Impact breakage of spherical, cuboidal and cylindrical agglomerates

L. Liu a, K.D. Kafui b, C. Thornton b,*

a Department of Engineering Technology, China University of Geosciences, Beijing 100083, China
b School of Chemical Engineering, University of Birmingham, Birmingham B15 2TT, UK

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ABSTRACT

A numerical study of the micro-mechanics of breakage of agglomerates impacting with a target wall has been carried out using discrete element simulations. Three agglomerates of different shapes are examined, namely spherical, cuboidal and cylindrical. Each agglomerate consists of 10,000 polydisperse auto-adhesive elastic spheres with a normal size distribution. The effect of agglomerate shape and impact site on the damage of the agglomerates under an impact velocity of 1.0 m/s for an interface energy of 1.0 J/m² is reported. It is found from the simulations that cuboidal edge, cylindrical rim and cuboidal corner impacts generate less damage than spherical agglomerate impacts. The cuboidal face, cylindrical side and cylindrical end impacts fracture the agglomerates into several fragments. Detailed examinations of the evolutions of damage ratio, number of wall contacts and total wall force indicate that the size of the contact area and the rate of change of the contact area play important roles in agglomerate breakage behaviour. Internal damage to the agglomerate is closely related to the particle deceleration adjacent to the impact site. However, the local microstructure may not be a decisive factor in terms of the breakage mode for non-spherical agglomerates.

1. Introduction

In particle technology, because of the relative surface area, there is a desire to have micron-sized particles but this then requires some form of granulation process to create millimetre-sized agglomerates that can be handled, stored and will flow easily. The consequent problem is to avoid breakage, in the form of fracture, crushing or attrition, during flow and storage of the agglomerates. Ideally, for fluid flowability, the agglomerates should be approximately spherical. However, some granulation techniques, e.g. roll compaction and attrition, during fluid flow produce extrudates that are not spherical and the collisional behaviour of non-spherical bodies is much more complex than that of spherical bodies. This has significant implications for the potential impact breakage of non-spherical agglomerates.

Experimental studies of agglomerate impact breakage have been reported by Subero and Ghadiri [1], Samimi et al. [2,3], Salman et al. [4], Fu et al. [5], Cheong et al. [6] and Antonyuk et al. [7]. However, the problem with such experiments is that the information gained is restricted to examining the post-impact particle size distribution, from which it is sometimes possible to reassemble the larger fragments to identify the fracture pattern. Due to the small length and time scales of an agglomerate impact it is not possible to examine in detail the actual fracture/breakage process. Numerical simulations are not restricted by such small length and time scales and consequently, over the past decade or so, this has encouraged the use of granular dynamics simulations, the discrete element method (DEM), to explore the detailed evolution of agglomerate breakage due to impact.

Yin [8] was the first to apply DEM to agglomerate impact breakage, as reported by Thornton et al. [9]. The simulations were limited in that they were 2D simulations but, nevertheless, it was demonstrated that, due to frictional energy dissipation in contact sliding, the energy required to break the interparticle bonds was orders of magnitude less than the initial work input, i.e. particle impact is not an energy efficient comminution process. It was found that the fraction of singlets produced was a power law function of the specific energy with an exponent of 5/8. Also, the size of the largest surviving fragment was found to be inversely proportional to the specific energy, in agreement with experimental data obtained for the fragmentation of centimetre-sized rock particles subjected to high velocity impacts of projectiles, Takagi et al. [10].

The first 3D simulations of agglomerate impact breakage were reported by Kafui and Thornton [11] for crystalline agglomerates, see also Kafui and Thornton [12]. By using such idealistic (regular array of primary particles) agglomerates it was clearly demonstrated from computer visualisations of the impact breakage that, for any given interparticle bond strength, there is an impact velocity that produces a complete set of fracture planes. Subsets of this fracture pattern are produced at lower impact velocities. Higher impact velocities do not produce extra fracture planes but the residual fragments are weakened due to internal bond breakage and this results in shattering at high impact velocities. It was shown that there is a shear-induced
weakening of a set of potential fracture planes during deceleration of the agglomerate. The pattern of weakened planes is dictated by the orientation of the agglomerate microstructure with respect to the impact direction. As the agglomerate recovers kinetic energy, further shear-induced bond breakage occurs along the same set of planes. At the end of the impact, depending on the amount of kinetic energy recovered, complete fracture occurs along some of the previously weakened planes. It was concluded that fracture is shear-induced and the agglomerate creates its own ‘flaw’ population during loading and, hence, ‘pre-existing flaws’ do not have a significant effect on agglomerate ‘strength’.

It was shown that the proportion of bonds broken during an impact was proportional to $\ln(\Gamma)$ where $\Gamma$ is the impact velocity and $V_0$ is the threshold velocity below which no significant damage occurred. Deviations from this scaling rule occurred at low velocities when agglomerate rebound occurred but there was, nevertheless, a small number of internal bonds broken and at very high impact velocities due to the inevitability that some small clusters, e.g. doublets and triplets, will survive. The threshold velocity $V_0$ was found to scale with $\Gamma^{1/2}$ were $\Gamma$ is the interface energy between contacting particles. It was also shown that the size distributions of the fragments produced by impact breakage exhibited a bilinear distribution on a double logarithmic plot against the normalised fragment size, in agreement with the experimental findings of Arbiter et al. [13] for impacts of sand–cement spheres. Independent of bond strength, the residue consisted of fragments of mass greater than 10% of the mass of the original agglomerate and the complement (or debris) of fragments of mass less than 10% of the initial agglomerate mass. For the complement (debris) the exponent of the power law relationship decreased if the bond strength was increased and the cumulative mass fraction undersize scaled with $(V/\Gamma)^2$. The size of the largest fragment (in terms of its mass) scaled with $(V/\Gamma)^{-3/2}$.

Three-dimensional simulations of normal loadings in a polycrystalline sphere agglomerate were performed by Ciocamoc [14] and reported by Thornton et al. [15]. From the simulation data produced 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. This was in contrast to the work reported by Ning et al. [16] who observed that fracture did not occur in any of their simulations. Using the same computer code, Subero et al. [17] attempted an experimental validation of their simulation results but, although agglomerate fracture occurred in a proportion of their physical experiments, fracture was never observed in their simulations.

Mishra and Thornton [18] 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.

Thornton and Liu [19] addressed the question as to how agglomerates break. It was observed that a generic feature of particle systems is that the force transmission is not uniformly distributed but tends to be focussed along discrete chains of particles, which align with the direction of maximum compression, Thornton [20], Thornton and Antony [21]. From simulations of the normal impact of a cuboidal agglomerate with a planar target wall it was demonstrated 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.

All the above published research was restricted to the consideration of normal impacts. Moreno et al. [22] reported DEM simulations of oblique impacts of spherical agglomerates. They found that, for a constant impact speed, the number of bonds broken and the amount of debris produced decreased as the impact angle became more oblique. They demonstrated that this was due to the decrease in the normal component of the impact speed and concluded that “the normal component of the impact speed is the dominant factor controlling the breakage of contacts”. However, it was also shown that, for the same number of bonds broken, the spatial distribution of damage (broken bonds) depended on the impact angle.

For non-spherical agglomerates, the damage mode and degree of damage depends not only on the impact speed, impact angle and interface energy but also on agglomerate orientation. However, because the orientation of non-spherical agglomerates introduces such a wide range of complexities, i.e. combined effects of orientation and impact angle, the paper is restricted to examining the impact breakage of cuboidal and cylindrical agglomerates resulting from normal impacts against a planar target wall with different agglomerate orientations.

## 2. Numerical methodology and simulation procedures

The granular dynamics model used in this study originated as the Distinct Elements Method (DEM), Cundall and Strack [23], Cundall [24]. The current version of the DEM code GRANULLE adapted to simulate agglomerates is capable of modelling elastic, frictional, adhesive or non-adhesive spherical particles with or without plastic yield at the interparticle contacts. In this study, the adhesive option with no plastic deformation at the contact is used. The contact interaction rules are based on the theoretical work of Johnson et al. [25], Savkoor and Briggs [26] and Thornton [27]. Details of the contact interaction equations may be found in Thornton and Yin [28].

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 $t+\Delta t$ involves the application of incremental force–displacement interaction laws at each contact, resulting in new interparticle forces which 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 $\Delta t$ used is a fraction of the critical time step determined from the Rayleigh wave speed for the solid particles, Thornton and Randall [29].

Each 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 all the agglomerates 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 agglomerates were to be impacted.

The procedures used to prepare the agglomerates were as follows. The primary particles were randomly generated in a specified spherical, cuboidal or cylindrical volume sufficiently large that there were no interparticle contacts. With interparticle friction set at a low value ($\mu = 0.01$), a low centripetal gravity field ($g = 1$ m/s$^2$) was introduced in order to bring the particles together over 40K cycles.
using a time step of $\Delta t = 8.52$ ns per cycle. The centripetal gravity field was then increased to $g = 10$ m/s 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 10K 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, as prepared, spherical agglomerate is illustrated in Fig. 1.

The final, as prepared, porosities of the spherical, cuboidal and cylindrical agglomerates were 0.395, 0.412 and 0.400 respectively, with corresponding values of bulk density of 1602 kg/m$^3$, 1557 kg/m$^3$ and 1591 kg/m$^3$. At the end of the preparation stage the respective coordination numbers of the spherical, cuboidal and cylindrical agglomerates were 5.124, 4.558 and 4.562, corresponding to 25,521, 21,831 and 22,092 contacts in the agglomerates. Fig. 2 shows views of the cuboidal and cylindrical agglomerates as prepared by the procedures described above. The dimensions of the three agglomerates were 0.54 mm diameter (spherical), 0.480 mm $\times$ 0.477 mm $\times$ 0.484 mm (cuboidal) and 0.500 mm diameter $\times$ 0.474 mm length (cylindrical).

### 3. Results of simulations

Numerical results of agglomerate impact simulations are presented to show the influence on the breakage behaviour of the agglomerate shape and the location on the agglomerate surface selected for the impact site. Some new terminologies, as defined in Thornton and Liu [19] and Mishra and Thornton [18], are adopted to describe the observed phenomena. The term “fracture” is reserved for breakage patterns in which clear fracture planes (cracks) are visible. The mode produces two or more large daughter fragments and is normally accompanied by some fines production adjacent to the impact site. If, for example, due to the high velocity used the large daughter fragments are themselves broken into small clusters of primary particles then the term “shattering” is used. An alternative mode of breakage, which will be illustrated later, is one in which there is no evidence from the simulation data of any attempted fracture and the end products consist of one large cluster centred in the upper part of the agglomerate with the remainder of the agglomerate reduced to small clusters of 1–10 primary particles. This type of breakage behaviour is termed “disintegration”. If the impact velocity is sufficient high, for example, that disintegration extends throughout the agglomerate and there is no “large” surviving cluster then this mode of breakage is referred to as “total disintegration”. If total disintegration occurs, the agglomerate simply collapses into a heap on the target wall, on the other hand, when shattering occurs, a significant number of small daughter fragments are projected at relatively high speeds away from the impact location.

#### 3.1. Breakage modes

All the impacts reported are collinear normal impacts. That is to say that the line orthogonal to the target wall at the initial point of
contact of the agglomerate with the wall passes through the centre of mass of the agglomerate. Impact with the wall was simulated by specifying, for all the primary particles, an initial velocity of 1.0 m/s in the direction orthogonal to the wall. Several researchers, Kafui and Thornton [11,12], Thornton et al. [15], Subero et al. [17], Mishra and Thornton [18] have adequately studied the effects of interface energy (bond strength) and impact velocity on the agglomerate strength and breakage which is not addressed here. In the present study the emphasis is directed to the effect of agglomerate shape and impact site.

Agglomerate breakage is illustrated by computer generated images of the configuration of the primary particles at the end of the impact with individual fragments indicated by different shades of grey; and by representing the agglomerate by the equivalent space lattice that is formed by connecting the centres of particles in contact by solid lines. In this manner, the impact breakage of the spherical agglomerate is shown in Fig. 3. It can be seen from the figure that, when impacted at a velocity of 1.0 m/s, the spherical agglomerate fractured resulting in three relatively large fragments (consisting of 4990, 2256 and 1083 primary particles) plus a significant amount of small debris adjacent to the impact site. If one used a different impact site one would expect some small differences in the detailed behaviour. Nevertheless, the results presented for the spherical agglomerate will be taken as typical and used as a benchmark for comparison with the results obtained for the non-spherical agglomerates.

For the cuboidal and cylindrical agglomerates, the target wall was repositioned in order to select different impact sites for collinear normal impacts. As shown in Fig. 4, the impact sites selected for the cuboidal agglomerate were (a) a corner of the agglomerate (b) an edge of the agglomerate and (c) a face of the agglomerate. For the cylindrical agglomerate impact sites were selected to provide (a) a rim impact (b) a side impact and (c) an end impact, see Fig. 5.

Figs. 6–8 illustrate the breakage of the cuboidal agglomerate. When a face of the agglomerate was impacted against the wall, see Fig. 6, the agglomerate fractured into four large fragments (3045, 2843, 1114 and 801 primary particles) together with small debris due to crushing adjacent to the wall. However, as can be seen in Fig. 7, fracture did not occur when the cuboidal agglomerate collided with the wall along one of its edges. Disintegration of the region of the agglomerate adjacent to the wall produced small debris with the largest cluster size of 15 primary particles. The large surviving cluster...
consisted of 9030 primary particles with no evidence of any internal damage. A similar breakage pattern occurred for a corner impact of the cuboidal agglomerate, see Fig. 8, but with a lower degree of disintegration adjacent to the wall.

The impact breakage of the cylindrical agglomerate is illustrated in Figs. 9–11. It can be seen that both the end impact and the side impact resulted in fracture but fracture was not observed for the rim impact.

In the case of the end impact, see Fig. 9, the agglomerate fractured into two large fragments (3975 and 3186 primary particles) and a medium sized fragment (607 primary particles) resulting from the bifurcation of the primary fracture, which immediately broke into four approximately equal parts; the remaining damage being small debris adjacent to the wall. In the side impact, see Fig. 10, aside from the...
small debris, fracture resulted in four large fragments (2818, 2012, 1608 and 1228 primary particles). Fracture did not occur when the impact was against the rim of the agglomerate, see Fig. 11, only disintegration into small debris adjacent to the impact site. The one large surviving cluster consisted of 9210 primary particles.

The above illustrations of agglomerate damage demonstrate that, for the agglomerate specification in terms of number of primary particles, bond strength and impact velocity, disintegration always occurs adjacent to the impact site and that this is where the small debris is produced. Whether fracture occurs or not depends on the impact site location. If fracture occurs then the fracture pattern and the consequent size and shape of the large surviving fragments depend on both the agglomerate shape and the location on the agglomerate surface used as the impact site.

3.2. Quantitative observations

Following Kafui and Thornton [11], the impact damage illustrated in Figs. 3, 6–11 can be quantified by a damage ratio defined as the ratio of broken bonds to the initial number of bonds prior to impact. Fig. 12 shows the time evolution of the damage ratio for all the impacts reported. It can be seen that the data sets for the non-spherical agglomerates fall into two groups. Group A consists of the cuboidal face, cylindrical end and cylindrical side impacts, all of which attain a final damage ratio of 0.32 which is significantly higher than the value of 0.205 obtained for the spherical agglomerate. In contrast, the final damage ratio for all Group B agglomerate impacts is about 0.185 which is slightly less than that of the spherical agglomerate impact. The figure shows that the damage ratio increases rapidly to the final asymptotic value except for the cuboidal edge and cuboidal corner impacts. In these two cases, there is a delay before the rapid increase in damage ratio occurs, most notable in the case of the cuboidal corner impact.

A possible reason for the significant different proportion of bonds broken during Group A and Group B impacts is the different nominal contact area with the target wall. This is examined in Fig. 13, which shows the time evolution of the number of primary particles in contact with the wall for (a) Group A impacts and (b) Group B impacts. For comparison, results for the spherical agglomerate are shown in both figures. It can be seen from Fig. 13(a) that, like the spherical agglomerate impact, in all three cases of Group A impacts (cuboidal face, cylindrical end and cylindrical side impacts) the number of wall contacts increases more or less monotonically to a final value that is equal to or greater than that of the spherical agglomerate. It might be expected that the cuboidal face impact should exhibit the greatest number of wall contacts. However, this is not the case because, as a consequence of preparing the agglomerate in a centripetal gravity field, the faces of the cuboidal agglomerate are in fact slightly curved, as can be seen in Fig. 2(a). Fig. 13(b) shows that, for cuboidal corner, cuboidal edge and cylindrical rim impacts, the number of wall contacts initially increases to a maximum value and then decreases to a constant asymptotic value. It is also noted that the number of wall contacts increases at a decreasing rate for all

![Fig. 12. Evolution of damage ratio during impact.](image)

![Fig. 13. Number of particle–wall contacts during impact.](image)
impacts except for the cuboidal corner impact for which the increase is linear.

The number of wall contacts affects the magnitude of the total force transmitted into the agglomerate from the wall and the consequent potential deceleration and damage. Fig. 14 shows the time evolution of the total wall force for (a) Group A impacts and (b) group B impacts. Again, the spherical agglomerate data is superimposed on both figures. Fig. 14(a) shows that the evolution of the total wall force is similar for Group A impacts and that of the spherical agglomerate. Although there are significant fluctuations, the general trend is that of an increase to a maximum force in about 10 µs followed by a gradual reduction to a negligible value corresponding to the self-weight of the residual agglomerate fragments. In contrast, the data obtained for Group B impacts shown in Fig. 14(b) exhibit a delay before the total wall force increases to a maximum value. This is more clearly seen in the cases of the cuboidal edge and cuboidal corner impacts. In both cases, the occurrence of the peak wall force coincides with the rapid increase in broken contacts shown in Fig. 12.

3.3. Fragment size distribution

In experimental studies, the results of impact breakage can be quantified by examining the fragment size distribution resulting from the impact event. Fig. 15 shows, for all the impacts simulated, a double logarithmic plot of cumulative mass fraction undersize against normalised mass in which the mass of each fragment is normalised by the initial agglomerate mass. The size distributions of the fragments show two distinct regions with a sudden change of slope (except for the cylindrical face impact — the reason for which is unclear) that distinguishes the large fragments (residue) from the complement of small fragments (debris). The bilinear form shown in Fig. 15 is in agreement with experimental data published in the literature, Arbiter et al. [13].

From DEM simulations of spherical agglomerate impacts, Kafui and Thornton [12] and Mishra and Thornton [18] demonstrated that the exponent for the debris is independent of the impact velocity but the amount of debris increases with increasing impact velocity. However, Fig. 15 illustrates that, for a given impact velocity, the amount of debris produced is dependent on agglomerate shape and impact site location. The smallest amount of debris is produced for the cylindrical rim impact and the largest amount occurs for the cuboidal face impact. The difference in the amount of debris produced by these two impact conditions is about a factor of four, which possibly indicates the limiting range of variation of potential debris production for general non-spherical agglomerates experiencing normal impact with a wall for the values of bond strength and impact velocity used in the current simulations. It is, however, notable that the exponent for the debris is independent of agglomerate shape and impact site location. This suggests that, for general non-spherical shapes, the exponent only depends on the bond strength. For the simulations reported here, with an interface energy $\Gamma = 1.0 \text{ J/m}^2$, the exponent for the debris is ca. 0.13. There is also a hint from Fig. 15 that the boundary between the residue and the debris might be dependent on agglomerate shape and impact site location but further simulations varying both the impact velocity and bond strength are required before this can be clarified.

4. Conclusions

Numerical simulations of a spherical agglomerate, a cuboidal agglomerate and a cylindrical agglomerate impacting with a target wall have been reported. The results have demonstrated that, for an impact velocity of 1.0 m/s and an interface energy of 1.0 J/m², fracture occurs if the cylindrical agglomerate is impacted against one end or the side, the cuboidal agglomerate is impacted against a face or if the agglomerate is spherical. When the cylindrical agglomerate was impacted against a rim or the cuboidal agglomerate was impacted against either an edge or a corner fracture did not occur. In these latter cases damage was restricted to local disintegration adjacent to the point of impact.
From detailed examinations of the evolutions of damage ratio, number of wall contacts and total wall force it is concluded that the size of the contact area and the rate of change of the contact area play important roles in agglomerate breakage behaviour. It has previously been demonstrated for spherical agglomerates by Mishra and Thornton [18] that the internal damage to an agglomerate is closely related to the particle deceleration adjacent to the impact site, which is dependent on the local microstructure. However, the local microstructure may not be a decisive factor in terms of the breakage modes for non-spherical agglomerates.

In all cases of agglomerate impact the cumulative probability of the post-impact fragment size distribution exhibited a bilinear form on a double logarithmic plot, distinguishing the residue from the debris, as found in laboratory experiments, Arbiter et al. [13]. The current simulation results have demonstrated that the exponent for the debris is independent of particle shape and impact location. This confirms previous studies in that the exponent of the debris is only dependent on bond strength (interface energy). However, the amount of debris is very sensitive to the impact location for non-spherical agglomerates.

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