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A stochastic approach for the simulation of collisions between colloidal particles at large time steps

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ABSTRACT

This paper presents a new approach for the detection and treatment of colloidal particle collisions. It has been developed in the framework of Lagrangian approaches where a large number of particles is explicitly tracked. The key idea is to account for the continuous trajectories of both colliding partners during a time step that is not restricted. Unlike classical approaches which consider only the distances between a pair of particles at the beginning and at the end of each time step (or assume straight-line motion in between), we model the whole relative, and possibly diffusive, trajectory. The collision event is dealt with using the probability that the relative distance reaches a minimum threshold (equal to the sum of the two particle radii). In that sense, the present paper builds on the idea of a previous work. However, in this first work, the collision event was simulated with a simplified scheme where one of the collision partners was removed and re-inserted randomly within the simulation domain. Though usually applied, this treatment is limited to homogeneous situations. Here, an extension of the stochastic model is proposed to treat more rigorously the collision event via a suitable evaluation of the time and spatial location of the collision and an adequate calculation of subsequent particle motion. The resulting collision kernels are successfully compared to theoretical predictions in the case of particle diffusive motion. With these promising results, the feasibility of simulating the collisional regime over a whole range of particle sizes (even nanoscopic) and time steps (from a ballistic to a purely diffusive regime) with a numerical method of reasonable computational cost has been confirmed. The present approach thus appears as a good candidate for the simulation of the agglomeration phenomenon between particles also in complex non-homogeneous flows.

1. Introduction

1.1. Agglomeration process

Agglomeration (also referred to as coalescence, coagulation, flocculation or aggregation) is related to the formation of larger particles upon collision and adhesion of two smaller particles. Particle agglomeration occurs in a wide range of situations such as meteorology (formation of clouds Gotoh and Fujii, 1998; Saffman and Turner, 1956), bioaggregates (in wastewater treatment facilities where coagulation is used during separation operations Bäbler and Morbidelli, 2007; Chu and Lee, 2004), filtration (agglomeration of colloidal particles Iimura et al., 2009), medical or pharmaceutical fields (for instance protein aggregation Bernacki and Murphy, 2009) as well as astrophysics (formation of planets Blum and Wurm, 2008). Within this wide-range subject, the present study is more specifically concerned with the simulation of agglomeration of colloidal particles (i.e. particles with sizes ranging from a few nanometres up to a few micrometres Elimelech et al., 1995) carried by complex flows (turbulent flows, wall-bounded flows, etc.).

In a way that is similar to the formation of multilayers of particles on a surface (Henry et al., 2012), the agglomeration phenomenon can be described as resulting from the interplay

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between two main mechanisms which are manifested in two different steps:

1. a collision step: this first step is governed by particle–fluid interactions, which influence the number of particle–particle encounters, their time of occurrence and their locations in space;
2. an adhesion step: this second step is governed by physico-chemical forces that act between particles when the separation distance is very small and that lead the colliding particles either to stick or to bounce off. These short-ranged physico-chemical forces are often accounted for using the DLVO theory (named after the work of Derjaguin and Landau (1941) and Verwey and Overbeek (1948)), which describes the interaction between two particles as the sum of van der Waals contributions and double-layer electrostatic interactions (Elimelech et al., 1995; Hunter, 2001; Israelachvili, 2011; Parsegian, 2005).

Since these two steps of agglomeration are of different nature and act at completely different scales, they are often treated separately. In this paper, attention will be focussed on the **simulation of the collision step** while the attachment step will be addressed in a subsequent paper.

1.2. Modelling approaches for particle collision

Various approaches have been proposed to simulate collisions between particles. These approaches can be classified into two main categories (Mohaupt et al., 2011):

1. The first approach consists in solving population balance equations for a given number of characteristic particle classes (Elimelech et al., 1995; von Smoluchowski, 1917). This approach thus provides information on macroscopic features of particle collisions (here the distribution of particle sizes). However, this approach requires a previous knowledge of the frequency of particle collisions (or the collision kernel β) for given hydrodynamic conditions. Formulas for the collision kernels have been derived in simple academic cases (more details in Elimelech et al. (1995)) but collision kernels in more complex situations have not been obtained yet;
2. In the second approach, referred to as particle-tracking approach, a large number of particles carried by a flow is explicitly tracked and the interactions between pairs of particles are evaluated. This approach thus gives insights into local (position-dependent) particle statistics such as the average size or velocity. Yet, the question that arises when using such particle-tracking approaches is to choose an appropriate method for the detection of particle collisions depending on the amount of information that is desired and on the numerical costs. A first method (Ho and Sommerfeld, 2002; Sommerfeld, 2001) consists in generating a fictitious particle every time step for each real particle and to evaluate the collision probability between this fictitious particle and the corresponding real particle using collision kernels derived from the kinetic theory of gases. A second method (Sundaram and Collins, 1996; Yeung and Pope, 1988) corresponds to the direct numerical simulation of particle collisions where collisions are evaluated using either an overlap condition (Chen et al., 1998; Sundaram and Collins, 1996) (interparticle distance smaller than the sum of the two radii) or a molecular dynamics-based algorithm (Sigurgeirsson et al., 2001) (geometric criteria for particles in the ballistic regime). This method allows to calculate the collision kernel as a result of a fully microscopic simulation and provides accurate predictions of collision kernels in various and complex conditions. However, it is limited to small time steps, i.e. in the ballistic regime where the time step Δt is much smaller than the particle relaxation time τ_p and is not appropriate to simulate collisions between nanoscale particles whose relaxation times are small.

1.3. Purpose of the paper

The purpose of the present study is to develop a new numerical method to simulate agglomeration of colloidal particles that remains valid in complex situations (turbulent flows, wall-bounded flows, etc.) where analytical formulas of the collision kernel do not exist. Numerical results of such collision kernels in complex situations can then be used as an input in classical population balance approaches. This numerical method should also be valid for inertial particles, while polydispersion in particle sizes should be treated without approximation. For that purpose, a particle-tracking approach is retained. With respect to the limitations of existing particle-tracking models, the aim of the present study is to put forward new ideas and to develop a corresponding algorithm for the detection of particle collisions using a direct method that is also valid for large time steps (thus allowing faster evaluations of the collision kernel than existing direct simulations). To that extent, a stochastic approach for the detection of particle collisions is chosen following the recent developments of Mohaupt et al. (2011). The key idea behind this approach is to consider the diffusive (random and continuous) particle trajectories during a (large) time step and to evaluate the probability that particles interact along two such trajectories. It has been shown to provide accurate predictions of the collision kernel independently of the time step and for various sizes of particles undergoing Brownian motion (Mohaupt et al., 2011). However, these promising results have been obtained with a simplified treatment of particle collisions (valid only for homogeneous flows): upon collision, one of the partners was removed and replaced randomly within the simulation domain. The particular aim of the present paper is thus to introduce a new stochastic model to simulate more rigorously the collision event that is valid for complex non-homogeneous situations. More specifically, knowing that a collision between a pair of particles has occurred, three main issues must be addressed:

a. When does the collision occur?
b. Where does the collision take place?
c. What is the motion of each particle after collision?

1.4. Organisation of the paper

Within this scope, the present paper is organised as follows. The modelling approach is presented in Section 2. A quick overview of the approach proposed previously by Mohaupt et al. (2011) is given in Section 2.1, followed by a generalisation to treat more specifically the collision event (time and space locations) and to account for particle motion after collision (Section 2.2). Then, numerical results obtained with the new stochastic approach for particle collisions are presented and discussed in Section 3. Numerical predictions of the collision kernels for monodispersed particles undergoing diffusive motion are compared to theoretical expectations that exist in some simplified situations in Section 3.1 to validate present ideas, followed by numerical results obtained for the collision kernels of initially polydispersed particles undergoing diffusive motion (Section 3.4).

2. Stochastic modelling approach for particle collisions

This section introduces the key notions of the present approach, where the trajectory of N particles is explicitly tracked and the collision event between each pair of particles is evaluated at every time step.