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Discrete element modelling of agglomerate impact using autoadhesive elastic-plastic particles

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ABSTRACT

In this study, the impact of agglomerates composed of autoadhesive, elastic-plastic primary particles are simulated using the discrete element method. Results obtained are compared to the impact breakage of an agglomerate of autoadhesive elastic particles. It is found that, for the same impact velocity, the elastic agglomerate fractures but the elastic-plastic agglomerate disintegrates adjacent to the impact site. For the elastic-plastic agglomerate, the impact damage increases with increase in material yield stress. It is also found that the particle size distribution of the debris is more accurately defined by a logarithmic function rather than the power law function commonly obtained for impacts of agglomerates composed of elastic particles.

1. Introduction

Particulate materials are frequently in the form of powders which are themselves agglomerations of much smaller sized primary particles. A common problem inherent in the handling of powders is the degradation resulting from attrition and/or fragmentation of agglomerates as they collide with each other and with the process equipment. Impact breakage has been studied experimentally for many years [1–9]. However, information from such experiments is normally restricted to post-impact examinations of the fragments and debris produced due to the short duration of an impact event. Numerical simulations of agglomerate impact fracture can overcome these restrictions and, therefore, have been extensively used to simulate impacts of agglomerates. Notable research findings have been made by Thornton and co-workers [10–18] by using the discrete element method [19,20] based upon contact mechanics [21]. Thornton et al. [10] reported results of 2D simulations of agglomerate impact and demonstrated that the energy required to break the interparticle bonds was orders of magnitude less than the initial work input. Three-dimensional simulations of impacts of a crystalline agglomerate were presented by Kafui and Thornton [14]. It was shown that the proportion of bonds broken during an impact was proportional to $\ln(V/V_0)$ where V is the impact velocity and V_0 is the threshold velocity below which no significant damage occurred. The threshold velocity V_0 was found to scale with $\Gamma^{3/2}$ were Γ is the interface energy between contacting particles. From 3D simulations of the normal impact of a polydisperse (irregular array) spherical agglomerate [11,12] it was shown that higher impact velocities lead to higher platen forces, local contact damage, number of broken bonds and amount of debris produced. It was demonstrated that rebound, fracture or shattering could occur depending on the magnitude of the impact velocity and the strength of the interparticle bonds.

Mishra and Thornton [15] demonstrated that dense agglomerates always fracture (above a critical impact velocity) but loose agglomerates always disintegrate. They showed that either fracture or disintegration may occur for agglomerates with an intermediate packing density and that the mode of breakage can change from disintegration to fracture by either increasing the interparticle contact density or by changing the location on the agglomerate surface that is used as the impact site. From simulations of the normal impact of a cuboidal agglomerate with a planar target wall, Thornton and Liu [16] showed that fracture occurs as a result of the heterogeneous distribution of the strong force transmission into the agglomerate that, due to the consequent heterogeneous distribution of particle decelerations, creates a heterogeneous velocity field. It was shown that this produces shear weakening along strong velocity discontinuities that subsequently become the potential fracture planes. If, for whatever reason, strong forces are unable to propagate into the agglomerate then fracture does not occur and the breakage mechanism is one of progressive disintegration.

Given the fact that in the processing industries not all granulation processes produce spherical or near-spherical agglomerates, simulations of the impact breakage of cuboidal and cylindrical agglomerates were presented by Liu et al. [18]. It was found from the simulations that cuboidal edge, cylindrical rim and cuboidal corner impacts generate less damage to the agglomerates. Detailed examinations of the evolutions of damage ratio, wall force and mass distribution of fines produced after impact indicated that the size of the initial contact area, the rate of change of the contact area, together with the local microstructure at the

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impact site play important roles in agglomerate breakage behaviour. Internal damage to the agglomerate is closely related to the particle deceleration adjacent to the impact site.

On the other hand, intensive research on agglomerate impact has also been carried out by many other researchers to examine various possible influence factors on agglomerate impact. These include particle size and bond strength [22,23], impact angle [24,25], interface energy [26] and energy dissipation [27]. There is perhaps one factor that hasn't been fully examined so far, i.e., particle plastic deformation at contacts during an agglomerate impact. We believe that this issue needs to be addressed in granular material impact because high stress concentration at particle contacts during particle collisions can occur, and the resultant inter-particle energy loss could directly affect the mechanisms of attrition and breakage of the agglomerate. Hence, this study focusses specifically on this problem and preliminary research results obtained are presented in the following sections.

2. Numerical methodology and agglomerate preparation procedures

2.1. Granular dynamics

The granular dynamics model used in this study originated as the distinct element method (DEM), [19]which was extended to 3D applications by the development of the program TRUBAL, Cundall [20].

In DEM simulations, the particle interactions are modelled as a dynamic process, the evolution of which is advanced using an explicit finite difference scheme to obtain the incremental contact forces and then the incremental displacements of the particles, both linear and rotational. Each cycle of calculations that takes the system from time t to time t + Δt involves the application of incremental force–displacement interaction laws at each contact, resulting in new interparticle forces that are resolved to obtain new out-of-balance forces and moments for each particle. Numerical integration of Newton's second law of motion yields the new linear and rotational velocities for each particle. A second integration yields the incremental particle displacements and, using the new particle velocities and positions, the calculation cycle is repeated in the next time step. The time step Δt used is a fraction of the critical time step determined from the Rayleigh wave speed for the solid particles. For complete details of the granular dynamics methodology the reader is referred to Thornton [21].

The version of the DEM code adapted to simulate agglomerates (and renamed GRANULE) is capable of modelling elastic, frictional, adhesive or non-adhesive spherical particles with or without plastic yield at the interparticle contacts. For the agglomerate impact simulations reported below we have adopted the adhesive, elastic contact force model of Thornton and Yin [28] and the adhesive, elastic-plastic contact force model of Thornton and Ning [29]. Full theoretical details of these models can be found in [28,29,21].

2.2. Preparation of an agglomerate

We have chosen to prepare a cuboidal agglomerate of particles in this research because it bears some 'attractive' characteristics such as having corners and edges which potentially allow us to be flexible to create an impact orientation which would likely exhibit structural changes that are sensitive to plastic deformation during an impact. In addition, for the chosen orientation, the motion is essentially planar and therefore cracks are easily visualised.

The agglomerate consisted of 10,000 primary particles (spheres) with an average diameter of 20 μm and particle size distribution as shown in Fig. 1. For the agglomerate the material properties of the primary particles were specified as: Young's modulus E = 70 GPa, Poisson's ratio $\nu = 0.3$, density $\rho = 2650$ kg/m^3 and interparticle friction coefficient $\mu = 0.35$. The same properties were specified for the stationary planar wall against which the agglomerate was to be impacted.

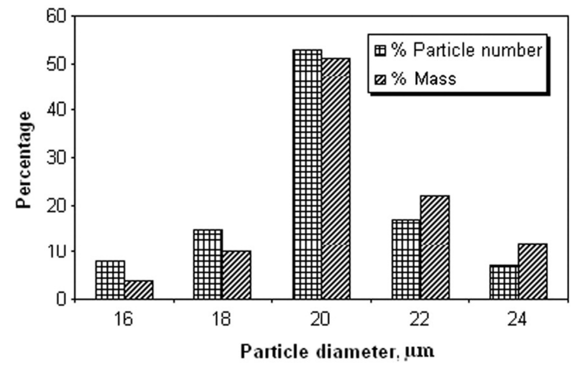
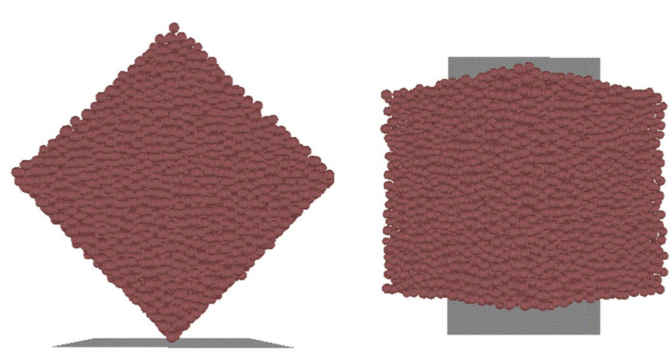


Fig 1. Particle size distribution in the agglomerate.

The procedures used to prepare the agglomerate were as follows. The primary particles were randomly generated in a specified cuboidal volume sufficiently large that there were no interparticle contacts. With interparticle friction set at a low value and using a time step of Δt = 8.52 ns per cycle, a centripetal gravity field was then increased to g = 10 m/s^2 and cycling continued. During this stage the decrease in porosity and increase in the number of contacts was monitored. After approximately 1 million cycles further changes in these two parameters were insignificant, at which point the time step was reduced by a factor of 10 and the interparticle friction coefficient was increased in steps of 0.02 to a final value of 0.35 with 10 K cycles being carried out for each step increase. At the same time, surface energy was introduced at the interparticle contacts. The final value of interface energy $\Gamma = 2\gamma = 1.0$ J/m^2 was obtained by step increases in the surface energy of the individual particles of $\Delta\gamma = 0.01$ J/m^2 initially and then $\Delta\gamma = 0.05$ J/m^2. The centripetal gravity was then reduced in small steps to zero. The final, as prepared, porosity of the cuboidal agglomerate was 0.42, with a corresponding bulk density of 1153.10 kg/m^3. At the end of the preparation stage the coordination number of the cuboidal agglomerate was 3.52, corresponding to 14,993 contacts in the agglomerate. Fig. 2 shows views of the cuboidal agglomerate as prepared by the procedures described above. The dimensions of the agglomerate were 0.497 mm × 0.445 mm × 0.447 mm. Details of the agglomerate properties can be found in Table 1.

3. Elastic agglomerate impact

For comparison, we first carried out impact simulations of an agglomerate composed of elastic particles onto a target wall. Plastic deformation of the particles was not allowed by defining the material yield



(a) (b)

Fig 2. Cuboidal agglomerate as prepared (a) front view (b) top view.