ice water and snowfall are needed to improve our understanding of the Earth’s climate and to better predict it. One promising approach is to evaluate ice water amount by measuring the scattering signatures at microwave frequencies by either active (e.g., Mace et al. 1998, Matrosov 1999, Wang and Sassen 2002) or passive (e.g., Weng and Grody 2000, Skofronick-Jackson 2003, Seo and Liu 2005) remote sensing. The availability of data from the cloud radar on CloudSat satellite (Stephens et al. 2002) and the high frequency microwave radiometers on NOAA satellites as well as the planned Global Precipitation Measuring satellite mission provides excellent opportunities to assess global cloud ice water amount and snowfall precipitation.

To develop an algorithm that converts the observed radar reflectivity or brightness temperature to ice water amount or snowfall rate, one must know the single-scattering properties, i.e., scattering cross sections and phase functions, etc., of the ice particles. In most retrieval algorithms, these properties need to be computed repeatedly many times and for particles with many sizes and shapes. It is quite challenging to accurately compute the single-scattering properties of ice crystals because of their complicated morphologies. There are several published methods for calculating the scattering of nonspherical particles (Mishchenko et al. 2000), such as the T-matrix method.
(Mishchenko et al. 1996), the finite difference time domain method (Tallove 1995, Yang and Liou 1996, 1998), and the discrete dipole approximation method (DDA, Draine and Flatau 1994). Due to the complexity of their shapes, computation of ice scattering is computationally inefficient and impractical to be used in physical retrieval algorithms, in which scattering needs to be evaluated many times for particles with various sizes and shapes. The author performed DDA modeling for selected frequencies and particle shapes in an effort to forming an empirical formula to compute the single-scattering properties accurately and efficiently (Liu 2004). Since then for the past several years, the author has been conducting DDA simulations for more particles shapes, broader particle size ranges, and over a wider range of frequencies. The results of these simulations has been arranged into a database containing single-scattering properties at frequencies from 15 to 340 GHz, with temperatures from 0 to -40°C, of particle sizes (maximum dimension) from 50 to 12,500 μm, and for 11 particle shapes. The database along with an easy-to-use reading program is now made available to interested investigators. A similar database that covers near- to far-infrared spectral regions has been reported by Yang et al. (2005). The current database covers microwave spectral region, complementary to the Yang et al. database.

**MODELING THE SCATTERING PROPERTY OF ICE PARTICLES.** The DDA model developed by Draine and Flatau (2000) is used to compute the single-scattering properties of ice particles. The DDA is a general method for computing the scattering and absorption by a particle of arbitrary shape, and has been used by many investigators for studying the scattering by interstellar grains and ice particles (e.g., Draine 1988; Evan
Simply stated, the DDA is an approximation of the continuum target by a finite array of polarizable points. The points acquire dipole moments in response to the local electric field. The dipoles also interact with one another via their electric fields. The principal advantage of the DDA is that it is flexible regarding the geometry of the target. The limitation is that the interdipole spacing must be sufficiently small compared to the wavelength in order to obtain desired accuracy, which requires large computer memory and long computation time for large particles.

We have performed DDA modeling for eleven types of ice particle shapes. In Fig. 1, examples of these ice particles are presented by collections of dots; each dot is a dipole in the DDA calculation. In deriving the single-scattering properties, all ice particles are assumed to be randomly oriented in space. The orientational average of a quantity, $Q$, can be calculated by (Draine and Flatau 2000):

$$
\langle Q \rangle = \frac{1}{8\pi^2} \int_0^{2\pi} d\beta \int_{-1}^{1} d\cos \theta \int_0^{2\pi} d\varphi Q(\beta, \theta, \varphi),
$$

where $\beta$, $\theta$, and $\varphi$ are the 3 angles to describe the orientation of the ice particle in the Draine and Flatau DDA model. All DDA model-calculated quantities presented in the database are orientationally averaged using calculations at 16 $\beta$s, 17 $\theta$s and 16 $\varphi$s.

The characteristics of the ice particles are listed in Table 1. In addition to particles’ maximum dimension, an equal-mass radius, $r_{\text{eff}}$, is also given in the table, which is defined by the radius of an “effective” ice sphere of the same mass but with a density of 0.916 g cm$^{-3}$. 

and Stephens 1995; Liu 2004; Kim 2006; Hong 2007). Simply stated, the DDA is an approximation of the continuum target by a finite array of polarizable points. The points acquire dipole moments in response to the local electric field. The dipoles also interact with one another via their electric fields. The principal advantage of the DDA is that it is flexible regarding the geometry of the target. The limitation is that the interdipole spacing must be sufficiently small compared to the wavelength in order to obtain desired accuracy, which requires large computer memory and long computation time for large particles.

We have performed DDA modeling for eleven types of ice particle shapes. In Fig. 1, examples of these ice particles are presented by collections of dots; each dot is a dipole in the DDA calculation. In deriving the single-scattering properties, all ice particles are assumed to be randomly oriented in space. The orientational average of a quantity, $Q$, can be calculated by (Draine and Flatau 2000):
Columns and plates. Five types of columns and plates are included (Fig. 1a); all have a hexagonal shape of basal plane, but differ in the ratio of length (or depth), L, to hexagonal diameter (distance between opposite vertices), d. The ratio of L/d is designed to be 4, 2, 1, 0.2 and 0.05 for long columns, short columns, block columns, thick plates and thin plates, respectively. As their maximum dimension increases, the L/d ratio does not change.

Rosettes. Rosettes (Fig. 1b) are represented by aggregates of hexagonal columns connected at the center. For this study, we construct rosettes with 3 to 6 bullets. The 3- and 4-bullet rosettes consist of 3 and 4 coplanar columns that display a “⊥” and a “+” shape, respectively. The 5- or 6-bullet rosette is constructed by adding one or two columns to a 4-bullet rosette in the direction perpendicular to the other 4 bullets. Columns that make up the same rosette have the same length and aspect ratio. But the aspect ratios for rosettes with different number of bullets are different depending on the area ratio – maximum dimension relations given below. To determine the aspect ratio of the columns, we use a relationship between the maximum dimension, $D_{\text{max}}$, and the area ratio, $A_r$, derived by Heymsfield and Miloshevich (2003):

$$A_r = a D_{\text{max}}^b,$$

where $a=0.125$ and $b=-0.351$ (in cgs unit), which are the values determined for rosettes based on Cloud Particle Imager measurements. $A_r$ is the projected area of an ice particle normalized by the area of a circle with diameter $D_{\text{max}}$. By letting (2) hold while $D_{\text{max}}$ varies, the aspect ratio of the columns with different lengths can be determined.
Snowflakes. Two types of snowflakes are considered. The first type is a sector-like particle (Fig. 1c), represented by 3 identical ellipsoids that share the same center, and whose longest axes are orientated $60^\circ$ apart. Given the maximum dimension of a snowflake $D_{\text{max}}$, the diameters of an ellipsoid in the other two dimensions are determined by the following relations (in cgs units):

$$A_r = 0.261 D_{\text{max}}^{-0.377},$$  \hspace{1cm} (3a)

and

$$\rho_e = 0.015 A_r^{1.5} D_{\text{max}}^{-1.0}.$$  \hspace{1cm} (3b)

$\rho_e$ is effective density defined as the mass divided by the volume of a circumscribed sphere. The relation (3a), given by Heymsfield and Miloshevich (2003), was derived based on surface measurement data for aggregate planar crystals (Kajikawa 1982). The relation of (3b) was derived by Heymsfield et al. (2002) for aggregates. Combining (3a) and (3b) makes $\rho_e$ approximately proportional to $D_{\text{max}}^{-1.6}$, similar to the relation given by Magono and Nakamura (1965). The top- and side-view of the images for $D_{\text{max}}$=100, 500, 1000 and 5000 $\mu$m of the sector snowflakes are shown in Fig. 1c.

The second type of snowflakes is dendrite as shown in Fig. 1d (top-view). As the particle size increases, the area ratio $A_r$ does not change. To determine the depth of the dendrites, equation (3b) is used, which results in a nearly constant value of $\sim 70$ $\mu$m for the depth of particles with maximum dimension from 75 to 11371 $\mu$m. The difference between the two types of snowflakes is that the ice volume is concentrated on 6 main
branches in the sector snowflakes, while it spreads more uniformly in the basal plane in the dendrite snowflakes.

It should be noted that for all the particles designed in this study, ice portion of the particle is made of pure ice with a density of 0.916 g cm$^{-3}$, not ice mixed with air bubbles.

Accuracy. There are two possible causes for an inaccuracy of the computed results: (1) the interdipole spacing not sufficiently small and (2) insufficient number of orientations in representing random orientation. To minimize error caused by the first problem, Draine and Flatau (2000) recommended a criterion of $|m|ks<0.5$, where $m$ is the refractive index, $k=2\pi/\lambda$ ($\lambda$: wavelength), and $s$ the interdipole spacing. In our computations, we followed $|m|ks<0.25$ in determining interdipole spacing to ensure adequate accuracy. An examination by further halving the interdipole spacing has been conducted for DDA computations of sector snowflakes. It is found that the difference between current results and those when further halving the spacing is less than 2% for absorption and scattering cross sections and asymmetry parameters for all frequencies and particle sizes. For backscatter cross section, the difference is slightly higher, but still less than 5%.

Currently, calculations for 16x17x16 particle orientations are performed to represent random orientation. To examine whether these many orientations are “random” enough, we further conducted calculations for sector snowflakes at doubled numbers of $\beta$s, $\theta$s and $\phi$s, i.e., 32x33x32 orientations. Results show that doubling the number of orientational angles does not cause measurable change (<1%) in absorption and scattering cross sections and asymmetry parameters. However, for backscatter cross sections
(therefore, for phase function at 180º direction as well), the difference between current results and those of doubled orientational angles increases dramatically with frequency and particle size. At frequencies below 150 GHz, the difference is less than 5% for all particle sizes; but it increases to over 20% for particle size of 10,000 µm at 340 GHz. Therefore, readers are cautioned that backscatter cross sections at frequencies over 150 GHz, particularly for particle size larger than 5,000 µm, contain significant error (up to 20%) in the current version due to the lack of “randomness”. We plan to conduct computations using more orientations in the future and announce the new results at the website which hosts the database. Fortunately, backscatter cross sections are used only for computing radar reflectivities; and currently available high-frequency radar is the W-band CloudSat radar with a frequency of 94 GHz. For this frequency, our comparison results show that the error due to this lack of randomness is less than 1.5%.

**WHAT ARE IN THE DATABASE?** Given a particle shape, the single-scattering properties of ice particles also depend on particle size, frequency and temperature. To build the database, the single-scattering properties have been computed at many “anchor” points defined by particle shape, size, frequency and temperature. These “anchor” points cover a broad range of particle sizes, frequencies and temperatures at reasonable increments, so that users can derive the scattering properties for any size, frequency and temperature through interpolation. In Table 2 and Table 3, we list the particles sizes, frequencies and temperatures used as “anchor” points for the DDA computations. It is noticed that the ice particles considered in this database are relatively large (≥50 µm in maximum dimension), since microwave scattering is insensitive to smaller particles. The
frequencies used in the computations resemble those used in current and future airborne and satellite radars and radiometers.

The following single-scattering properties are computed: the absorption cross section ($C_{abs}$), the scattering cross section ($C_{sca}$), the backscatter cross section ($C_b$), the asymmetry parameter ($g$), and the phase function [$P(\cos\Theta)$, where $\Theta$ is referred to as scattering angle that is the angle between incident and observing directions]. Absorption and scattering cross sections, in unit of area, are quantities describing how much incident radiation is absorbed or scattered to all directions by the particle. Backscatter cross section (also in unit of area) describes the scattered energy to the opposite direction of the incident radiation, a necessary quantity to assess radar reflectivity. The phase function is a physical quantity that describes the angular distribution of scattered energy, while the asymmetry parameter describes the degree of symmetry of scattered energy distributed with respect to the plane dividing forward and backward hemispheres. The phase function archived in this database is normalized, so that $\frac{1}{2} \int_{-1}^{1} P(\cos\Theta)d\cos\Theta = 1$.

Figure 2 shows examples of the normalized (a) absorption, (b) scattering, (c) backscatter cross sections, and (d) the asymmetry parameter for several selected particle shapes at 340 GHz, as a function of the size parameter, $x = \frac{2\pi r_{eff}}{\lambda}$, where $\lambda$ is wavelength. For easy viewing purpose, the absorption, scattering and backscatter cross sections are normalized by $\pi r_{eff}^2$ in these plots. The above parameters of corresponding to spheres of the same mass but with radii of $r_{eff}$ (i.e., solid sphere) are also shown in the diagrams, which clearly illustrates the inaccuracy of using spheres as a shortcut to represent nonspherical ice particles. Figure 3 shows examples of phase functions of
selected ice particles at 150 GHz. The phase function evolves from a Rayleigh-like for small particles to a more forward-peaked pattern as particle size increases.

The database is downloadable from: http://cirrus.met.fsu.edu/research/scatdb.html. Along with a data file containing the computed results, a subroutine program (scatdb.c, which can be called by either C or Fortran programs) is provided to read and interpolate (if needed) the scattering properties at required frequencies, temperatures, and particle sizes. In many applications, the scattering properties required by users may not match exactly with those calculated at the “anchor” points. In these cases, the subroutine will perform a linear interpolation using values at the nearby “anchor” points.

SUMMARY. This article serves as an announcement of the availability of a useful database that contains the single-scattering properties at microwave frequencies of ice particles with a variety of shapes. The database contains the scattering properties at frequencies from 15 to 340 GHz, with temperatures from 0 to -40°C, of particle sizes (maximum dimension) from 50 to 12,500 μm, and for 11 particle shapes. The database along with an easy-to-use reading program is now made available to interested investigators, so that they can perform radiative transfer modeling without repeating the lengthy computation of nonspherical scattering. This paper explains how the database is derived and how it can be accessed. The address of the website that hosts this database is http://cirrus.met.fsu.edu/research/scatdb.html.

Limitations and future improvements. There are several limitations of this database. First, the eleven types are only a fraction of ice particle shapes observable in nature. As our knowledge based on in situ measurements increases, results for additional ice particle
shapes will be added to this database. Second, many ice particles have preferential orientations when falling due to aerodynamic balance. The preferential orientation is particularly important for backscatter cross sections that radars observe. Future addition to the database should include single-scattering properties for preferential orientated particles, particularly at radar frequencies. In relation to this addition, many modern radars observe polarized signatures; therefore, inclusion of depolarization properties will be also beneficial. Finally, improving the accuracy of the DDA results by reducing interdipole spacing and increasing orientational angles is needed for frequencies higher than 150 GHz to ensure the backscatter cross sections with an accuracy of a few percent. We will keep readers informed by posting any improvements made to the database at the aforementioned website.

ACKNOWLEDGEMENTS. The author is very grateful to Drs. B. T. Draine and P. J. Flatau whose DDA model is used for the computation of the scattering properties. The development of the database has been supported by DOE ARM DE-FG02-03ER63526, NASA TCSP NNG05GJ17G, and NASA PMM NNX07AD63G.

REFERENCES


Table 1. Characteristics of ice particles.

<table>
<thead>
<tr>
<th>Shape Name</th>
<th>Shape No.</th>
<th>Range of maximum dimension, $D_{\text{max}}$ (µm)</th>
<th>Range of equal-mass sphere radius, $r_{\text{eff}}$ (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Long Column (L/d=4)</td>
<td>0</td>
<td>121 - 4835</td>
<td>25 - 1000</td>
</tr>
<tr>
<td>Short Column(L/d=2)</td>
<td>1</td>
<td>83 - 3304</td>
<td>25 - 1000</td>
</tr>
<tr>
<td>Block Column (L/d=1)</td>
<td>2</td>
<td>66 - 2532</td>
<td>25 - 1000</td>
</tr>
<tr>
<td>Thick Plate (L/d=1/5)</td>
<td>3</td>
<td>81 - 3246</td>
<td>25 - 1000</td>
</tr>
<tr>
<td>Thin Plate (L/d=1/20)</td>
<td>4</td>
<td>127 - 5059</td>
<td>25 - 1000</td>
</tr>
<tr>
<td>3-Bullet Rosette</td>
<td>5</td>
<td>50 - 10000</td>
<td>19 - 1086</td>
</tr>
<tr>
<td>4-Bullet Rosette</td>
<td>6</td>
<td>50 - 10000</td>
<td>19 - 984</td>
</tr>
<tr>
<td>5-Bullet Rosette</td>
<td>7</td>
<td>50 - 10000</td>
<td>21 - 1058</td>
</tr>
<tr>
<td>6-Bullet Rosette</td>
<td>8</td>
<td>50 - 10000</td>
<td>21 - 1123</td>
</tr>
<tr>
<td>Sector Snowflake</td>
<td>9</td>
<td>50 - 10000</td>
<td>25 - 672</td>
</tr>
<tr>
<td>Dendrite Snowflake</td>
<td>10</td>
<td>75 - 12454</td>
<td>33 - 838</td>
</tr>
</tbody>
</table>
Table 2. Maximum dimension (in μm) of ice particles used for DDA computations

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Long Columns</strong></td>
<td>121, 242, 484, 967, 2417, 3626, 4835</td>
</tr>
<tr>
<td><strong>Short Columns</strong></td>
<td>83, 165, 330, 661, 1652, 2478, 3304</td>
</tr>
<tr>
<td><strong>Block Columns</strong></td>
<td>66, 132, 263, 527, 1316, 1974, 2632</td>
</tr>
<tr>
<td><strong>Thick Plates</strong></td>
<td>81, 162, 325, 649, 1623, 2434, 3246</td>
</tr>
<tr>
<td><strong>Thin Plates</strong></td>
<td>127, 253, 506, 1012, 2529, 3794, 5059</td>
</tr>
<tr>
<td><strong>3, 4, 5, 6-Bullet Rosettes</strong></td>
<td>50, 100, 200, 300, 400, 500, 750, 1000, 1500, 2000, 2500, 3000, 3500, 4000, 5000, 6000, 7000, 8000, 9000, 10000</td>
</tr>
<tr>
<td><strong>Sector Snowflakes</strong></td>
<td>50, 100, 200, 300, 400, 500, 750, 1000, 1500, 2000, 2500, 3000, 3500, 4000, 5000, 6000, 7000, 8000, 9000, 10000</td>
</tr>
<tr>
<td><strong>Dendrite Snowflakes</strong></td>
<td>75, 101, 201, 277, 369, 526, 621, 759, 854, 976, 1073, 1430, 2076, 3113, 3558, 4151, 4981, 6227, 8302, 12454</td>
</tr>
</tbody>
</table>
Table 3. Frequencies and Temperatures used in the DDA computations

<table>
<thead>
<tr>
<th>Frequency (GHz)</th>
<th>13.4, 35.6, 94, 85.5, 118, 150, 166, 183, 220, 340</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature (°C)</td>
<td>0, -10, -20, -30, -40</td>
</tr>
</tbody>
</table>
Figure Captions:

Fig.1 Shapes of (a) columns and plates, (b) rosettes, (c) sector snowflakes and (d) dendrite snowflakes. The drawings are made of small dots that are the dipoles used in DDA model simulations.

Fig.2 Normalized (a) absorption, (b) scattering and (c) backscattering cross sections, and (d) asymmetry parameters at 340 GHz and -10 ºC for selected particles. Parameters of equal-mass spheres are also shown.

Fig.3 Phase functions for (a) long columns, (b) 6-bullet rosettes, (c) sector snowflakes, and (d) dendrite snowflakes at 150 GHz and -10ºC. In each diagram, five phase functions are drawn; each corresponds to an ice particle with its maximum dimension as shown in the legend.
Fig.1  Shapes of (a) columns and plates, (b) rosettes, (c) sector snowflakes and (d) dendrite snowflakes. The drawings are made of small dots that are the dipoles used in DDA model simulations.
Fig. 2 Normalized (a) absorption, (b) scattering and (c) backscattering cross sections, and (d) asymmetry parameters at 340 GHz and -10 °C for selected particles. Parameters of equal-mass spheres are also shown.
Fig. 3 Phase functions for (a) long columns, (b) 6-bullet rosettes, (c) sector snowflakes, and (d) dendrite snowflakes at 150 GHz and -10℃. In each diagram, five phase functions are drawn; each corresponds to an ice particle with its maximum dimension as shown in the legend.