Systematic correlation between aerodynamic shape factor and optical properties

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There are many scientific researches of the influence of non-spherical aerosol particles to optical properties and fluid dynamics. Either for the optics or the fluid dynamics exist semi-theoretical approaches up to complex numerical simulations.

To obtain an physically consistent, plausible approach, we have to consider the morphology entirely, e.g. an optical closure with an particle number size distribution measured with an aerodynamic based instrument. When an aerodynamic shape factor is used to correct the size distribution, using Mie theory to calculate optical properties of this particle population must be critically questioned.

Because simulations of optical properties for arbitrary shaped particles (especially discrete dipole approximation) need a lot of numerical power, we have to find an useful but simple optical shape factor. Simultaneously, to further simplify the fact of particle morphology, we have to analyse the correlation between this optical shape factor and the aerodynamic shape factor. This would lead to a simple but useful approach to consider the manifold influence of the particle morphology.

Numerical simulations

In a first step, numerical simulations were accomplished for a moderate number of particle shapes, from simple ellipsoids, cylinders, cuboids (prolate and oblate) up to realistic looking arbitrary shaped particles.

To calculate the aerodynamic shape factor, we used a modified version of “stkSolver” (Fernandez, 2006). The results of some characteristic shapes, such as a cube or cylinders, are in a good agreement with values from literature.

Depending on the particle shape the optical properties were calculated using T-Matrix method (MIESCHKA, Rother, 2009) or DDA (ADDA, Yurkin & Hoekstra, 2011). The maximum simulated size parameter was 30, which is a moderate value to investigate the influence of particles morphology to coarse mode particles (lowest super micron range).

Results

With a focus on the systematic deviations for dust events, the primary aim is to investigate the influence of particle shape to the scattering coefficients. For all particle shapes, the scattering coefficients were calculated using fictive log normal distributed particle populations with a mean size parameter from 0.3 to 10.

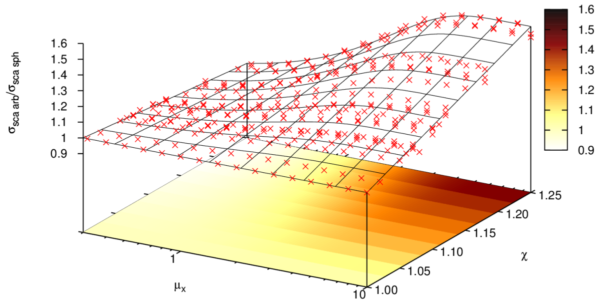

Figure 1. 2D scattering plot of the signal increase for the scattering coefficient of the arbitrary shaped particle to the volume equivalent sphere as a function of the mean size parameter μ_x and the aerodynamic shape factor χ.

The numerical results show a good correlation of the aerodynamic shape factor and the increase of the scattering coefficients relative to the volume equivalent sphere for all particle shapes and mean size parameters larger than approx. 3. Smaller particles act like the volume equivalent sphere, independently of their morphology.

This surprising result is based on the fact that larger particles scale with their geometrical cross section in contrast to smaller particles, which scale with the volume (Pollack & Cuzzi, 1979). In general, for non spherical particles the ratio of orientation averaged cross section equivalent diameter to the volume equivalent diameter increases. The aerodynamic shape factor itself can also be approximated using inter alia these both diameters (Leith, 1997), which leads to this positive correlation. As a consequence, the aerodynamic shape factor seems to be already sufficient to estimate the signal increase of the scattering coefficient for non spherical particle.

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