Computer Physics Communications 192 (2015) 70–90

Contents lists available at ScienceDirect

Computer Physics Communications

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

Accurate modelling of flow induced stresses in rigid colloidal aggregates

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ARTICLE INFO

Article history:
Received 15 September 2014
Received in revised form
6 February 2015
Accepted 21 February 2015
Available online 2 March 2015

Keywords:
Colloidal aggregates
Stress distribution
Breakup
Colloids
Emulsions and suspensions
Computer simulation of molecular and particle dynamics

ABSTRACT

A method has been developed to estimate the motion and the internal stresses induced by a fluid flow on a rigid aggregate. The approach couples Stokesian dynamics and structural mechanics in order to take into account accurately the effect of the complex geometry of the aggregates on hydrodynamic forces and the internal redistribution of stresses. The intrinsic error of the method, due to the low-order truncation of the multipole expansion of the Stokes solution, has been assessed by comparison with the analytical solution for the case of a doublet in a shear flow. In addition, it has been shown that the error becomes smaller as the number of primary particles in the aggregate increases and hence it is expected to be negligible for realistic reproductions of large aggregates.

The evaluation of internal forces is performed by an adaptation of the matrix methods of structural mechanics to the geometric features of the aggregates and to the particular stress–strain relationship that occurs at intermonomer contacts. A preliminary investigation on the stress distribution in rigid aggregates and their mode of breakup has been performed by studying the response to an elongational flow of both realistic reproductions of colloidal aggregates (made of several hundreds monomers) and highly simplified structures. A very different behaviour has been evidenced between low-density aggregates with isostatic or weakly hyperstatic structures and compact aggregates with highly hyperstatic configuration. In low-density clusters breakup is caused directly by the failure of the most stressed intermonomer contact, which is typically located in the inner region of the aggregate and hence originates the birth of fragments of similar size. On the contrary, breakup of compact and highly cross-linked clusters is seldom caused by the failure of a single bond. When this happens, it proceeds through the removal of a tiny fragment from the external part of the structure. More commonly, however, breakup takes place through a sequence of bond failures that start at the periphery of the aggregates and then moves toward the interior according to a crack propagation mechanism. A gradual transition between these two modes of breakup has been found as the density of the aggregates increases.

1. Introduction

The breakup of aggregates by hydrodynamic stresses in a colloidal suspension strongly influences the size and the morphology of the dispersed phase. The modelling of such process has evolved and improved greatly in the last decades. At present accurate simulation of single breakup events can be obtained by Discrete Element Methods (DEMs), where the equations of motion are solved for each primary particle of the aggregate taking into account body forces, hydrodynamic interactions and colloidal forces. In this approach contact forces, exchanged by each pair of touching primary particles, are mimicked through spring–dashpot mechanisms that reproduce the effect of elasticity, adhesion and friction and extend the original DEM developed by Cundall and Strack for granular materials [1] to colloidal aggregates suspended in a fluid.

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http://dx.doi.org/10.1016/j.cpc.2015.02.022
0010-4655/

Different levels of complexity and accuracy characterise the Discrete Element Methods developed so far for the study of breakup. At the simplest level, hydrodynamic interactions are described by the free-draining approximation [2,3], where each primary particle experiences the Stokes drag force as if no other particle were present in the flow. More refined methods take into account the screening of the hydrodynamic forces by the external parts of the aggregate on the basis of the fraction of surface area of the primary particles directly exposed to the external fluid flow [4,5]. A more accurate description is obtained through Stokesian dynamics, which is based on a first-order multipole expansion of the exact solution of the Stokes flow [6–8]. Concerning contact forces, some models only consider normal adhesion forces [4,6,9], that is, forces acting along the centre–centre line between two primary particles. The inclusion of tangential forces, bending and torsional moments is quite recent and adds considerable complexity to the method [2,10,11].

All DEM approaches for breakup, even the simplest ones, require substantial computational resources, because processes acting at very different scales must be simulated simultaneously. Hydrodynamic interactions and the large scale motion of the aggregate take place on lengths of the order of the size of the aggregate, whereas contact forces and local deformations of the contact area act on distances that can be smaller than 1 nm. As a consequence, the time step must be extremely small in comparison to the duration of the process and the simulations are very slow. Hence, this type of simulation can be applied only to a small number of breakup events and, even if it provides highly detailed and valuable information, it is not able to take into account the large statistical variability of the elements of a population of aggregates or the very different histories experienced by different aggregates in a turbulent flow. To overcome this problem, Vanni and Gastaldi [12] proposed a different approach, in which aggregates are modelled as rigid bodies. The method is much faster than the aforementioned DEMs, but retains many of their features. It allows the simulation of many single breakup events in reasonable time and has been applied to extract reliable statistics from large populations of aggregates. Indeed, the internal deformations of an aggregate are likely to be very small before the occurrence of breakup or restructuring.

When an aggregate is modelled as a rigid body, the dynamics of the system are determined only by the equations of motion of the whole aggregate. The small scale motions at intermolecular contacts, due to surface forces or local deformations, are not considered in this approach, making the problem much better conditioned. The methods of structural mechanics can then be employed to determine how the hydrodynamic forces are redistributed as internal stresses over the solid matrix. At this point, by comparing the internal force acting at each contact with the pull-off value required for breaking the bond or the critical stress required for mutual sliding, rolling or twisting, one can determine the occurrence of breakup or restructuring. As shown in previous works, the calculation of internal stresses, and hence the determination of the breakup condition in laminar flows [12–14] or the breakup rate in turbulence [15], is accomplished very easily for aggregates with isostatic structures. From a mechanical point of view such structures are statically determined and simple force and torque balances on the single primary particles allow direct calculation of the internal stresses from the hydrodynamic forces [12, 16]. In the presence of hyperstatic configurations, however, the problem becomes more complex and its solution requires a stress–strain model for the structure of the aggregate. The development and integration of such a model with a Stokesian dynamic method to calculate hydrodynamic forces are the subjects of this paper.

The paper is organised as follows. We first describe the implementation of Stokesian dynamics, which allows the prediction of the motion of an aggregate immersed in a fluid flow and the calculation of the hydrodynamic forces acting on each primary particle. Subsequently, linearised stress–strain relationships for the internal interactions are obtained from contact mechanics. Such relationships are then recast in a matrix form well suited for the fast evaluation of internal stresses from hydrodynamic forces, in a way similar to that used in structural mechanics. Finally, in order to show its potential, the method is applied to the study of the stress on simple structures and aggregates immersed in an elongational flow.

2. Hydrodynamic forces and particle motion

2.1. Stokesian dynamics and determination of hydrodynamic forces

In our simulations a single rigid aggregate made of p primary particles is immersed in an unbounded Newtonian fluid subject to a linear flow. The aggregate is carried passively by the fluid flow and the effects of Brownian motion and body forces are negligible in comparison to the interaction between aggregate and shear flow. The undisturbed flow field is $\mathbf{u}^\infty = \boldsymbol{\Gamma}^\infty \cdot \mathbf{x}$, where all the components of the velocity gradient tensor are known functions of time:

$$\boldsymbol{\Gamma}^\infty = \begin{bmatrix} \dfrac{\partial u_x^\infty}{\partial x} & \dfrac{\partial u_x^\infty}{\partial y} & \dfrac{\partial u_x^\infty}{\partial z} \\ \dfrac{\partial u_y^\infty}{\partial x} & \dfrac{\partial u_y^\infty}{\partial y} & \dfrac{\partial u_y^\infty}{\partial z} \\ \dfrac{\partial u_z^\infty}{\partial x} & \dfrac{\partial u_z^\infty}{\partial y} & \dfrac{\partial u_z^\infty}{\partial z} \end{bmatrix}. \tag{1}$$

The tensor $\boldsymbol{\Gamma}^\infty$ can be decomposed as follows:

$$\boldsymbol{\Gamma}^\infty \cdot \mathbf{x} = \mathbf{e}^\infty \cdot \mathbf{x} + \boldsymbol{\omega}^\infty \times \mathbf{x}$$

where the rate of strain tensor is the symmetrical part of $\boldsymbol{\Gamma}^\infty$, $e_{ij}^\infty = (\Gamma_{ij}^\infty + \Gamma_{ji}^\infty)/2$, and the components of the angular velocity of the fluid are related to the antisymmetrical part of the gradient:

$$\omega_1^\infty = (\Gamma_{32}^\infty - \Gamma_{23}^\infty)/2 \qquad \omega_2^\infty = (\Gamma_{13}^\infty - \Gamma_{31}^\infty)/2 \qquad \omega_3^\infty = (\Gamma_{21}^\infty - \Gamma_{12}^\infty)/2.$$

Stokesian dynamics provides a simple way to calculate the action of the fluid on each monomer of the simulated aggregate [17,18]. This technique relates the velocities of a swarm of spherical particles to the hydrodynamic forces acting on them through a mobility matrix. In