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Discrete element modeling of the microstructure of fine particle agglomerates in sheared dilute suspension

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HIGHLIGHTS

- The initial agglomerates are generated by the Cluster–Cluster Aggregation (CCA) algorithm.
- Break-up and restructuring of loose fractal agglomerates under shear are studied by the DEM.
- The fragmentation number is validated from the hydrodynamical and chemical contexts, and the particle size.
- The packing density of the agglomerates is studied as a function of the fragmentation number.
- The particle size and the chemical context do not affect the exponents of the power laws.

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ABSTRACT

The fragmentation and restructuring under shear of agglomerates of fine mineral particles are studied with the Distinct Element Method. The model used takes into account contact forces, van der Waals forces, and hydrodynamic forces computed with the free-draining approximation. A loose initial agglomerate is submitted to a constant shear rate until reaching a quasi-stationary state, where the number, size and structure of fragment of agglomerates can be considered as constant. The influence of shear stress and size of particles on the characteristics of agglomerates at equilibrium is studied. Fragmentation is controlled by a non-dimensional number, depending on the radius of the particles, shear rate and maximal adhesion force.

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1. Introduction

The agglomeration of fine particles in suspensions plays a crucial role in a lot of industrial applications like pharmaceutical, food processing, water treatment, civil engineering.... It has in particular a determining influence on the rheological behavior of suspensions. Indeed, agglomeration leads to the formation of large porous composite particles containing part of the free water of the suspension and modifying also the particle size distribution of the suspended particles. It is very important to know the characteristics of these agglomerates so as to apply rheological models allowing us to predict the suspension viscosity [1,2].

Agglomeration of fine particles in a resting fluid is quite well understood [3] and leads to the formation of loose and deformable agglomerates. However, under shear, agglomerates tend to restructure and change into denser composite particles containing water.

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In most of the previous studies on the fragmentation of the particle agglomerate in a fluid flow, it has been explained that the fragmentation process is dominated by a static or dynamic balance between the cohesive forces (or the cohesive strength of the agglomerate) and the hydrodynamic force (or hydrodynamic stress). This fragmentation process has already been studied by a lot of experimental [4–8] and theoretical and numerical approaches [9–14]. In a shear flow, some researchers pointed out that the relation between hydrodynamic shear stress characterized by the product of the fluid viscosity by shear rate, and the final (stable) agglomerate size obeys the power law [4,15]. The final size of the agglomerate for a given flow condition is largely dependent on the initial agglomerate structure [9,10]. The exponent of the power law is called fracture. Based on the balance theory between driving and resisting forces, some similar dimensionless numbers have already been proposed in the literature to predict the final agglomerate size [9–11,16–18] but have also been used to develop a breakage kernel [19]. It has already been previously observed that when the final agglomerate size is scaled with the dimensionless number, almost all data are aligned on a single straight line [9,10]. The authors emphasize that some data tend to deviate from the master line which they explain by the non-linearity of the behavior of constituent particles in the simulation [9] or do not explain [10]. If all studies agree on the establishment of a final size of agglomerates, a quite large dispersion is obtained in the literature on the values reported for the fracture exponent of the power law, and the explanation for this dispersion does not enjoy consensus. Many researchers have suggested certain key ideas for reflection on this dispersion. Recently, Eggersdorfer et al. [12] attributed the offset of the data to different primary particle sizes, bond strength and level of description of the hydrodynamic force because the inter-particle force as well as the hydrodynamic force change with the primary particle size and their ratio influences the steady state agglomerate size. Harshe and Lattuada [19] emphasize that the fracture exponent depends on the type and magnitude of the inter-particle interactions taken into account.

The mechanisms involved in the restructuring have already been explored. In the field of colloidal science, the restructuring of particle agglomerates has been often reported from a viewpoint of the change in space-filling properties [8,20,21]. Generally, the space-filling properties of agglomerates are expressed by the fractal dimension. Harada et al. [18,22] studied by discrete numerical simulations, the restructuring from a viewpoint of the coordination number for the non-fractal agglomerates in a shear flow. The authors have demonstrated that a loose non-fractal agglomerate increases the coordination number and it turns into a dense agglomerate owing to the fluid stress. However, in the case of fractal agglomerates, the internal connectivity may be changed with its fractal dimension and its packing density kept constant. Becker et al. [11] showed that tangential forces significantly affect restructuring behavior and neglecting tangential forces leads to a strong overestimation of the restructuring effects. The transition from the rotational regime to the restructuring regime for the colloidal aggregates exposed to a shear flow has been investigated by Becker et al. [23]. Their results show that the probability that an aggregate being affected by restructuring changes depends on the numbers of primary particles.

The kinetics of fragmentation and the evolution of aggregates' size and fractal structure have been particularly studied. If the prediction and control of the size of the agglomerates in the shear field are required, this information is not sufficient to precisely characterize their microstructure. Indeed, less attention has been paid to the density of agglomerates which characterizes the quantity of water trapped inside composite particles. Despite the role played by the restructuring process on the structural change of the fractal agglomerates under shear, very little attention has been paid to the characterization of a contact network formed by the constituent particles. Also, the influence of the primary particle size has not been explored in detail. These three points have to be specified anyway if one wants to apply existing rheological models to predict the viscosity of suspensions.

The aim of this paper is to develop a DEM simulation of agglomerates in sheared dilute suspensions in order to identify the influence of shear rate, physicochemical context and primary particle size on the size, structure and density of agglomerates. The paper is organized as follows: the DEM model is described in Section 2; simulation conditions and numerical methods used for the characterization of agglomerates are presented in Section 3; results and discussion are presented in Section 4 and compared to the literature.

2. DEM model presentation

The DEM was initially developed by Cundall and Stack [24]. Since this seminal work, it has considerably developed and it is now widely used for the simulation of granular materials. In our simulations, an initial loose agglomerate of fine spherical mono-sized particles of radius a is immersed into a fluid and submitted to a constant shear rate.

2.1. Equations of motion

$$m_i \frac{\mathrm{d}\mathbf{V}_i}{\mathrm{d}t} = \sum_{j=1}^{N} \mathbf{F}_{ij} + \mathbf{F}_{i,h} \tag{1}$$

$$I_i \frac{\mathrm{d}\boldsymbol{\omega}_i}{\mathrm{d}t} = \sum_{j=1}^{N} \mathbf{T}_{ij} + \mathbf{T}_{i,h} \tag{2}$$

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