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Analysis of aerodynamic dispersion of cohesive clusters

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HIGHLIGHTS

- DEM coupled with CFD has been used to investigate aggregate dispersion.
- Dispersion behaviour is dependent on the relative aggregate size.
- If the relative aggregate size is small, the aggregate will disintegrate.
- For larger aggregates, the dispersion process switches to surface erosion.

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ABSTRACT

The aerodynamic dispersion of bulk powders is important for a number of applications including particle characterisation, and the delivery of therapeutic drugs via the lung using dry powder inhalers (DPIs). Complete aerodynamic dispersion of cohesive clusters is very challenging to achieve, due to large interparticle attractive forces compared to dispersive forces.

In this paper the distinct element method (DEM) coupled with continuum models for the fluid phase flow to simulate fluid–solids interactions is used to investigate the aerodynamic dispersion of different sized cohesive clusters in a uniform fluid flow field. The simulations have shown that aggregate dispersion behaviour is dependent on the relative aggregate size (i.e. the ratio of aggregate diameter to primary particle diameter). If the aggregate size is small, it appears as though the aggregate disintegrates; however, for larger aggregates, the dispersion process switches to a gradual peeling of the particles from the surface layers. These two dispersion processes have been analysed through investigating dispersion rate and it has been shown that the dispersion rate decreases as the aggregate size increases. Furthermore, different regions within the aggregates have been studied and confirm that for larger aggregates the surface particles disperse more rapidly than internal particles; however, for smaller aggregates, dispersion is essentially occurring everywhere in the aggregate.

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1. Introduction

The complete dispersion of powders to their constituent entities is important for a number of industries, including pharmaceutical, bulk chemical and food. Aerodynamic dispersion is receiving much attention due to its importance for particle characterisation and drug delivery via the lungs from dry powder inhalers (DPIs). The dispersion of fine cohesive powders is challenging because of large attractive forces, such as van der Waals, electrostatics and liquid bridges (Visser, 1989), compared to dispersing forces, such as drag and impaction.

Recently, two reviews related to aerodynamic dispersion are available and provide a comprehensive critique of the current state of theoretical and experimental understanding (Calvert et al., 2009; Masuda, 2009). Aggregated clusters experience several type of forces due to rapid acceleration, deceleration, turbulent eddies, impact on surfaces etc. Kousaka et al. (1979) concluded that dispersion by impaction (particle—particle and particle–wall) is the most effective and that dispersion by acceleration can be effective, provided the velocity difference between the fluid and particles, the relative velocity, is sufficiently large. There are several theoretical approaches based on a force balance that evaluate the separating force acting at a contact point between two particles when accelerated in a uniform flow field (Kousaka et al., 1979, 1992; Yuu and Oda, 1983); however, these basic models are not directly applicable to the dispersion of cohesive aggregates of a large number of particles.

Computational simulations involving the distinct element method (DEM) coupled with computational fluid dynamics (CFD) for simulating two phase flows have received much attention (Xu and Yu, 1997; Moreno-Atanasio et al., 2007). With respect to deformation and breakage of loose aggregate assemblies in fluid

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flow fields, a number of computational studies are available that focus on liquid systems (Zeidan et al., 2007; Higashitani et al., 2001; Fanelli et al., 2006a, 2006b). Increasing attention has been given to the behaviour of loose aggregate clusters dispersed in air (Iimura et al., 2009; Tong et al., 2010; Calvert et al., 2011). Iimura et al. (2009) investigated the dispersion of particle aggregates in air and water. The investigation shows dispersion behaviour only qualitatively; and hence a greater understanding is necessary with respect to particulate dispersion in air to quantify the condition for a complete dispersion. Tong et al. (2010) introduced an index based on the ratio of impact energy and cohesion energy and showed that the dispersion efficiency correlated well with the index. Furthermore, Moreno-Atanasio and Ghadiri (2006) defined a mechanistic model that described aggregate breakage due to impact based on an energy approach, which related the number of broken contacts in a particle assembly to impact velocity, inter-particle adhesion energy and particle properties. A quantitative evaluation of aggregate dispersion by acceleration in a uniform flow field was conducted by Calvert et al. (2011). It was shown that the dispersion of aggregates occurred once a threshold relative velocity was reached. To analyse the effect of surface energy on particle dispersion, a model was developed that expressed the extent of dispersion to the ratio of the fluid resistance force acting on a sphere to the bond strength binding the particles together. This approach resulted in a dimensionless dispersion index (DI) which incorporated the Weber number, which is also present in the impact model of Moreno-Atanasio and Ghadiri (2006), and a second parameter for the size ratio between the aggregate diameter and primary particle diameter (Eq. (1)):

$$DI = \frac{\rho_f D_{Agg} u_r^2}{\Gamma} \left(\frac{D_{Agg}}{d}\right) \quad (1)$$

where ρ_f is the fluid density, Γ is the interface energy, u_r is the relative velocity, D_{Agg} is the aggregate diameter and d is the primary particle diameter.

The effect of aggregate size was also briefly addressed by Calvert et al. (2011) who showed qualitatively that the loose aggregate dispersion behaviour was dependent on the aggregate size. It seemed that small aggregates dispersed by disintegration, whereas large aggregates dispersed by particles gradually peeling from the cluster surface. For the latter, Calvert et al. (2011) only provided a qualitative description of the dispersion behaviour. In this paper the dispersion behaviour of loose aggregates of different size ratios, accelerated in a uniform flow field, is further investigated with a quantitative approach that evaluates the difference in dispersion rate as aggregate size increases; furthermore, different regions within the aggregates are studied and the rate of dispersion in these regions is shown.

2. Simulation details

The distinct element method (DEM) coupled with computational fluid dynamics (CFD), based on the commercial code produced by Itasca, PFC3D, has been used to investigate the two phase interaction of the particles and the fluid. Details regarding the simulation approach can be found in Calvert et al. (2011).

To investigate the dispersion behaviour as a function of aggregate size, four assemblies have been generated in exactly the same way, but with different particle numbers and hence different aggregate diameters. For each loose aggregate, the primary particles, with properties shown in Table 1, were randomly generated and brought together by applying a centripetal acceleration towards a point in the centre of the cluster until a stable coordination number was achieved. The interface energy and particle friction were then progressively introduced between particles to the required level. Subsequently, the centripetal acceleration was gradually removed from the particle assembly. Details of the four loose aggregate assemblies, which have been investigated, are shown in Table 2.

Table 1
Particle and fluid properties.

Diameter	100 μm
Density	2500 kg/m^3
Normal stiffness	7.9×10^4 N/m
Shear stiffness	7.9×10^4 N/m
Contact damping (-)	0.16(dimensionless)
Friction coefficient (-)	0.3(dimensionless)
Fluid density	1.225 kg/m^3
Fluid viscosity	1.8×10^{-5} Pa s

Table 2
Loose aggregate properties.

Loose aggregate	*A*	*B*	*C*	*D*
Number of particles	500	1000	2000	8000
Aggregate diameter (mm)	0.966	1.22	1.52	2.37
Contact number (coordination number)	1494 (5.976)	2994 (5.988)	5894 (5.894)	23,608 (5.902)

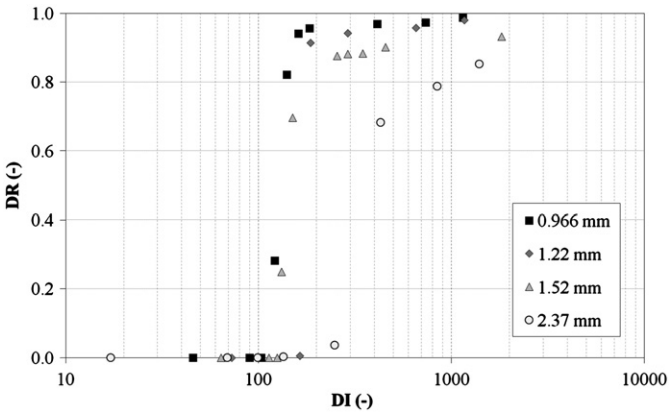

Fig. 1. Relationship between the dispersion ratio and dispersion index for the different loose aggregates shown in Table 2 and interface energy 0.1 J/m^2 after 3×10^{-4} s.

3. Aggregate dispersion

To evaluate the state of aggregate dispersion, a parameter termed dispersion ratio (DR) has been defined. DR relates the number of broken bonds in a specific aggregate after a given amount of time compared with the initial number of bonds. Calvert et al. (2011) investigated DR as a function of DI (Eq. 1) and showed a good unification of data obtained for the different interface energies. This indicated that DI could be used to define the onset of loose aggregate dispersion due to acceleration by a fluid flow.

The dispersion index incorporates a size ratio term which leads to a similar unification of data. In Fig. 1 the dispersion ratio is given as a function of the dispersion index for all the loose aggregates in Table 2 for interface energy, 0.1 J/m^2. A good unification of the data is seen for the smaller aggregates. However, as the aggregate size increases the data shifts to higher values of DI. Calvert et al. (2011) showed qualitatively that as the

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