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The applicability of physical optics in the millimetre and sub-millimetre spectral region. Part I: The ray tracing with diffraction on facets method

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ABSTRACT

Future satellite missions, from 2022 onwards, will obtain near-global measurements of cirrus at microwave and sub-millimetre frequencies. To realise the potential of these observations, fast and accurate light-scattering methods are required to calculate scattered millimetre and sub-millimetre intensities from complex ice crystals. Here, the applicability of the ray tracing with diffraction on facets method (RTDF) in predicting the bulk scalar optical properties and phase functions of randomly oriented hexagonal ice columns and hexagonal ice aggregates at millimetre frequencies is investigated. The applicability of RTDF is shown to be acceptable down to size parameters of about 18, between the frequencies of 243 and 874 GHz. It is demonstrated that RTDF is generally well within about 10% of T-matrix solutions obtained for the scalar optical properties assuming hexagonal ice columns. Moreover, on replacing electromagnetic scalar optical property solutions obtained for the hexagonal ice aggregate with the RTDF counterparts at size parameter values of about 18 or greater, the bulk scalar optical properties can be calculated to generally well within $\pm 5\%$ of an electromagnetic-based database. The RTDF-derived bulk scalar optical properties result in brightness temperature errors to generally within about ± 4 K at 874 GHz. Differing microphysics assumptions can easily exceed such errors. Similar findings are found for the bulk scattering phase functions. This finding is owing to the scattering solutions being dominated by the processes of diffraction and reflection, both being well described by RTDF. The impact of centimetre-sized complex ice crystals on interpreting cirrus polarisation measurements at sub-millimetre frequencies is discussed.

1. Introduction

The application of sub-millimetre radiometry to the study of microphysics of ice clouds has been an active area of research since about the latter part of the 1990s. For example, studies by [1–4] have shown that the sub-millimetre part of the spectrum is very sensitive to the column-integrated ice water content (IWC), the ice water path (IWP), and the size distribution function of ice particles (PSD). This is because atmospheric ice at sub-millimetre frequencies is weakly absorbing, relative to scattering; therefore, the upwelling radiance emitted from below the ice cloud (i.e. from the surface, the gaseous atmosphere, the water, and the mixed phase cloud below the cirrus) is largely scattered, rather than absorbed. This means that the scattered radiance received by a radiometer above the ice cloud will be depressed, relative to clear-sky radiance (owing to the radiance being scattered out of the line of sight of the instrument as a result of multiple scattering and internal cloud scattering).

However, as frequency increases, so does the water vapour continuum [5]. This increase in the water vapour continuum will depend on the location and/or the time of year and may ultimately limit the sensitivity of the sub-millimetre region to particular properties of ice cloud microphysics. This is because the brightness temperature depressions caused by an increase in atmospheric water vapour loading may also be large and compete with the brightness temperature depressions caused by the ice cloud in certain situations, such as semi-transparent cirrus occurring lower in the atmosphere. However, to account for this water vapour loading effect on brightness temperature depressions, it is usual to retrieve water vapour loading from the microwave region, but this also requires an accurate understanding of the water vapour continuum, not only throughout the microwave region, but also

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throughout the sub-millimetre region. Unfortunately, the current understanding of the water vapour continuum in both microwave and sub-millimetre regions is poor [6], as brightness temperature differences between water vapour continuum models can be as large as 5 K across the microwave and sub-millimetre spectrum [7].

As previously discussed, atmospheric ice at sub-millimetre frequencies is weakly absorbing; therefore, the observed brightness temperature depressions are weakly dependent on the temperature of the atmosphere, but are, instead, more directly related to the IWP [1]. This direct dependence of brightness temperature depression on ice cloud microphysics is a distinct advantage of the sub-millimetre region over the infrared and microwave regions of the spectrum. As the IWP is not directly related to the measured radiance in those two spectral regions, the interpretation of the measurement strongly depends on prior assumptions about the size, orientation, shape and mass of the ice crystals. In the case of the infrared region, the measurement is also dependent upon the temperature of the atmosphere, and in the case of radar reflectivity, its interpretation depends on assumptions about the mass and size of ice crystals. In the latter case, both the mass and the size of ice crystals can be simply related to radar reflectivity through the Rayleigh–Gans approximation [8–10]. However, measurements from across the spectrum should be seen as complementary. For instance, the solar and infrared region will be sensitive to IWP values as low as about 0.5 and as high as about 1000 g m^{-2} [11]. Radar reflectivity will be sensitive to the middle and upper ranges of solar and infrared IWP sensitivity, but it will also significantly exceed the upper range in solar and infrared sensitivity by a number of factors. The sub-millimetre region will be sensitive to a continuum of IWP between radar reflectivity, and solar and infrared sensitivities. Thus, the sub-millimetre region can act as an important constraint on retrievals of ice cloud properties using radar, solar and infrared radiometric measurements. This is why sub-millimetre instrumentation is required on board aircraft, such as the International Sub-millimetre Airborne Radiometer (ISMAR) [12,13], and in space to measure the total amount of ice mass contained in Earth's atmosphere. Ultimately, such measurements will help to constrain both climate and numerical weather prediction (NWP) models in their prediction of ice mass and the characteristic size of the PSD through their assumed ice microphysics properties.

Of course, the interpretation of microwave and sub-millimetre brightness temperature depressions will still depend on assumptions about the PSD, ice crystal shape, mass and orientation of the hydrometeors, all of which are currently subject to a considerable degree of uncertainty; see, for instance, the following review articles by [14,15], and references contained therein. The main difficulty in interpreting millimetre and sub-millimetre radiometry is relating the measured brightness temperature depression to an assumed crystal geometry that is consistent with observed mass– and density–size relationships. This further requires representative PSDs that are valid in the mid-latitudes and tropics. In the microwave region, various microphysics assumptions can lead to very large differences in simulated cirrus brightness temperatures. For instance, in Ref. [16] it is shown that at frequencies centred on 183 GHz, and by assuming a number of PSD parameterisations and density–size relationships, these various assumptions can lead to simulated upwelling brightness temperature differences at top-of-the-atmosphere (TOA) greater than 12 K and 30 K, respectively. Moreover, more recent work by Ref. [17] has shown that different PSD assumptions to represent the centre microphysics of Hurricane Irene can also lead to brightness temperature differences between the model and observations on the order of about 50 and 70 K at about 183 GHz at TOA. In the sub-millimetre region, Ref. [18] shows that on assuming realistic microphysical variability to generate a variety of cloud states constrained by radar measures of IWC, simulated brightness temperature differences of about 40 and 70 K between about 334 and 874 GHz, respectively, can be realised between the differing cloud states. This range in brightness temperature differences in the sub-millimetre region, between the cloud states, also demonstrates the sensitivity of this spectral region to ice microphysics, such as PSDs, ice crystal shape, and density.

To facilitate the simulation of cirrus brightness temperatures at millimetre and sub-millimetre frequencies, there are now a couple of publicly available single-scattering databases of ice crystals. See, for instance, the databases developed by Refs. [19] and [20]. These databases are based on the discrete dipole approximation (DDA), which was developed by Ref. [21], to calculate the single-scattering properties of their assumed ice crystal models. The application of the DDA method at the time limited either the range in frequency or the maximum dimension of ice crystals that could be considered in the construction of each of the databases. In the case of Ref. [19], the frequency does not exceed 340 GHz, and in the case of Ref. [20], the maximum dimension of ice crystals does not exceed 2 mm. Aircraft-based cirrus and ice cloud field campaign in-situ measurements have shown that the maximum dimensions of ice crystals can be significantly greater than 2 mm. Indeed, ice crystal aggregates can grow to maximum dimensions of several centimetres; see, for instance, Refs. [22–24]. However, the databases described above do consider a variety of ice crystal shapes, such as solid and hollow hexagonal ice columns, three-dimensional bullet rosettes, sector snowflake models, and hexagonal ice aggregates, among others. Moreover, Ref. [19] considers four temperatures, between 0 °C and −40 °C, whereas Ref. [20] considers a single temperature of −30 °C. Recently, Ref. [25] has demonstrated that absorption by atmospheric ice at sub-millimetre frequencies has a strong dependence on temperature. A further source of uncertainty in the calculation of single-scattering properties of atmospheric ice is their assumed dielectric properties in microwave and sub-millimetre regions. For instance, Ref. [26] notes differences in the absorption properties of ice crystals having the same mass of ice between Refs. [19,20], which was found to be due to different complex refractive indices being used to construct the two single-scattering databases. Moreover, Ref. [26] recommends the complex refractive indices of atmospheric ice compiled by Ref. [27] to calculate the single-scattering properties of ice crystals at millimetre and sub-millimetre frequencies.

A more recent single-scattering database of atmospheric ice has been made available by [28]. In that paper, 16 ice crystal models are considered, including single solid and hollow hexagonal ice columns, solid hexagonal plates, solid and hollow bullet rosettes, and hexagonal ice aggregates consisting of column and plate aggregations, among other ice crystal models. The maximum dimensions of each of the ice crystal models range between 2 and 10,000 μm, in 24 bins, where the latter sizes are more resolved. The assumed microphysical properties of the ice crystal models that comprise the database are described in Ref. [29]. The single-scattering properties of the various randomly oriented ice crystal models have been calculated at four temperatures, ranging between −113 and −3 °C, and between the frequencies of 1 and 874 GHz, assuming the complex refractive indices for ice compiled by Ref. [30]. The single-scattering calculations are based on the invariant imbedding T-matrix method of Ref. [31], at most size parameters in the database. At a few of the larger size parameters, the improved geometric optics method of Ref. [32] is applied at the higher frequencies in the database. At these particular size parameters, so-called “edge effects” are applied to the efficiency factors and to the single-scattering albedo to account for the above-edge and grazing incidence of rays, occurring either above the particle or at its edge, respectively [29,33,34]. These effects must be parameterised into the physical optics method, as it does not