On the Use of Scattering Kernels to Calculate Ice Cloud Bulk Optical Properties

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ABSTRACT

Nonspherical ice crystal optical properties are of fundamental importance to atmospheric radiative transfer through an ice cloud and the remote sensing of its properties. In practice, the optical properties of individual ice crystals need to be integrated over particle size distributions to derive the bulk optical properties of ice clouds. Given a particle size distribution represented in terms of size bins, the conventional approach uses the microphysical and optical properties of ice crystals at the bin centers as approximations to the bin-averaged values. However, errors are incurred when the size bins are large. To reduce the potential errors, a kernel technique is utilized to calculate the bulk optical properties of ice clouds by computing the bin-averaged values instead of using the bin-center values. Comparisons between the solutions based on the conventional method and the kernel technique for different numbers of size bins from in situ measurements demonstrate that the results computed from the kernel technique are more accurate. The present study illustrates that, for a given size distribution, 40 or more size bins should be used to calculate the bulk optical properties of ice clouds by the conventional method. Although the accuracy of bulk-scattering properties can be improved by using finer bin resolutions in the single-scattering property computation, the advantage of using a precomputed database of scattering kernels allows efficient computation of ice cloud bulk optical properties without losing the accuracy.

1. Introduction

Ice clouds remain one of the key uncertainty sources in the study of the atmospheric radiation budget and atmospheric remote sensing (Liou 1986; Lynch et al. 2002; Wendisch et al. 2007; Minnis et al. 1993a,b; Baum et al. 2000, 2005; Baran 2009, and references cited therein). These clouds also pose a challenge to atmospheric radiative transfer and remote sensing studies. As the optical properties of ice crystals are fundamental to quantifying the radiative properties of ice clouds, the atmospheric research community has made a significant effort to investigate the single-scattering properties of ice particles (Takano and Liou 1989a; Macke et al. 1996; Yang and Liou 1996; Borovoi and Grishin 2003; Baran et al. 2001; Baran 2004; Um and McFarquhar 2007; Zhang et al. 2009). For practical applications to atmospheric radiative transfer and remote sensing involving ice clouds, the single-scattering properties (i.e., the phase matrix, single-scattering albedo, asymmetry factor, and extinction cross section) of individual ice crystals need to be integrated over particle size and shape distributions to derive the bulk optical properties (Ebert and Curry 1992; Fu 1996; Key et al. 2002; McFarquhar et al. 2002; Baum et al. 2000, 2005). For example, Field et al. (2005, 2007) developed a moment estimation parameterization of the particle size
distribution for ice clouds, which had been used by Baran (2009) and Baran et al. (2011) to compute the bulk scattering properties for ice clouds.

In situ measurements (Heymsfield and Platt 1984; Heymsfield et al. 2002) of the ice crystal size distributions are essentially provided in terms of discrete bins. For each bin, the number concentration of ice crystals is assumed to be a constant. The conventional method of integrating the single-scattering properties of ice crystals over the size distribution is to use the microphysical properties (volume and area) and the single-scattering properties at bin centers, although some bins are quite large (e.g., the bin width may be as large as several hundred microns). In the literature, a coarse bin resolution of 5 bins (Takano and Liou 1989b; King et al. 2004) and relatively fine bin resolutions of 27 bins (Nasiri et al. 2002), 38 bins (Fu 1996), and 45 bins (Baum et al. 2005) have been used to discretize the size distribution. Nasiri et al. (2002) compared the bulk optical properties of ice clouds derived from using 5 and 27 bins to simulate the ice cloud microphysical and optical properties. Their results indicate that the ice cloud effective particle size and optical properties calculated from a given size distribution tends to be sensitive to the number of size bins. The intent of our study is to investigate the impact of resolving the bin variation of the single-scattering properties of ice crystals on the corresponding bulk scattering properties by utilizing the scattering kernel technique, which has been used to calculate the bulk optical properties of dustlike particles in the studies of King et al. (1978), Dubovik and King (2000), and Dubovik et al. (2006). This paper is organized as follows: Section 2 presents the formulas for computing the bulk optical properties of an ice crystal ensemble by the kernel technique, section 3 contains the results and discussion, and section 4 is a summary of the study.

2. Bulk optical properties of ice clouds
   and the kernel technique

The ensemble (or population) averaged single-scattering properties of individual ice crystals within ice clouds are usually referred to as the bulk optical properties of the clouds. In this study, the number concentration of ice crystals is indicated in terms of \( n(L) \), where \( L \) is the

![Figure 1](http://journals.ametsoc.org/doi/pdf/10.1175/JTECH-D-11-00034.1)

**FIG. 1.** Examples of size distributions discretized with (a) 5 bins (King et al. 2004) and (b) 38 bins (Fu 1996). (c),(d) As in (a),(b), respectively, but logarithmic scales are applied to the abscissas of (c),(d).
maximum dimension of an ice crystal. The quantity $n(L)$ is specified in terms of discrete bins and Fig. 1a shows one of the size distributions used in deriving ice cloud optical properties used for the Moderate Resolution Imaging Spectroradiometer (MODIS) collection 4 cloud product (King et al. 2004). Figure 1b shows one of the size distributions used by Fu (1996) that compiled 28 size distributions from the literature (Heymsfield and Platt...
1984; Mitchell and Arnott 1994). Figures 1c and 1d are the same as Figs. 1a and 1b, respectively, except that a logarithmic abscissa scale is used. From Fig. 1, it is evident that some of the size bins, particularly those for large particles, are quite coarse. Thus, using ice crystal microphysical (volume and projected area) and optical properties at the bin centers as surrogates for their bin-averaged counterparts may lead to substantial errors in deriving the bulk optical properties. To avoid the potential errors, the kernel technique can be employed. Dubovik and King (2000) and Dubovik et al. (2006) have formulated this technique for application to the calculation of the bulk optical properties of nonspherical dustlike particles. Following Dubovik and King (2000) and Dubovik et al. (2006), we briefly outline the kernel technique for application to the bulk optical properties of ice clouds.

For a given size distribution, the bulk scattering phase matrix of an ice cloud can be calculated as follows:

$$\mathbf{P}_{ij} = \frac{\int_{L_{\text{min}}}^{L_{\text{max}}} P_{ij}(\theta, L) Q_{\text{sc}}(L) A(L) n(L) dL}{\int_{L_{\text{min}}}^{L_{\text{max}}} Q_{\text{sc}}(L) A(L) n(L) dL}, \quad (1)$$

where the subscripts $i$ and $j$ indicate the $(i, j)$ element of the scattering phase matrix, the term $Q_{\text{sc}}$ indicates the scattering efficiency factor, and $A$ is the projected area of the particle.

Because the size distribution is specified in terms of discrete size bins and $n(L)$ does not vary within a given size bin, it follows that

![Figure 4](https://journals.ametsoc.org/doi/abs/10.1175/JTECH-D-11-00034.1)

**FIG. 4.** The scattering cross-section kernel as a function of size parameter at three wavelengths for (top) 5 and (bottom) 30 bins. The smoothed curved lines show the kernel of 4390 size bins, the step lines show the fine kernel calculated from the kernel technique, and the circles show the coarse kernel computed from the conventional method.
The scattering phase function kernel at the scattering angles of (top) 1° and (bottom) 60° as a function of size parameter at three wavelengths for (left) 5 and (right) 30 bins. The smoothed curved lines show the kernel of 4390 size bins, the step lines show the fine kernel calculated from the kernel technique, and the circles show the coarse kernel computed from the conventional method.

\[
\overline{K}_{ij} = \frac{\sum_{m=1}^{N} n_m \int_{L_{\text{min},m}}^{L_{\text{max},m}} P_{ij}(\theta, L) Q_{\text{sca}}(L) A(L) \, dL}{\sum_{m=1}^{N} n_m \int_{L_{\text{min},m}}^{L_{\text{max},m}} Q_{\text{sca}}(L) A(L) \, dL},
\]

where the term \( m \) indicates the size bin, \( N \) is the total number of the size bins used to discretize the size distribution, the terms \( L_{\text{min},m} \) and \( L_{\text{max},m} \) denote the lower and upper size limits for the \( m \)th bin, \( K_{ij,m} \) is the so-called kernel for the \((i, j)\) scattering phase matrix element, and \( K_{\text{sca},m} \) is the kernel for the scattering cross section.

The conventional approach for averaging the optical properties of individual ice crystals over the size distribution is to approximate the kernels using the relevant optical and microphysical properties at bin centers (e.g., in the following forms for \( K_{ij,m} \) and \( K_{\text{sca},m} \)):

\[
K_{ij,m} = P_{ij}(\theta, L_{\text{mid}}) Q_{\text{sca}}(L_{\text{mid}}) A(L_{\text{mid}}),
\]

\[
K_{\text{sca},m} = Q_{\text{sca}}(L_{\text{mid}}) A(L_{\text{mid}}),
\]
where \( L_{\text{mid},m} = (L_{\text{max},m} + L_{\text{min},m})/2 \) is the bin-center size for the \( m \)th bin. Since only the optical properties at bin centers are utilized, the kernels calculated from Eqs. (3) and (4) are much coarser.

In the present kernel method, \( K_{ij,m} \) and \( K_{\text{sca},m} \) are given by

\[
K_{ij,m} = \frac{1}{(L_{\text{max},m} - L_{\text{min},m})} \int_{L_{\text{min},m}}^{L_{\text{max},m}} P_{ij}(\theta,L)Q_{\text{sca}}(L)A(L) \, dL,
\]

(5)

\[
K_{\text{sca},m} = \frac{1}{(L_{\text{max},m} - L_{\text{min},m})} \int_{L_{\text{min},m}}^{L_{\text{max},m}} Q_{\text{sca}}(L)A(L) \, dL.
\]

(6)

Similarly, the kernels for the extinction cross section, volume, and projected area can be defined and are denoted as \( K_{\text{ext},m} \), \( K_{\text{vol},m} \), and \( K_{\text{area},m} \), respectively. The integrals in Eqs. (5) and (6) are computed based on numerical summation. The “subbins” of the \( m \)th bin in the numerical summation are consistent with the size bins of the ice crystal single-scattering property database that will be discussed in detail in section 3. It is evident from Eqs. (5) and (6) that the present kernels represent the bin-averaged values of integrands and resolve the variations of ice crystal optical and microphysical properties for each size bin. Mathematically, the relative errors in the conventional method arise from neglecting the variations of the number concentration, the optical properties, and the microphysical properties within size bins, whereas the errors in the kernel method are due only to neglecting the number concentration variation.

Because the conventional approach is, in principle, to approximate the kernels, it is a simplified kernel technique. However, in this paper, we refer to the kernel method as a special term for the approach based on Eqs. (5) and (6). To avoid ambiguity, the kernels calculated from the conventional method based on Eqs. (3) and (4) are referred to as “coarse kernels” and their counterparts based on Eqs. (5) and (6) as “fine kernels.”

3. Results and discussion

Ice crystals have various sizes and shapes (or habits) (Baran 2009; Zhang et al. 2004). For simplicity without the loss of generality, we will assume ice crystals to be hexagonal columns. The hexagonal column model for ice crystal habit has been extensively used in studies concerning ice clouds, particularly in the parameterization of the bulk optical properties (e.g., Ebert and Curry 1992; Minnis et al. 1993a,b; Fu 1996). The aspect ratios are taken from Mitchell and Arnott (1994) and Auer and Veal (1970):

\[
a/L = \begin{cases} 
0.35, & \text{for } L < 100 \mu m \\
3.5L^{-1/2}, & \text{for } L \geq 100 \mu m.
\end{cases}
\]

(7)

For a randomly oriented hexagonal column, \( A \) in Eqs. (1)–(6) is \( \frac{1}{4} \) of the surface area of the particle.

To derive the bulk scattering properties, the individual ice crystal optical properties are required. We consider three wavelengths at 0.66, 3.78, and 12.0 \( \mu m \), at which the refractive indices are 1.3078 + 1.66 \( \times 10^{-4} \), 1.384 306 + 7.055 \( \times 10^{-3} \), and 1.2762 + 4.133 \( \times 10^{-1} \) (Warren and Brandt 2008), corresponding to slight, moderate, and strong absorption, respectively. We use the Amsterdam DDA (ADDA) code (Yurkin et al. 2007) based on the discrete dipole approximation method (Purcell and Pennypacker 1973) and an improved geometric optics method (IGOM) (Yang and Liou 1996) to solve the light scattering by small and large ice crystals. Additionally, we incorporate the edge effect (Nussenzveig and Wiscombe 1980; Bi et al. 2011) into the IGOM solutions for the extinction and absorption efficiencies in the form of

\[
Q_{\text{ext,adjusted}} = Q_{\text{ext,IGOM}} + \frac{a}{x^{2/3}}.
\]

(8)

\[
Q_{\text{abs,adjusted}} = Q_{\text{abs,IGOM}} + \frac{b}{x^{2/3}}.
\]

(9)
where the subscripts ext and abs indicate extinction and absorption. The quantity $x$ is the size parameter and is defined in terms of the length of a hexagonal column as follows:

$$ x = \frac{\pi L}{\lambda} \quad (10) $$

where $\lambda$ is the wavelength of the incident light. The coefficients $a$ and $b$ in Eqs. (9) and (10) are determined to smooth the transition from the ADDA results to their IGOM counterparts. The presence of the edge effect of light scattering by nonspherical particles without local curvature is explained in Bi et al. (2010).

Figure 2 shows the extinction and absorption efficiencies computed from the ADDA (red line), the IGOM (green line), and their adjusted IGOM counterparts (blue line). Ice has negligible absorption at the 0.66-$\mu$m wavelength, and thus the absorption efficiency is not shown. Figure 2 indicates that the edge effect is important, and the incorporation of this effect leaves no discontinuity between the ADDA and IGOM results.

In the present study, a single-scattering property database is developed with a fine resolution with respect to the particle size (4390 size bins, specifically). The particle sizes, in terms of the maximum dimension $L$, range from 1 to 3500 $\mu$m with a step of 0.1 $\mu$m when $L \leq 100$ $\mu$m and a step of 1 $\mu$m when $L > 100$ $\mu$m. The bin resolutions are also used in the numerical evaluation of the integrals in Eqs. (5) and (6). Based on 4390 size bins, “exact” bulk-scattering properties can be obtained and are employed as a reference to assess the accuracy of the results computed from the conventional approach and the kernel technique with different numbers of size bins.
To derive the bulk-scattering properties, we generate three continuous particle size distributions by fitting three chosen particle size distributions in Fu (1996) (see Fig. 3). Given a size distribution, based on the definition of kernels, the commonly defined effective particle size (Foot 1988; Baum et al. 2000; King et al. 2004) can be calculated as follows:

\[ D_e = \frac{3}{2} \sum_{m=1}^{N} n_m K_{\text{vol},m}(L_{\text{max},m} - L_{\text{min},m}) \]

The effective particle sizes associated with the three generated size distributions are 20.1, 116.1, and 185.2 \( \mu m \), respectively. The values of the three effective particle sizes are not the same as those reported by Fu (1996) because, although the ice crystal shapes are also assumed to be hexagonal, the aspect ratios defined in Fu (1996) and in the present study are different.

To test the errors for both methods in the cases of different numbers of size bins, we discretize the size distributions into a number of size bins. To be more specific, three continuous size distributions as shown in Fig. 3 are discretized into 5, 10, 20, 30, 40, 50, 60, 70, 80, 90, and 100 size bins in equal logarithmic steps from 1 to 3500 \( \mu m \). We recalculate the bulk properties using the kernel method and the conventional method for each number of size bins. By comparing the results with the benchmark based on 4390 size bins, we investigate the relative errors of both methods and examine at which number of size bin the conventional method and the kernel method give similar results.

Figure 4 shows the comparisons of scattering cross section kernels as a function of size parameter calculated by using the kernel technique and the conventional
method for the cases of 5 and 30 size bins, respectively, at 0.66-, 3.78-, and 12.0-μm wavelengths. The scattering cross section kernels (smooth lines) based on 4390 size bins calculated from the conventional method are also included. The step lines show the fine kernels calculated from the kernel technique and the circles show the coarse kernels computed from the conventional method. The colors represent different wavelengths. The kernels computed from the conventional method and the kernel technique are different values within a wide size bin. The solution based on the kernel method is an accurate bin-averaged value, whereas its counterpart from the conventional method is an inaccurate approximation. However, the differences of the two solutions decrease with the decrease of the size-bin width, as is illustrated by the lower panel of Fig. 4.

Figure 5 shows the scattering phase function kernel at the scattering angles 1° and 60° as a function of size parameter at three wavelengths. From Fig. 5, the differences between the kernels from the conventional and the present methods, especially for coarse size bins, can be seen. Therefore, the advantage of the present kernel method over the conventional method is that more accurate bulk-scattering properties can be obtained even if a coarse bin resolution is used.

Figure 6 shows the comparison between the relative errors of the effective particle sizes calculated from the kernel technique and the conventional approach as functions of the number of discrete size bins for the three size distributions shown in Fig. 3. The relative error of the effective particle size is defined as \( \delta_D = \left| \frac{D_{e} - D_{eo}}{D_{eo}} \right| \times 100\% \), where \( D_{e} \) indicates the effective particle size calculated from either the conventional method or the kernel method and \( D_{eo} \) indicates the “true” effective particle size calculated from a fitted continuous distribution based on 4390 size bins. From Fig. 6, it is evident that the relative errors of the effective particle size from the conventional approach exceeds 10% when using less than 10 bins, and the relative errors of the effective particle size calculated from the kernel technique are much smaller for all the three particle size distributions. The results indicate the kernel technique can significantly improve the accuracy of effective particle size, particularly when the number of size bins is smaller than 40. For both methods, the relative differences decrease with the increase in the number of size bins. The
difference between the two methods is less than 1% when the number of size bins is larger than 40.

Figures 7–9 show the comparison of the relative errors of the extinction efficiency, asymmetry factor, and albedo, calculated from both the kernel technique and the conventional approach as functions of the number of discrete size bins for a set of three particle size distributions at the three wavelengths of 0.66, 3.78, and 12.0 $\mu$m. The absorption of ice particles is negligible at the 0.66-$\mu$m wavelength and the single-scattering albedo is 1.0, which is not shown in Fig. 9. The relative error is defined as $\delta = |F - F_o|/F_o \times 100\%$, where $F$ indicates the bulk optical properties (the extinction efficiency, asymmetry factor, and single-scattering albedo) calculated from both the kernel technique and the conventional method for 5–100 size bins and $F_o$ indicates the value calculated based on 4390 size bins. From Fig. 7, the differences of the extinction efficiency between the two methods are obvious for a small number (<30) of size bins. The values of the relative errors from the kernel technique are much less than those from the conventional approach and indicate that the kernel technique can improve the accuracy of the bulk extinction efficiency for cases using fewer size bins. The difference decreases with an increase in the number of size bins used. Both methods get similar results when the number of size bins is larger than 50. Note that both relative differences are under 0.5% for the 40 size bins case.

As an important quantity in radiative transfer simulation, the asymmetry factor ($g$), the first moment of the scattering phase function, indicates the relative strength of forward scattering. The radiative fluxes, especially for shortwave fluxes, at the surface and the top of the atmosphere are highly sensitive to the uncertainties in the asymmetry factor. Vogelmann and Ackerman (1995) investigated the sensitivity of net shortwave fluxes to the uncertainties in cirrus cloud scattering properties and found that uncertainties on the order of 1% in a typical cirrus cloud asymmetry factor ($g \sim 0.8$) could lead to uncertainties on the order of 2.5% in net surface fluxes.
Fu (2007) showed that the uncertainties in the global cloud albedo are approximately ±0.06 in conjunction with the uncertainties of ±0.05 in an asymmetry factor of 0.8. Figure 8 is similar to Fig. 7 but compares the relative errors associated with the bulk asymmetry factor. The differences in the asymmetry factor derived from the two methods are obvious for the size bins less than 30 and indicate that the kernel technique can also improve the accuracy of the bulk asymmetry factor when using fewer size bins. The relative differences decrease with an increase in the number of size bins used. The relative differences between both methods can be under 0.2%, which is much less than the requirements determined in previous studies (Vogelmann and Ackerman 1995; Fu 2007), when the number of size bins is larger than 40. Both methods get similar results when the number of size bins is larger than 50.

From Fig. 9, it can be seen that the relative errors of the single-scattering albedo calculated from the kernel technique are less than those from the conventional approach, and the differences of the single-scattering albedo between the two methods are obvious for the size bins less than 30. The kernel technique can improve the accuracy of the single-scattering albedo when using fewer size bins. The relative errors from both methods are under 0.1% for the number of size bins larger than 30, but both methods get similar results when the number of size bins is larger than 40.

Figures 10–12 show the comparison of the bulk phase functions calculated from both methods for various numbers of size bins at the 0.66-, 3.78-, and 12.0-μm wavelengths. It can be seen that the biggest difference of the bulk phase functions from both methods occurs with 10 size bins, and the difference tends to be smaller with an increase in the number of size bins. When the number of size bins is 60, the phase functions obtained from both methods are approximately the same.

Figures 7–12 show the deviations of the scattering properties from both methods for three given size distributions with the so-called true effective particle sizes of 20, 116, and 185 μm. However, since the effective particle sizes calculated from two methods are different and also deviate from the true values, the compared scattering properties actually correspond to different
effective particle sizes. Figure 13 shows the single-scattering albedo versus the effective particle size calculated from both methods for different numbers of size bins at the wavelengths 3.78 μm (left column) and 12 μm (right column). The red circles indicate the results calculated from the kernel technique and the blue squares indicate the results based on the conventional approach. When the effective particle sizes calculated from two methods are similar, the corresponding single-scattering albedo values are in agreement. However, the ranges of the effective particle sizes computed from both methods are quite different. Nasiri et al. (2002) showed that using different bin resolutions for a given size distribution in the simulation of the bulk scattering properties of ice clouds can modify the reflectance simulation. However, since the effective particle size and single-scattering properties vary consistently, as clearly illustrated by Fig. 13, the net effects may have little impact on the relation between the simulated reflectance and effective particle size (i.e., the dependence of the simulated reflectance on the effective particle size) (King et al. 2004).

4. Summary

To study the differences of the bulk single-scattering properties of ice crystals derived from the kernel technique and the conventional approach, three wavelengths at 0.66, 3.78, and 12.0 μm, corresponding to cases with slight, moderate, and strong absorption, respectively, are considered. The shape of an ice crystal is assumed to be a hexagonal column. The optical properties of individual ice crystals are calculated from the ADDA code and an improved geometric optics method (IGOM). The edge effects are incorporated in the IGOM solutions for the extinction and absorption efficiencies.

“Exact” bulk-scattering properties are first obtained based on 4390 size bins. Both the kernel technique and the conventional approach are utilized to calculate the bulk optical properties of ice clouds based on various size bins from 5 to 100 and then compared with the exact results. It is demonstrated that the kernel technique can uncover more delicate kernel information and improve the accuracy of the bulk microphysical and optical properties of
ice crystals when the number of size bins is less than approximately 30. However, the differences are much smaller when using more than 40 size bins and both methods give similar results, which implies that more than 40 size bins should be used to calculate the bulk optical properties of ice clouds by the conventional method.

It is not efficient to obtain bulk scattering properties in various applications based on the single-scattering database of fine-bin resolution. A more proper approach is to compute the scattering kernels from the scattering database of fine bin resolution. Consequently, bulk scattering properties can be efficiently obtained from the database of scattering kernels without losing accuracy.

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