Powder Technology 253 (2014) 207–215

Contents lists available at ScienceDirect

Powder Technology

journal homepage: www.elsevier.com/locate/powtec

The chord length distribution of a dumbbell shaped aggregate: Analytical expression

Frédéric Gruy [a,*], Soong-Hyuck Suh [b]

[a] Ecole Nationale Supérieure des Mines, 158 Cours Fauriel, 42023 Saint-Etienne, France
[b] Department of Chemical Engineering, Keimyung University, Daegu 704-701, Republic of Korea

ARTICLE INFO

Article history:
Received 12 June 2013
Received in revised form 12 November 2013
Accepted 16 November 2013
Available online 25 November 2013

Keywords:
Chord length distribution (CLD)
Dumbbell
Aggregation
Anomalous diffraction

ABSTRACT

Dumbbell shaped aggregates are small particles synthesized in precipitation reactors. Their characterization by optical methods needs the chord length distribution (CLD) of such a shape. We present in this paper the analytical calculation of two CLDs corresponding to two different definitions of CLD. Comparison with Monte-Carlo simulations is presented. Good agreement is found between the exact calculation and simulations.

1. Introduction

Many manufacturers use solid micro-particles in suspension for various applications: ceramics, paintings, pharmaceutics, cosmetics, food and chemicals. Particle sizing can be performed by physical methods based on the scattering between the particles and an incident electromagnetic wave. The scattered wave is depending on the particle morphology and on the ratio between the refractive indices of particle material and suspending medium. Depending on the particle material and the selected method the measured signal may be straightforwardly related to the chord length distribution (CLD) of the randomly orientated particle set. This is illustrated by three examples:

- Small-Angle Scattering (SAS) measurements [1] are suitable for nano- and micro-particles interacting with X-rays. This method can be extended to the optically soft micro-particles interacting with light [2].
- Focused Beam Reflectance Measurements (FBRMs) are among the most widely used techniques for particle sizing [3]. It uses a focused beam of laser light that scans across particles passing in front of the probe window to measure a chord length distribution. The interpretation of the signal is only based on the reflected light. This method is suitable for particle size higher than 5 μm.
- Spectral Turbidimetry, i.e. extinction measurement, is an optical method to measure the light scattering or extinction cross section of particles. In the case of large micro-particles (>1 μm) and very small optical contrast, extinction or forward scattering can be explained in the framework of anomalous diffraction approximation [2]: then the scattering cross section is expressed as an integral including the particle CLD. Anomalous diffraction approximation was applied to a sphere, an infinitely long circular cylinder, a prism column, a hexagonal crystal of ice, ellipsoids and a finite cylinder [4].

Depending on the physical principles of measurement the definition of the CLD for a given object changes: 3D isotropic uniform flow of infinite straight lines in the case of SAS and turbidity measurements, or 2D isotropic uniform flow of infinite straight lines for each projected area in the case of FBRM.

The CLD of convex and non-convex bodies has been studied from a mathematical point of view. Explicit expressions have been obtained for bounded 2D or 3D convex domains: disk, triangle, rectangle, regular polygon [5], sphere, hemisphere [6], cylinders of various cross sections [7,8], spheroids, and polyhedron [9]. Moreover, Aharonyan [10] obtained an explicit expression for the orientation-dependent CLD for any bounded convex body.

Non-convex bodies have paid less attention than convex ones. Mazzolo et al. [11] discussed the CLD in the context of reactor physics. They show 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 [12] studied the CLD of an infinitely long circular hollow cylinder that is a special case of non-convex body; the corresponding calculation is based on basic principles. Gille [13] also considered two parallel circular cylinders

* Corresponding author.
E-mail address: fgruy@emse.fr (F. Gruy).

0032-5910/$ – see front matter
http://dx.doi.org/10.1016/j.powtec.2013.11.022

separated by a short distance and calculated the 3D-correlation function that is related to CLD. Vlasov [14] introduced the notion of signed chord distribution for convex and non-convex bodies. He started from the work of Dirac transforming the six-dimensional integral of pairwise interaction potential for a convex body into a simpler expression including the CLD; he extended it to a non-convex body. He showed that the expression of the integral is much more complicated than the one for convex body: it can be decomposed into several terms (integrals), each one related to the various segments of the given chord inside the non-convex body. He formally deduces the expression of the CLD for the non-convex case.

Among the particle shapes observed in industrial processes, small clusters of spherical particles are often present. By the past we calculated [15] the CLD for a two-sphere aggregate. In this paper we extend this calculation to a set of two spheres penetrating each other. For instance, these dumbbell-like particles appear in the precipitation of inorganic compounds performed at high supersaturation and weak aggregation conditions. Polymeric colloids with such a morphology are also synthesized [16].

Section 2of this paper develops a methodology in order to calculate the CLD of a dumbbell shaped aggregate. It is followed by a comparison with Monte Carlo Simulations in Section 3. Section 4 is devoted to concluding remarks.

2. Calculation of the chord length distribution

A straight line may intersect more than one time across a non-convex body. As a consequence, two CLD can be defined:

- The multiple chord distribution (MCD) where each segment interval on the same line is considered as one chord length separately. FBRM measurements are associated to 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. SAS and turbidity measurements are associated to OCD.

Even if the latter ones only consider OCD, we will present both OCD and MCD calculations with 3D uniform flow of lines. The corresponding procedure is similar to the one used for a two-sphere aggregate [15].

Throughout the paper, the chord length distribution (density) is written $D(l)$. $D(l)dl$ is the number of chords within the l-range $[l, l+dl]$. $D(l)$ is normalized, i.e. $\int_0^{l_{max}} D(l)dl = 1$.

2.1. Definition of the different geometrical areas

In the following of the paper, points will be denoted by lower-case letter (except the origin O of the coordinate system), line by upper-case letter, area by upper-case letter within parentheses and a volume by upper-case letter within brackets.

The dumbbell projection on a plane is considered. θ ($0 \le \theta \le \pi/2$) is the angle between the line binding the centers of the two spheres (radius value equal to one) and the projection plane (coordinates x,y). The distance between the two sphere centers is denoted δ. The center of one of the two spheres is chosen as the origin O of the coordinate system (Fig. 1). The projection of the dumbbell is represented in Fig. 2a–b for two values of the θ angle and for a semi-plane. The circles C1 and C2 represent the projection of the spheres (disks (C1) and (C2)) whereas the dashed curve (ellipse later called E1 in the paper) represents the projection of the circular junction J between the two spheres. Let us consider a chord (perpendicular to the projection plane). According to the location of its intersection (x,y) point with the plane this line may cross:

- one single sphere: the point belongs to (P1)
- the junction between the two spheres: the point belongs to (PJ)
- or successively the two spheres: the point belongs to (P12).

The (Pf) area that is bounded by C2 (and C1) and E1 is fictitious. Its definition will be detailed hereafter.

The previously defined areas correspond to a full plane.

The ellipse E1 has some interesting properties:

- the coordinates of E1 center are $(2\delta \cos(\theta),0)$
- the ellipse intersects the circles at the two b1 and b2 points (in fact four points if one considers the other semi-plane). The coordinates of the b2 point are $(\delta/(2\cos(\theta)), (1-\delta^2/(4\cos^2(\theta)))^{1/2})$. The tangent at this point is common to the circle and the ellipse.
- as the θ-angle increases E1 tends to a circle. E1 does not intersect C1 and C2 for $\theta > \theta_{E1} = a\cos(\delta/2)$
- the equation of the E1 ellipse is:

$$(x-\delta\cos(\theta)/2)^2/\sin^2(\theta) + y^2 = 1-\delta^2/4 \quad (1)$$

- E1 and C2 intersect the horizontal axis at b1* and b1** respectively. The area defined by b1, b1* and b1** is the one-fourth of (Pf).

2.2. Decomposition of the CLD

The CLD may be written as a sum of several partial CLDs.

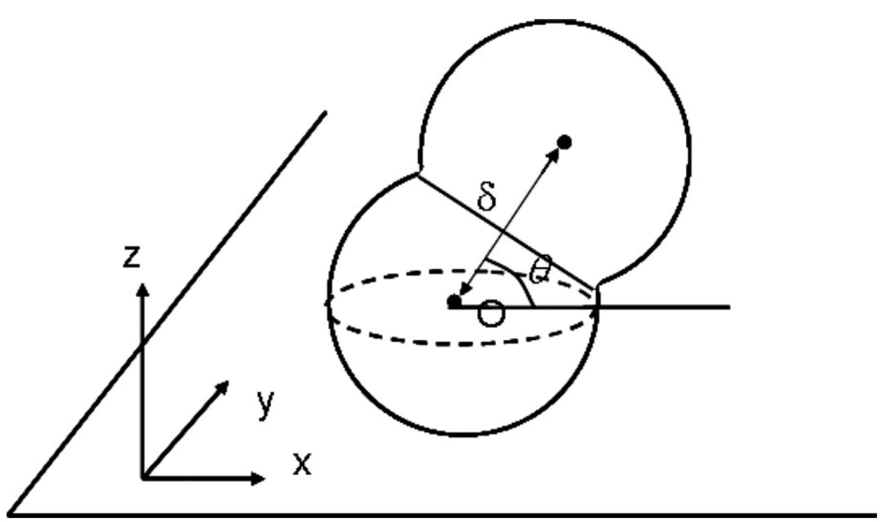

Fig. 1. 3D drawing of the dumbbell shaped aggregate.