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Particle-based modeling of aggregation and fragmentation processes: Fractal-like aggregates

Jens C. Zahnow *, Joeran Maerz, Ulrike Feudel

Theoretical Physics/Complex Systems, ICBM, University of Oldenburg, 26129 Oldenburg, Germany

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ABSTRACT

The incorporation of particle inertia into the usual mean field theory for particle aggregation and fragmentation in fluid flows is still an unsolved problem. We therefore suggest an alternative approach that is based on the dynamics of individual inertial particles and apply this to study steady state particle size distributions in a 3D synthetic turbulent flow. We show how a fractal-like structure, typical of aggregates in natural systems, can be incorporated in an approximate way into the aggregation and fragmentation model by introducing effective densities and radii. We apply this model to the special case of marine aggregates in coastal areas and investigate numerically the impact of three different modes of fragmentation: large-scale splitting, where fragments have similar sizes, erosion, where one of the fragments is much smaller than the other and uniform fragmentation, where all sizes of fragments occur with the same probability. We find that the steady state particle size distribution depends strongly on the mode of fragmentation. The resulting size distribution for large-scale fragmentation is exponential. As some aggregate distributions found in published measurements share this latter characteristic, this may indicate that large-scale fragmentation is the primary mode of fragmentation in these cases.

1. Introduction

In recent years there has been a great effort to investigate the advection of inertial particles in fluid flows [1–6]. Understanding the behavior of inertial particles like aggregates, dust or bubbles moving in incompressible flows plays an important role in such diverse fields as cloud physics [7], engineering [8], marine snow and sediment dynamics [9,10] as well as wastewater treatment [11]. The dynamics of individual inertial particles is dissipative. This leads to a behavior that is very different from passive tracers, for example to a preferential accumulation in certain regions in space, i.e. on attractors [12–14]. Previous studies concentrated mainly on non-interacting particles, in spite of the fact that accumulation leads unavoidably to mutual interactions of different kinds.

It is well known that as a result of collisions between particles, aggregates can be formed that consist of a large number of primary particles. In many areas of science the formation of such aggregates and their break-up due to shear forces in the flow plays a very important role, e.g. in sedimentation of particles in oceans and lakes [15], chemical engineering systems such as solid–liquid separation [16,17], aggregation of marine aggregates [18] and flocculation of cells [19].

Most approaches of aggregation and fragmentation models are based on the pioneering work of Smoluchowski [20] and use usually a mean field approach with kinetic rate equations to model these processes (see e.g. Jackson [9]). However, for particles with inertia a field theory for the particle velocity has not yet been formulated. The existence of caustics, meaning that the dynamics of inertial particles would lead at some points to a multi-valued particle velocity field [21,22], has prevented such an approach so far. While attempts have been made to incorporate particle inertia in approximate ways in a mean field approach [23,24], no completely satisfying solution has been found yet.

Here we therefore choose a different, individual particle-based approach, where the dynamics of finite size particles are taken directly into account. The approach has recently been introduced in Ref. [25], and discussed in more detail with respect to different flows in [26]. In the present study we adopt this approach to study the long-term behavior of particle size distributions that develop from a balance between aggregation and fragmentation. In particular, we examine the influence of fragmentation and aggregate structure on these size distributions.

In most previous works the particles were considered to be spheres with a specific density. In many realistic cases, for example for marine aggregates, this is a crude approximation. The complex structure of particles can have a great influence on particle dynamics as well as aggregation and fragmentation processes. Both the actual motion of aggregates and the probabilities for aggregation and fragmentation are influenced by the structure of

* Corresponding author. Tel.: +49 441 7983904.
E-mail addresses: zahnow@icbm.de, jens.c.zahnow@uni-oldenburg.de (J.C. Zahnow).

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the particles. In the context of a mean field approach, a complex particle structure has been incorporated in the past in terms of a density modification for the particles, e.g. by Kranenburg [27] or Maggi et al. [28]. However, so far there have been very few attempts to treat this problem for inertial particles in a flow. Wilkinson et al. [29] used a model for fractal particles in an aggregation model for dust particles during planet formation. Our present work expands the consideration of spherical particles to model more realistic aggregates. We focus specifically on the problem of aggregation and fragmentation in systems where the aggregates can be described as having a *fractal-like structure*, as is for example the case for marine aggregates [27]. By this we mean that on average there exists a power-law relationship between the characteristic length and the mass of such aggregates. The exponent of the power law is called the fractal dimension. Such a characterization in terms of a fractal dimension leads to a modification of the radii and effective densities of the aggregates compared to a solid sphere of the same mass. Nevertheless, we still treat them as effectively spherical for the particle motion, allowing us to apply the Maxey–Riley equations of motion [30] with modified parameters.

In this work we choose a parameterization of our model for the case of a suspension of marine aggregates in the ocean. In this way we can study our modeling approach for a specific case, but we emphasize that our model is a general one that can in principle be used for a wide range of applications where aggregation and fragmentation of solid particles play a role. The concept of a fractal-like structure has been found to be a reasonable first approximation in many different applications, ranging from colloidal systems to the flocculation of cells [31]. A different application would require a different parameterization of the model, but the general approach introduced here would remain the same.

Since the fractal dimension of marine aggregates can vary greatly in natural systems [28], we examine its effect on the steady state particle size distributions in our model. We find that while the shape of the size distributions does not depend strongly on the fractal dimension, the average particle size and relaxation time towards the steady state depend strongly on this parameter.

Even though to a certain extent methods from dynamical systems theory can usefully be applied, we mention that the entire problem is much more complex than that of any usual dynamical system. While particles of a single size move on specific attractors, aggregation and fragmentation lead to repeated transitions from one attractor to another one, depending on the aggregate size. The skeleton of the new dynamics is therefore a superposition of the different attractors, with transient motion in between. The structure of the individual attractors and their superposition in turn influence the aggregation probabilities due to different local concentrations of particles. Fragmentation is also affected by the particle dynamics, because shear forces can be locally different in the flow. Therefore, break-up may depend on whether an attractor for a certain particle size lies in a region with high shear or not.

We show that the combination of aggregation and fragmentation of fractal-like aggregates, superimposed on inertial advection dynamics, leads to a convergence to a steady state in the particle size distribution. This steady state is unique for a given set of parameters. Mainly, we compare three different types of splitting, uniform fragmentation, erosion and large-scale fragmentation. These splitting modes differ in the size of the fragments that are created during break-up. While erosion leads to one large and one relatively small fragment, large-scale fragmentation leads to two fragments of similar size. We find that the transient dynamics as well as the size distribution in the steady state depend strongly on the splitting mode. The steady state size distribution found for large-scale fragmentation conforms best to observation reported in the literature for the break-up of marine aggregates in tidal areas [32], indicating that this may be the primary mode of fragmentation in these cases.

Section 2 describes the complete model for advection, aggregation and fragmentation that is used in this work. The equations of motion for heavy spherical particles (Stokes equation) are used, but with modified parameters to take a fractal-like structure into account. Rules governing the aggregation and fragmentation are introduced. Finally, the model is applied to a simple 3D synthetic turbulent flow field.

Section 3 then presents a complete analysis of the influence of all major system parameters on the resulting steady state size distributions, the average aggregate size in steady state and the relaxation time towards the steady state. Namely, these parameters are aggregate strength, fractal dimension of the aggregates and total particle mass in the system.

Section 4 contains a discussion of the limitations of the model and the conclusions.

2. Advection, aggregation and fragmentation model

In this section we will present the modeling approach used in this study, that describes the motion, aggregation and fragmentation of finite size particles. Firstly, the equations of motion used for the advection of spherical particles heavier than the surrounding fluid are presented. Secondly, a model to account for the fractal-like structure of real aggregates is described. Thirdly, a full model to include aggregation and fragmentation in this context is introduced. Finally, a simple 3D synthetic turbulent flow field is chosen, that will be used to study the aggregation and fragmentation model in detail.

2.1. Equations of motion for spherical particles

For simplicity, we consider all primary (smallest, unbreakable) particles to be spherical and denser than the ambient fluid. We emphasize that the equations of motion presented here for spherical particles will in the following also be used to describe the motion of aggregates which usually cannot be assumed to be spherical [27]. However, to account for properties related to the fractal-like structure of aggregates some modifications to the equations of motion (in the form of modified parameters) will be introduced in the next section. While this represents only a very simplified model and the surface forces acting on particles with a complex structure are an extremely complex problem where to date no satisfying expressions exist, we believe that this is a reasonable starting point. On the one hand, if one wants to employ the model discussed here to a specific case where better expressions are known, this can easily be adapted without changing the general idea of our approach. On the other hand, it has been found in many cases (see for example [25,26]) that changes in the motion of the individual particles usually do not lead to significant changes in the dynamics of the particle ensemble and in particular in the collision rates which are relevant for the overall size distribution in an aggregation–fragmentation system.

Finite size particles usually do not follow exactly the motion of the surrounding fluid, instead inertia effects lead to deviations of the particle motion from that of the fluid. For small particle Reynolds numbers the equations of motion for spherical particles of finite size are the Maxey–Riley equations [30]. This implies that locally the flow around the particle is laminar, even though the overall fluid flow can still be turbulent. While inertia effects can be fairly small for the primary particles in the case of marine aggregates (see Section 2.6), the influence of particle inertia increases with aggregate size and can become quite important for larger marine aggregates.