Colloids and Surfaces A: Physicochem. Eng. Aspects 482 (2015) 154–164

Contents lists available at ScienceDirect

Colloids and Surfaces A: Physicochemical and Engineering Aspects

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

Inertia tensor as morphological descriptor for aggregation dynamics

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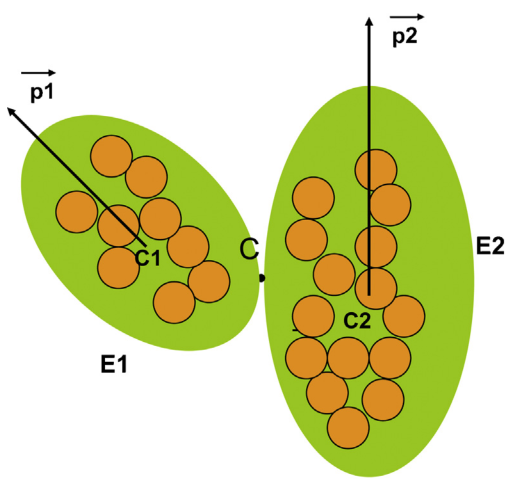
HIGHLIGHTS

- Morphological descriptors of particles based on the inertia tensor.
- Variation of descriptor values during the collision of aggregates.
- Descriptors distribution for aggregates built in a 2D shear flow.

GRAPHICAL ABSTRACT



$$\left(M_1,\lambda_1,\varepsilon_1\right)+\left(M_2,\lambda_2,\varepsilon_2\right)\rightarrow\left(M_1+M_2,\lambda_{(1+2)},\varepsilon_{(1+2)}\right)$$

ARTICLE INFO

Article history:
Received 15 January 2015
Received in revised form 17 April 2015
Accepted 18 April 2015
Available online 30 April 2015

Keywords:
Aggregation
Inertia tensor
Anisotropy
Equivalent ellipsoid
Aggregation kernel

ABSTRACT

Multidimensional population balance modelling is a powerful tool to study the dynamics of the precipitation and particularly the aggregation of particles. This approach involves the selection of internal parameters describing the particle. Among them, morphological or geometrical descriptors are required. In this paper, the inertia or gyration tensor is considered and evaluated for the modelling of aggregation. An equivalent ellipsoid to the aggregate is defined from the tensor. First, a general expression for the inertia tensor of the aggregate resulting from the collision of two aggregates is presented. In this framework, the collision event becomes the collision between two equivalent ellipsoids and leads to a larger ellipsoid. Second, the inertia tensor and the characteristics of the equivalent ellipsoid are explicitly calculated in the case of shear aggregation in a two-dimensional space. An approximate calculation is also presented and checked. Finally, the shear aggregation of a set of disks in a two-dimensional space is simulated using simultaneously this modelling of the collision event and Monte-Carlo simulations for all the collisions. This is compared with classical Monte Carlo simulations where the colliding particles are clusters of disks. Physical properties of the cluster population as, for instance, the distribution of elongation or anisotropy factor at different times are presented.

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http://dx.doi.org/10.1016/j.colsurfa.2015.04.034
0927-7757/

Nomenclature

$\vec{a}$	vector between the centres of mass of two particles
a	semi-major axis of ellipse
b	semi-minor axis of ellipse
A	anisotropy factor defined by [9,10]
A_{ij}	anisotropy factor defined by [11]
B	coefficient in Eq. (35)
D_f	fractal dimension
$\underline{\underline{D_E}}$	diagonal matrix for ellipsoid
$\underline{\underline{D_I}}$	diagonalized inertia tensor
$\underline{\underline{D_{I,m}}}$	diagonalized inertia tensor after averaging
$\underline{\underline{I}}$	inertia tensor of the particle
k_{12}	contribution to K_{12} (Eq. (14))
K_{12}	kernel of aggregation
L	penetration length
M	particle mass
N	number of primary particles per aggregate
P	configuration probability
$\vec{p}$	orientation vector of ellipsoid
R_i	square root of diagonal elements of $\underline{\underline{D_I}}$
R_g	gyration radius
U_i	semi-axis i of equivalent ellipsoid
V	particle volume
$\vec{v}$	particle velocity
$\vec{x}$	position vector of particle
x,y,z	space coordinates
Greek letters	
$(\alpha,\beta,\gamma,\delta)$	subscripts for configuration of two-ellipse set
ε	porosity
ϕ	solid volume fraction or density
$\dot{\gamma}$	shear rate
κ	permeability
λ	elongation
ρ	mass density
θ	orientation angle
Superscript	
app	approximate
(i)	for tensor (particle i)
Subscript	
$\underline{X}$	tensor X
eq	equivalent
i	for scalar or vector (particle i)
i,k	k component of vector (particle i)
k,l	k,l element of the tensor or matrix
m	lower integration boundary (Eq. (15))
M	upper integration boundary (Eq. (15))
symbol	
$\langle\ \rangle$	average

1. Introduction

Aggregation of particles in a suspension is due to the binary collisions between two particles. The resulting aggregate or cluster is a branched and porous object consisting of primary particles, usually considered as identical. Most often, the morphology of the cluster is described by using the fractal theory: it is defined by the radius of the primary particle, its number of primary particles and the fractal dimension. The last quantity is a real number within the 1–3 range. It is determined from simulations of colliding particles obeying a given collisional mechanism or from an experimental characterization tool as X-ray scattering (SAXS) device. Even if the fractal hypothesis was successful for describing the dynamics of aggregation, the fractal dimension is not the only morphological parameter to be relevant. The fractal dimension of stochastic aggregates is a statistical quantity; it either refers to a population of aggregates (as in SAXS analysis) or to a sufficiently large single aggregate (as in the analysis of microscope images); in addition fractal dimension is related to several morphological parameters (e.g. radius of gyration or mobility radius – when measured against aggregate mass, or interparticle distance (pair correlation) – when using box-counting or SAXS data). Moreover, the relation between its value and the nature of the collisional mechanism is not so obvious.

A convex particle, as a spherical primary particle, or a non-convex one, as an aggregate, may be described by several morphological parameters, the relevance of which depending on the considered physical phenomenon. These parameters can be organized as a vector or as a tensor. The theory of scalar or Tensorial Minkowski Functionals (TMF) provides the rigorous framework for such parameter set. Mecke et al. [1,2] have applied the integral geometry in various fields of physics. They underlined that the inertia tensor does not belong to the TMF because it does not possess all the mathematical properties. However, inertia tensor is similar to TMF. Porosity, anisotropy and orientation of an object are geometrical and textural characteristics that investigators have frequently considered. Inertia tensor seems an interesting candidate for introducing these quantities. This is a more popular concept among physicists than the Minkowski functionals.

Torres et al. [3] have, for instance, performed simulations of 3-D shear aggregation. They found a fractal dimension value equal to 1.83 and they observed the non spherical shape of the aggregate. Moreover they have calculated the inertia tensor (normalized by the square of the gyration radius) for clusters with a number N of primary particles smaller than 4100. They have observed that the semi-axes of the equivalent ellipsoid were in the ratio 1/1.6/3.1 whatever the origin of the particle collision (Brownian motion, shear flow, elongation flow).

Investigators defined two quantities: inertia tensor [4] and gyration tensor [5]. The first one considers the mass and the position vector distributions inside the particle. The second one that has, in fact, the same definition is often used for systems, polymers or aggregates, consisting in monomers or identical primary particles; in this case it only depends on the position vector distribution. The words "inertia tensor" will be used later on in this paper.

One considers a set of N points with Cartesian coordinates x_k, y_k, z_k or $x_{k,1}$, $x_{k,2}$, $x_{k,3}$ and a mass equal to one in a three-dimensional space. The origin of the coordinate system is the centre of mass. The inertia tensor is defined by the expression [4–8]:

$$\underline{\underline{I}} = \sum_{k=1}^{N} \begin{bmatrix} x_{k,2}^2 + x_{k,3}^2 & -x_{k,1}x_{k,2} & -x_{k,1}x_{k,3} \\ & x_{k,1}^2 + x_{k,3}^2 & -x_{k,2}x_{k,3} \\ & & x_{k,1}^2 + x_{k,2}^2 \end{bmatrix} \tag{1}$$

or

$$I_{i,j} = \sum_{k=1}^{N} -x_{k,i}x_{k,j} + \delta_{ij}\vec{x}_k^{\,2} \tag{2a}$$

The continuous formulation of the tensor component is

$$I_{i,j} = \int_{[V]} \left(-x_i x_j + \delta_{ij}\vec{x}^2\right) \mathrm{d}V \tag{2b}$$