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Chord length distributions of non convex bodies: Dumbbell and diabolo like-particles

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ABSTRACT

The scattering of an electromagnetic wave by a particle is directly related to its Chord Length Distribution (CLD) in certain cases. Whereas the CLD of convex bodies, e.g. sphere, ellipsoids, cylinders..., can be easily calculated, few studies have been conducted on the CLD of non convex bodies which are more difficult to ascertain. Two non convex bodies built from two spheres, i.e. dumbbells and diabolos, were considered. Firstly, we describe original algorithms designed for calculating the intersection between a straight line and these particles. Then the corresponding CLDs are calculated by using the Monte-Carlo method. Analysis of the deviation of these CLDs from the CLD of the sphere can identify precisely the main features due to some local non convexity. The corresponding items are expressed as a function of a non convexity parameter.

1. Introduction

Many manufacturers use solid micro-particles in suspension for various applications: ceramics, paintings, pharmaceutics, cosmetics, food and chemicals. Particle size can be evaluated by physical methods based on the scattering of an incident electromagnetic wave as it strikes the particle. The scattered wave depends on the particle morphology as well as on the ratio between the refractive indices of both the material and suspension medium. Depending on the material, the particle morphology and the selected method, the signal measured may be straightforwardly related to the Chord Length Distribution (CLD) of the set of the randomly orientated particles. This is applied for Small-Angle Scattering (SAS) measurements [1,2], Focused Beam Reflectance Measurements (FBRM) [3], Spectral Turbidimetry, i.e. extinction measurement [4].

Whereas a straight line passes just once through a convex body, it may intersect more than one time across a non convex body. As a consequence, there are two chord length distributions which can be defined as:

– The Multiple Chord Distribution (MCD) where each segment interval on the same line is considered as one chord length separately. FBRM measurements and experiments in the field of SAS are associated with MCD.

– The one chord distribution (OCD) where the sum of chord lengths for all intersected intervals is used as the definition of the chord length. Turbidity measurements are associated with OCD.

The CLD of convex and non-convex bodies has been studied mathematically [5–7]. Explicit expressions have been obtained for bounded 2D or 3D convex domains: disc, triangle, rectangle, regular polygon [8], sphere, hemisphere [9], cylinders of various cross sections [10,11], spheroids [12], polyhedron [13,14].

However, to the best of our knowledge little attention has been paid to non convex bodies compared to convex ones. Mazzolo et al. [15] discussed the CLD in the context of reactor physics. They showed that some relations between lower moments of CLD and simple geometric properties as volume, surface, ... of the body remain valid for non-convex bodies whereas higher CLD moments do not obey the simple relations valid for convex bodies. Gille [16] studied the CLD of an infinitely long circular hollow cylinder that is a special case of non convex body; the corresponding calculation was based on basic mathematics. Vlasov [17] introduced the notion of signed chord distribution for convex and non-convex bodies. He started from the work of Dirac to reduce the six-dimensional integral of pairwise interaction potential for a convex body into a simpler expression including the CLD; then he extended this to a non convex body, showing that the expression of the integral is much more complicated than the one for a convex body. In the case of non convex body the integral can be decomposed into several terms (integrals), each related to the various

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segments of the given chord inside the non convex body. Vlasov formally deduced the expression of the CLD for the non-convex case. Gruy et al. analytically calculated the CLD of a two-sphere cluster [18] and a dumbbell [19].

There are some results linking CLD's with scattering experiments, particularly SAS-measurements, for non convex particles. This aspect has been analysed by Gille [20]. The geometric and physical quantity directly related to the SAS-intensity is the correlation function $\gamma(r)$. The function $r^2\gamma(r)$ is proportional to the distance distribution function. For instance, using cylindrical models, Gille [21] has studied the relation between non-convex particles and SAS. He derived explicitly the correlation function for two touching circular cylinders and deduced the second derivative γ'' that is proportional to the CLD for convex particles. When analysed he found five contributions for γ'': each corresponding to a chord crossing a given sub-space: either traversing a sole cylinder, both cylinders or the space between the two cylinders.... Therefore, this example proves that the CLD is related to the scattering intensity in a more complex manner for the case of non convex particles as opposed to convex particles. Kaya [22], Kaya and De Souza [23] have studied barbells and dumbbells and the related convex particles, i.e. capped cylinders. They calculated the corresponding form factors. Senesi and Lee [24] have indirectly studied non convex bodies. They presented a general method to calculate the scattering functions of polyhedra. These are calculated by breaking the body into sets of pieces. This work included the calculation of concave bodies. Ciccariello et al. [25a,25b] have considered the small-angle scattering from anisotropic samples and have found a simple expression between the scattering intensity and the absolute values of Gaussian curvature at particular surface points. They show that this equation is also valid for non convex particles. This corpus of work emphasizes the links between scattering theory and stochastic geometry, integral geometry and differential geometry.

Among the particle shapes observed in suspensions during a precipitation or crystallization process, small clusters of spherical particles are often present [19]. The contact between the two spheres in the cluster can be a single point or a neck due to sintering. This type of particle is one of the simplest cases of non convex bodies. Therefore, in this paper, we explore the properties of their CLD's and the relationship between CLD and convexity. Due to the complexity and difficulty of exact analytical calculation, CLD's will be obtained from Monte-Carlo Simulations (MCS).

The rest of the paper is organized as follows: section two introduces the algorithms used for MCS. The data issued from MCS for some non convex bodies are presented and discussed in the section three, followed by a conclusion and perspectives for future work in section four.

2. Chord length distributions by Monte-Carlo simulations

Our work focuses on OCD calculations with 3D uniform flow of lines.

Note: throughout the paper and the literature, the chord length distribution (density) is written $D_l(l)$ where $0 \leqslant l \leqslant l_{\max}$. $D_l(l)dl$ is the number of chords within the l-range $[l, l + dl]$. $D_l(l)$ is usually presented as normalized, i.e. $\int_0^{l_{\max}} D_l(l)dl = 1$.

In this article three kinds of particles are considered and compared, that are bodies of revolution along the x-axis. They are composed of spheres or parts of a sphere. The centres of spheres are symmetrically located along the x-axis. The origin of the coordinate system is the symmetry centre of the particle. The three particles are:

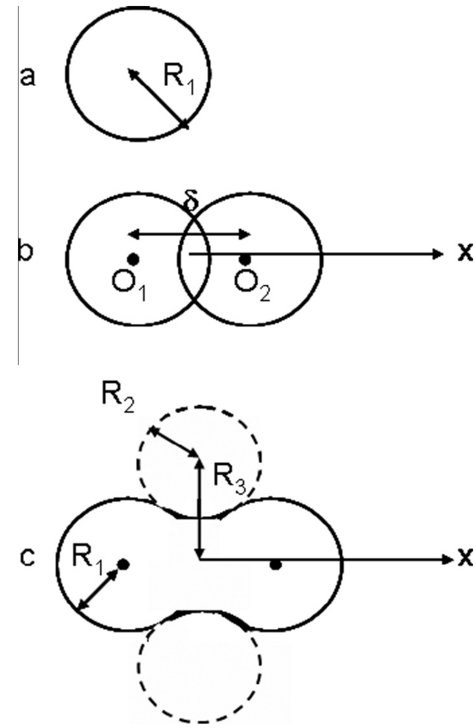

Fig. 1. Sphere (a), Dumbbell (b) and the Diabolo (c).

- Sphere with radius R_1 (Fig. 1a).
- Cluster of two overlapping spheres (Fig. 1b); the radius of spheres is R_1 and the distance between the two centres is denoted δ. This type of cluster will be designated dumbbell [19]. A particular case is the cluster of two touching spheres: $\delta = 2R_1$.
- A cluster of two touching spheres where the neck (or overlap) is partially filled with matter (Fig. 1c); the radius of spheres is R_1 and the upper boundary of the neck is a part of a torus with a minor radius R_2; as the torus is tangentially linked to the spheres, the major radius R_3 obeys the expression $R_3 = \sqrt{R_2^2 + 2R_2R_1}$. This type of cluster will be called a diabolo. An example is the convex body corresponding to $R_2 \to \infty$, i.e. a capsule. The cluster of two touching spheres corresponds to $R_2 \to 0$.

A MCS software was employed to generate an isotropic uniform random line across the geometric object, and to collect the chord length segments. The same framework for the Monte Carlo Simulations (MCS) of the different particle shapes has been used.

All the distances are normalized by R_1 (then, $R_1 = 1$). Consider a sphere with radius 2 and its centre located at the origin. The way used to define the random straight line is the following: A direction and a point belonging to the plane orthogonal to that direction and tangent to the sphere are considered. The coordinate system of the plane is composed of the point of tangency and the vectors from the usual spherical coordinate system. The line will be defined by the two angles, polar θ and azimuthal ϕ, and the two coordinates x_P, y_P of the point in the plane. Four random numbers [26] are chosen for the values of the variables $\cos\theta$, ϕ, x_P and y_P. The line intersects the sphere at two points denoted M_1 and M_2. This algorithm is known to provide a translation and rotation invariant density [27].

Depending on the particle, the straight line between M_1 and M_2 may intersect the particle 0, 2, 4 or 6 times. The intersection points will be analytically determined and the corresponding distances calculated. The details of these calculations based on the analytic