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How accurate is the Discrete Dipole Approximation for melting ice particles? A comparison against exact scattering techniques

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The number of single scattering databases containing realistically shaped ice particles increased dramatically during the last decade. The particle types comprised in those databases are largely dominated by pristine, non-spherical ice crystals and ice crystal aggregates. Very few initial attempts have been made toward simulating rimed particles and partially melted snowflakes due to the additional complexity given by the simulation of riming and melting dynamics. In particular, the modeling of the melting process requires a huge theoretical and computational effort due to the large number of physical interactions that have to be accurately simulated.

Single scattering properties of complex shaped ice particles at microwave frequencies have been generally computed using the Discrete Dipole Approximation (DDA) technique which assumes arbitrarily shaped particles to be represented by a cluster of polarizable cubic regions and has been found to adequately represent particle electromagnetic scattering in the single-phase ice case if a sufficiently high resolution of the particle modeling with respect to the simulated electromagnetic wavelength is used. On the other hand, the accuracy of the DDA method in case of melting ice particles has been debated due to the huge gradients in dielectric permittivity between water and ice at microwave frequencies that can potentially introduce numerical instabilities.

The accuracy of the DDA technique for representing scattering properties of melting particles has been investigated in the special case of layered spheres for which an analytical solution of the scattering problem exists. In the presented numerical experiments, the layered sphere has been designed with a progressively thinner outer water shell to investigate the effect of geometric misrepresentation of spherical shapes and to analyze the response of simulated scattering properties to increasing dielectric gradients.

In order to separate the distinct sources of modeling error, namely the geometric representation problem and the intense dielectric gradient, tests with increased volumetric resolution have been performed. The performances of the DDA algorithm has been tested for very large particles (up to 20 mm wide) and up to high frequencies (220 GHz). An in-depth analysis has been carried out by comparing internal electric fields in cases where largest discrepancies in the simulated radiative properties have been observed.

As expected, largest errors are found when the outer water layer is thinnest. With increasing particle diameter the relative error in the computed scattering properties appears to decrease, suggesting that the geometrical misrepresentation of the spherical shell by clusters of cubes is the main source of simulation error. This was confirmed by the reduced computational error obtained by increasing the DDA volume resolution. Results suggest that the numerical error introduced by DDA in the computation of the scattering properties of melting ice particles is small within the parameter range investigated. These uncertainties can be considered to be negligible considering uncertainties introduced by other unknowns such as particle size and shape.