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Assessing the uncertainties of the discrete dipole approximation in case of melting ice particles

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ABSTRACT

We studied the applicability of the Discrete Dipole Approximation (DDA) for scattering by partially melted snowflakes in the microwave region. The DDA accuracy in the case of a liquid water coated ice sphere was tested at various particle sizes, water layer thicknesses, frequencies and DDA grid resolutions. We found that the backscattering and absorption cross section show the largest biases with respect to the Mie reference. The highest discrepancies were found for the thinnest water coating and the lowest frequency. We applied a previously published method to separately analyze the errors due to the representation of particle shape and discretization. The accuracy of the DDA seems to decrease particularly when only a single dipole is used to represent some structural element of the target with large refractive index. A similar behavior was also found by testing the variation of the scattering properties of complex shaped melting snowflakes at different grid resolutions. From both experiments we conclude that single isolated water dipoles should be avoided when modeling the scattering properties of melting snowflakes in the microwave using DDA. Although we found that a stability criterion which is commonly used for pure ice particles is not sufficient for melting particles, the DDA results in general converge to the exact Mie solution when shape and discretization errors are reduced by using a refined grid.

1. Introduction

A key requirement of cloud and precipitation remote sensing techniques in the microwave is an accurate knowledge of the hydrometeors' scattering and absorption properties. During the last decade, the number of available scattering databases for various frozen hydrometeors has largely increased [1]. A growing number of databases not only include single idealized ice crystals but also complex particles such as aggregates, rimed, and melting particles. The majority of these datasets utilize the Discrete Dipole Approximation (DDA) because open-access software packages are available (e.g. DDSCAT, [2] or ADDA, [3]); DDA has further been extensively tested for various particle geometries and size parameters.

Melting ice particles are of particular interest for microwave remote sensing applications. The large difference of the refractive index between ice and liquid water dramatically alters the scattering and absorption properties of the ice particles during the melting process. The so-called radar bright-band is mainly a result of the onset of melting as the snow particles fall through the melting layer (ML). The characterization of the scattering and absorption properties of the ML is an important issue e.g. for remote sensing of rainfall from space ([4–6] among others). Scattering properties of melting ice particles also play an important role for the detection and classification of hail (dry versus melting hail) using polarimetric precipitation radars (e.g., [7]).

Only a few datasets currently exist which use DDA to calculate the scattering properties of complex melting snowflakes [8–11]. The most common way to calculate the scattering properties of melting particles is to approximate them with spheroidal shapes and assuming an effective refractive index of the air-ice-liquid water mixture inside [12–15]. Especially when higher frequencies are used, it has been found that these approximations becoming inaccurate. For example, [10] compare spheroids calculated using the T-Matrix method [16] to realistically shaped snowflakes calculated with the generalize multiparticle Mie solution [17]. They find large differences (up to 7dB at Ka-Band) which they suspect to be related to how the effective medium approximation is used. Also melting hail and graupel are usually approximated with layered spheres or spheroids [7] but comparisons with DDA simulations reveal some differences especially for polarimetric variables [18].

This study was partly motivated by discussions of a larger group of scattering experts and ice particle scattering database developers at the recent First International Summer Snowfall Workshop [1]. A particular discussion topic was related to the question under which conditions DDA is a suitable technique to simulate ab-

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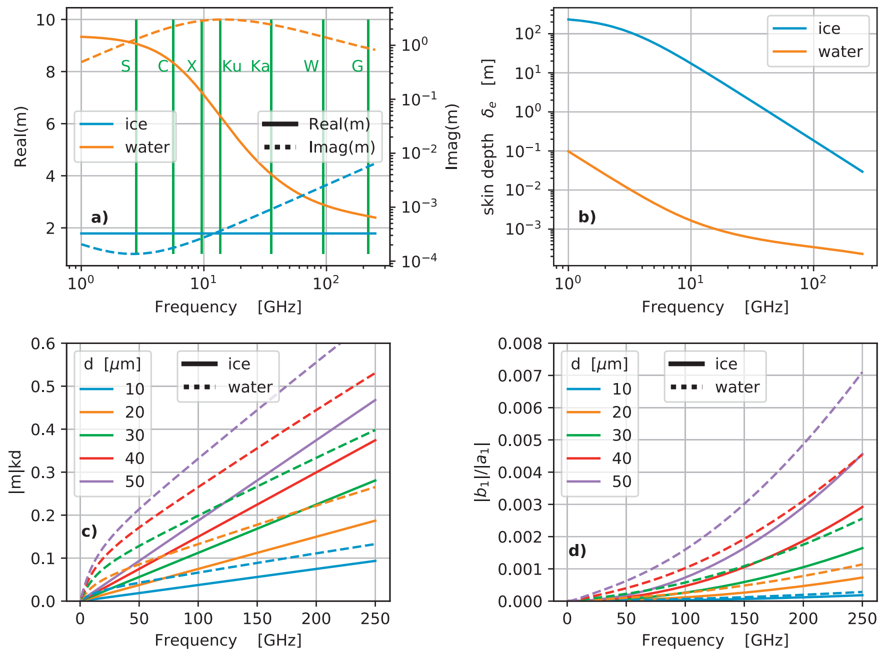

Fig. 1. (a) Real (continuous line, left axis) and imaginary (dashed line, right axis) part of the refractive index of water (orange) and ice (blue) at 0° as a function of frequency. The seven frequencies used in the present studies are marked as vertical lines. (b) Skin depth δ_e as a function of frequency for water and ice. (c) DDA discretization parameter $|m|kd$ as a function of the frequency of the incident electromagnetic wave for ice (continuous line) and water (dashed lines). The different colors correspond to different values of the inter-dipole spacing d ranging from 10µm to 50µm. (d) Relative magnitude of the induced magnetic dipole moment with respect to the electric moment; the line-style is the same as in panel (c). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

sorption and scattering properties of melting ice particles. As discussed e.g. in [19], two main sources of errors in DDA calculations have been intensively investigated: How well is the shape of the particle represented by a finite number of regular elements in a cubic lattice? A common example for this “shape error” is the attempt to approximate the shape of a sphere by the cubic DDA grid (Fig. 2). The second error source is related to the question how many dipoles are needed in order to discretize the electromagnetic field within the particle. For example, if we want to calculate the scattering properties of a cube, the shape error would be null but we still would need to decide how many dipoles to include in order to accurately represent the spatial variations of the electromagnetic field inside the volume element. Yurkin et al. [19] investigated the importance of both error sources using various discretization of spheres with a single refractive index. They found that for different scattering variables the shape or the discretization error can dominate and hence both errors have to be taken into account.

The applicability of DDA to a particular scattering problem is commonly verified by ensuring that $|m|kd < 0.5$ [2]; which m being the complex refractive index, k the wavenumber, and d the inter-dipole distance. Using $d < 40$ µm conforms with this criterion for liquid water and ice up to 220 GHz as shown in Fig. 1. The particular threshold value for the $|m|kd$ parameter has been derived by DDA experiments on weakly absorbing particles [20] and might not be sufficient when a substance with high refractive index (e.g. water at microwave) are employed. Draine [21] originally proposed two separate criteria (both related to the discretization error) for checking the validity of DDA results. The first criteria ensures that the characteristic scale of variation of the electric field within the particle, i.e. the *skin depth* $\delta_e = 1/k\mathrm{Im}(m)$ is large compared to d. The second criteria verifies the assumption that the scatterer is composed of electric dipoles neglecting the magnetic dipole effects. The skin depth for water is two to three orders of magnitude smaller than for ice at microwave frequencies (Fig. 1) and ranges from 1cm at S-band to 0.2 mm at G-band. The relative magnitude of the magnetic dipoles effect is estimated by assuming the DDA polarizable volumes to be equivalent volume spheres and computing the ratio between magnitude of the coefficients b_1 and a_1 of the relative Mie series expansion [22]. In Fig. 1 it is shown that the relative magnitude of the magnetic dipoles is always at least two orders of magnitude smaller than the correspondent electric dipole even for the coarsest used resolution (50 µm).

A common approach to assess the DDA uncertainty is to compare DDA simulations for homogeneous spheres or spheroids with exact solutions such as Mie theory or T-Matrix method. Considering the obvious problem of approximating a sphere with a cubic lattice and taking into account the strong interference effects due to the spherical shape, one can see a sphere as the most challenging test for the DDA. In case of melting ice particles, we have to use a structure of ice and liquid water which have very different m in the microwave. In order to not introduce additional uncertainties with effective medium approximations, we will use an ice spheres with an outer layer of liquid water for which exact Mie solutions can be calculated. Tyynelä et al. [23] also compared DDA with layered ice spheres and find large differences; the DDA errors in general increase with smaller thicknesses of the liquid layer and are largest for absorption cross sections. Unfortunately, they did not further investigate how fine the dipole grid has to be in order to keep the errors below a certain threshold. Zubko et al. [22] find similar to [21] for absorbing particles that the dipole resolution should be a few times smaller than the depth of the skin layer.

In this study, we extend the tests done by previous studies to provide some useful guidelines for future scattering calculations of complex melting particles [24,25]. At first, we simulate liquid coated spheres at sizes between 4 mm and 2 cm and various thicknesses of the liquid layer for 7 frequencies covering typical precipitation and cloud radar frequencies. These calculations allow us to infer how the errors change with varying discretization and representation of the shape. We also perform experiments with a complex melting snowflake structure using DDA and only changing