A single scattering study using aggregates of spheres in random orientation

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The particle shape influences the efficiencies of scattering (Q_{sca}) curves versus size parameter (X) and consequently on the overall single scattering properties of a sample of particles in random orientation. In order to show how the influence of the shape works, a model consisting of aggregates of different numbers of spheres has been used to fit laboratory measurements of fly ashes.

INTRODUCTION

Single scattering properties of a distribution of particles in random orientation depend on different parameters such as refractive index, size, shape, internal structure, as well as the degree of fluffiness of the particles. The measurements carried out in the scattering laboratory [1] and those obtained from astronomical observations [2] provide information on the overall scattering properties of a sample formed by small particles in random orientation. Individually identifying or "untangling" the way in which each parameter is affecting the overall scattering properties is difficult since these parameters have a collective influence on the measurements. In order to better understand how the single scattering properties observed are affected by these parameters, a lot of research has been carried out [3-7]; however, some questions remain open. The problem of single scattering by a distribution of small particles in random orientation can be approached by different techniques. We chose the DDA (Discrete Dipole Approximation). Despite it is not suitable for performing calculations for particles bigger than the wavelength of the incident light, on the current computers, in a reasonable time (days), it has the potential to reproduce any particle shape. We can fix all parameters of the model except for one and then vary it to study the response of the system. In this work, we present an attempt to fit a set of scattering laboratory measurements [1] by modeling it with a distribution of different aggregates of spheres. Nevertheless, our main goal is not to exactly fit the laboratory measurements, but to show how the particle shape is influencing Qsca; and therefore, the way it is determining the size average of the elements of the scattering matrix.

MODEL

We have modeled the system by using Eq. (1), which gives the scattering matrix as a function of the scattering angle θ, for a certain wavelength λ, under the assumption of independent scattering

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$$Fij(\lambda,\theta) = \int_{r_1}^{r_2} F^{ij}(\lambda,\theta,r)n(r)dr\,. \quad (1)$$

In Eq. (1), *n(r)* is the size distribution as a function of the radius, r_1 and r_2 correspond to the smallest and largest particles in the distribution respectively, and $F^{ij}(\lambda,\theta,r)$ is one of the elements of the scattering matrix for a single particle of radius *r*.

CALCULATIONS

As mentioned, we have compared our calculations with laboratory measurements of fly ashes. The peculiar shapes of the particles involved in these measurements [1] have motivated the used model. Upper side in Fig. 1 show what these shapes are like. Regarding the eight aggregates of spheres shown in this image, the four on the left are made of a smaller number of spheres than those on the right. The shape average was performed by considering all these aggregates and a single sphere, with the same weight. Calculations corresponding to all aggregates have been carried out by DDA, and those for the single sphere have been also performed by Mie theory, for a wavelength of 0.633 μm in all cases. The value of the refractive index used was 1.5+0.001i, as given in [1]. The size distribution function n(r) was chosen a power law with negative exponent equal to -1.8, r_1=0.1 μm and r_2=1.0 μm. We have divided this range into 35 radii equally spaced intervals. The truncation of the size distribution to these values was a consequence of the computational limitations with the DDA code. The calculations were averaged over 2000 orientations to mimic the random orientation, and the number of dipoles was chosen so that the accuracy condition $|mkd| < 0.5$ was fulfilled [8].

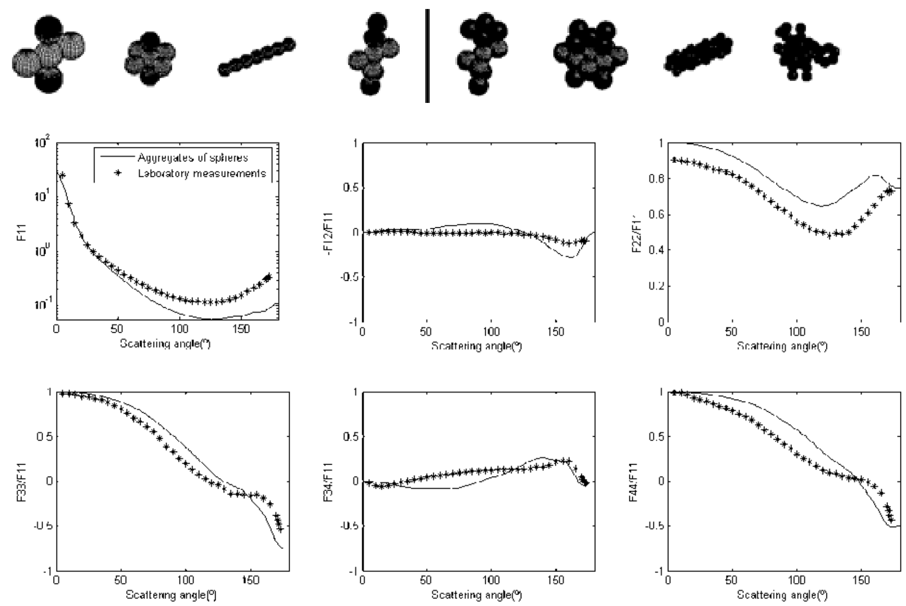

Figure 1. Eight aggregates made of 5, 7, 7-linear, 9, 14, 19, 25 and 36 spheres (top) and a comparison of laboratory measurements of fly ashes with our size and shape averages from 0.1 to 1.0 μm considering the eight aggregates and a single sphere equally weighted (bottom).

RESULTS AND DISCUSSION

In Fig. 1 (bottom), we show the comparison of our results with the laboratory measurements, size and shape averaged, considering the eight aggregates of spheres shown on the upper side of this figure, plus a single sphere. In Fig. 2, we can see the overlapped images of the size averaged results for each of the aggregates of spheres (blue and green lines) and for a single sphere (dashed black line). From Fig. 2, it comes out that the contribution of the aggregates of less number of spheres (≤9) is necessary to approach the laboratory measurements (see in Fig. 2 the blue and green lines). On the other hand, we note that the real size distribution, as given in the reference [1], has constituents with X larger than 10.

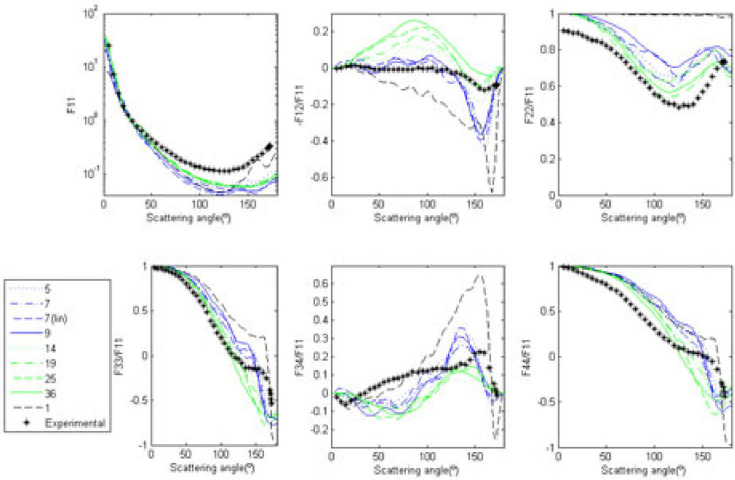

Figure 2. Comparison of laboratory measurements of single scattering matrix elements of fly ashes with our size averages from 0.1 to 1.0 μm for each one of the aggregates of spheres (blue and green lines) and for a single sphere (dashed black line).

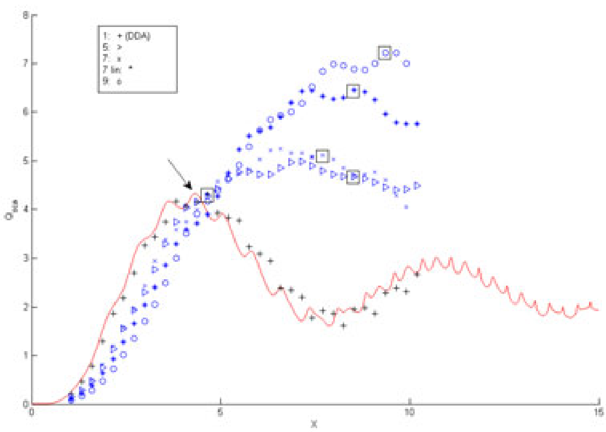

Figure 3. Q_{sca} versus X for the aggregates with a number of spheres ≤ 9 (5: **×**, 7: **>**, 7-linear: ***** and 9: **o**) and a single sphere (DDA: **+** and Mie: solid red line). The square on Q_{sca} curve of aggregates with number of spheres of 1, 5, 7, 7-lin and 9 are considered in the "same" state of oscillation to that marked by an arrow on the Q_{sca} curve of the single sphere (red line).

In Fig. 1, we see a not perfect fit of the results of DDA to the measurements, the calculations
stopping at r_2=1.0 μm. In particular, the deviation of the calculated values from the measurements points to a Rayleigh-like behaviour. From Fig. 2, we infer that the more spheres the aggregates are made of, the more the calculated values resemble Rayleigh features of the scattering matrix elements as functions of the scattering angle. This is suggesting us an explanation for the unperfected fitting: when aggregates are made of a large number of spheres, the curve of Q_{sca} as a function of X changes so that we are skipping some of its main features by cutting our size distribution at r_2=1.0 μm. In order to prove this, we present on Fig. 3 the Q_{sca} curves for the four aggregates with a number of spheres ≤ 9 till X=10, along with the Q_{sca} curve of the single sphere, calculated till X=15. A progressive displacement to the right and rising of the Q_{sca} curves is observed when the number of spheres of the aggregates increases. Due to this displacement, some of the features of Q_{sca} that correspond to r > 1.0 μm are lost in our calculations, and this effect becomes more important as the number of spheres of the aggregates increases. The result is a Rayleigh-like behaviour because only the first oscillation of the curve of Q_{sca} is been considered for the size distribution.

REFERENCES

[1] O. Muñoz, H. Volten, J.F. Haan, W. Vassen, and J.W. Hovenier. Experimental determination of scattering matrices of randomly oriented fly ash and clay particles at 441.6 nm and 632.8 nm. J. Geophys. Res. **106** (2001).

[2] L. Kolokolova, H. Kimura, N. Kiselev, and V. Rosenbush. Two different evolutionary types of comets proved by polarimetric and infrared properties of their dust. Astron. Astrophys. **463** (2007).

[3] H. Kimura, L. Kolokolova, and I. Mann. Light scattering by cometary dust numerically simulated with aggregate particles consisting of identical spheres. Astron. Astrophys. **449** (2006).

[4] T. Nousiainen. Optical modeling of mineral dust particles: A review. J. Quant. Spectrosc. Radiat. Transf. **110** (2009).

[5] R. Vilaplana, F. Moreno, and A. Molina. Study of the sensitivity of size-averaged scattering matrix elements of non-spherical particles to changes in shape, porosity and refractive index. J. Quant. Spectrosc. Radiat. Transf. **100** (2006).

[6] F. Moreno, O. Muñoz, D. Guirado, and R. Vilaplana. Comet dust as a size distribution of irregularly shaped, compact particles. J. Quant. Spectrosc. Radiat. Transf. **106** (2007).

[7] Y. Shen, B.T. Draine, and E.T. Johnson. Modeling porous dust grains with ballistic aggregates. II. Light scattering properties. Astron. Astrophys. **696** (2009).

[8] B.T. Draine, P.J. Flatau. Discrete-dipole approximation for scattering calculations. J. Opt. Soc. Am. A. **11** (1994).