

SHAPE DEPENDENCY OF THE EXTINCTION AND ABSORPTION CROSS SECTIONS OF DUST AEROSOLS MODELED AS RANDOMLY ORIENTED SPHEROIDS

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ABSTRACT. We present computational results on the shape dependency of the extinction and absorption cross sections of dustlike aerosol particles that were modeled as randomly oriented spheroids. Shape dependent variations in the extinction cross sections are largest in the size regime that is governed by the interference structure. Elongated spheroids best fitted measured extinction spectra of re-dispersed Saharan dust samples. For dust particles smaller than $1.5 \mu\text{m}$ in diameter and low absorption potential, shape effects on the absorption cross sections are very small.

1. Introduction

For a better assessment of the radiative impact of mineral dust aerosols, accurate wavelength dependent complex refractive indices in the UV/VIS spectral region of natural dust samples are needed [1]. These are the basic input parameters for the calculation of the single scattering properties of dust aerosols. In a laboratory aerosol chamber study, we have measured wavelength-resolved aerosol extinction and absorption coefficients of five Saharan dust aerosol samples with different mineralogical compositions [2]. The elemental and mineralogical composition of the soil samples was thoroughly characterized by bulk and single particle X-ray Fluorescence and X-ray Diffraction analyses. Applying an inversion scheme based on a spheroidal dust model, we have retrieved complex refractive indices from the optical measurements with the simultaneously recorded aerosol number size distributions as the required input data. Our findings show that the absorption potential of the dust samples crucially depends on the content of iron oxides like hematite and goethite. We analyze how accurately these retrieved complex refractive indices agree with those calculated by applying mixing rule approaches using tabulated refractive indices of the identified mineralogical constituents. In this extended abstract, we present selected results on the shape dependency of the optical cross sections of the dust aerosols which had

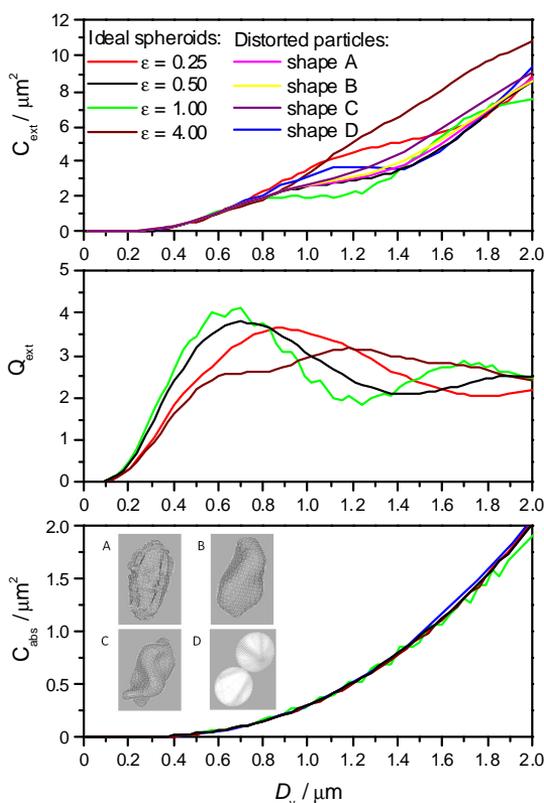


Figure 1. Shape dependent extinction and absorption cross sections (top and bottom panels) as well as extinction efficiencies (middle panel) for ideal spheroids and distorted particle shapes. Random particle orientation is assumed. See text for details.

to be considered in the retrieval procedure. A complete overview about the experiments is given in our full manuscript [2].

2. Modeling

The shape dependent extinction and absorption cross sections of the spheroidal dust particles were computed for 29 logarithmically equidistant aspect ratios, ϵ , between 0.25 (prolate shape) and 4.0 (oblate shape). For each aspect ratio, three dimensional look-up tables were calculated, covering 88 logarithmically spaced size parameters between 0.02 and 50, 11 linearly spaced grid points between 1.3 and 1.7 for the real part of the complex refractive index, and 15 logarithmically spaced values between 0.0001 and 0.1 for the imaginary part of the complex refractive index. The computations were done, if stable convergence was guaranteed, with the T-matrix code by Mishchenko and Travis [3]. Above

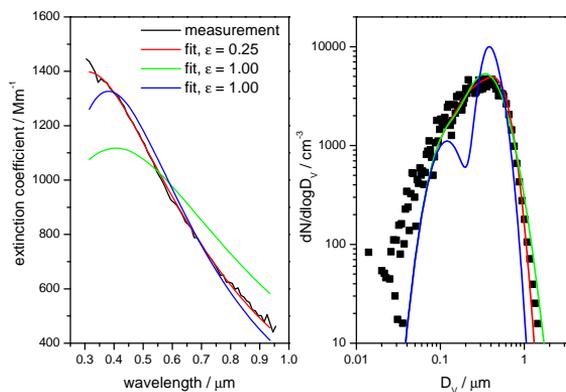


Figure 2. Measured extinction spectrum (left panel) and number size distribution (right panel) of a re-dispersed Saharan soil sample from Morocco (black line and black squares) in comparison with best fit results for different particle shapes (coloured lines).

the convergence limit, the calculations were continued with a ray tracing model including diffraction and applying edge corrections to account for the limitations of the geometric optics approximation. In addition to the idealized spheroids, selected test calculations were also done for distorted spheroids and aggregate like particles with the discrete dipole approximation (DDA) using the DDSCAT 6.0 FORTRAN software package [4].

3. Results

Fig. 1 shows selected shape-dependent results for the extinction and absorption cross sections, C_{ext} and C_{abs} , as well as the extinction efficiency, Q_{ext} , for some ideal and distorted spheroids (shapes A, B, and C; bottom panel) as a function of the equal volume sphere diameter D_v (wavelength 500 nm, complex refractive index $1.5 + 0.014i$). The distortions were introduced with the HyperFun polygonizer (<http://www.hyperfun.org>) starting from an ideal $\epsilon=0.5$ spheroid as the original shape. Up to a D_v of about $0.7 \mu\text{m}$, the spread of the individual traces for C_{ext} is low (top panel). Above $0.7 \mu\text{m}$, we enter the size range that is governed by the interference structure and the results for the extinction cross sections of the various particle shapes start to diverge significantly, as can be better seen in the middle panel where the extinction efficiencies are plotted. Changing the aspect ratio of the spheroids leads to much larger variations in C_{ext} than introducing particle distortions by the polygonizer. The trace of C_{ext} for the aggregate like particle (shape D, modeled as two touching ellipsoids), being a better representation for the habit of irregularly formed natural dust grains, is up to a D_v of $1.1 \mu\text{m}$ very similar to that of the most elongated spheroid ($\epsilon=0.25$), a result that may explain the findings from Fig. 2 which are discussed below. Up to a D_v of about $1.5 \mu\text{m}$, the absorption cross sections (bottom panel) are proportional to the particle volume and, therefore, do not show any variation with ϵ as long as D_v is kept constant.

The left panel of Fig. 2 shows an exemplary extinction spectrum of re-dispersed Saharan dust particles from Morocco (black line). Their concomitantly measured number size distribution is shown in the right panel (black squares). For different assumptions on the particle shape, we have tried to simultaneously fit both the extinction spectrum and the number size distribution. Two fit results for spherical particles ($\epsilon=1$, green and blue lines) are shown. The fit example in green shows that Mie theory is unable to reproduce the measured habitus of the extinction spectrum for a size distribution that is similar to the measured one. A better agreement with the measured extinction spectrum is only obtained when significantly distorting the measured number size distribution (blue line). On the contrary, both measurements can be accurately reproduced with spheroids of $\epsilon=0.25$. As part of the aerosol number size distribution extends into the size regime that is dominated by the interference structure, an elongated spheroid is obviously a much better shape representation than a sphere to model the extinction spectrum of dust grains in this size regime. This seems reasonable because the trace for C_{ext} of the aggregate particle in Fig. 1 closely agrees with that of the $\epsilon=0.25$ spheroid for the range of particle sizes covered by the experiment.

References

- [1] I.N. Sokolik, O.B. Toon, "Incorporation of mineralogical composition into models of the radiative properties of mineral aerosol from UV to IR wavelengths", *J. Geophys. Res. (Atmos.)* **104**, 9423–9444 (1999)
- [2] R. Wagner, K. Kandler, K.I. Lieke, C. Linke, T. Müller, M. Schnaiter, M. Vragel, "Complex refractive indices of Saharan dust samples at visible and near UV wavelengths: a laboratory study", *to be submitted*, (2011)
- [3] M.I. Mishchenko, L.D. Travis, "Capabilities and limitations of a current FORTRAN implementation of the T-matrix method for randomly oriented, rotationally symmetric scatterers", *J. Quant. Spectrosc. Rad. Transfer* **60**, 309–324 (1998)
- [4] B.T. Draine, P.J. Flatau, "Discrete-Dipole Approximation for Scattering Calculations", *J. Opt. Soc. Am. A* **11**, 1491–1499 (1994)

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Paper presented at the ELS XIII Conference (Taormina, Italy, 2011), held under the APP patronage; published online 15 September 2011.

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