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Numerical simulation of the impact-breakage behavior of non-spherical agglomerates

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A B S T R A C T

A numerical study of the breakage behavior of non-spherical agglomerates is presented in this paper. Six agglomerates of various shapes (e.g., spherical, regular tetrahedral, cuboidal, regular octahedron, regular dodecahedron and regular icosahedrons) with different sphericities are examined using discrete element method (DEM) simulations. First, appropriate parameters for the simulation model are obtained based on uniaxial compressive experiments and single coal rock impact test. Then, a series of numerical simulations is performed to examine the breakage behavior of the non-sphere agglomerates produced. The study shows that better breakage performance can be obtained with a higher impact velocity. The collision behaviors of the non-spherical bodies are relatively more complex compared to those of spherical bodies. Detailed examinations of the evolutions of the damage ratio and wall force indicate that the size of the contact area plays an important role in the breakage behavior of the agglomerates. Most of the maximum wall forces and final damage ratios show a decreasing trend when the face-impact, edge-impact and vertex-impact modes are used. However, these values are still significantly larger than those of spherical agglomerates. The simulation results show that the debris and fragments created after the agglomerates fracture have independent shapes and impact modes. The value of the detected two features decrease as sphericity increases when the face-impact mode is used but increase with the sphericity when the edge- and vertex-impact modes are used. Minor changes in sphericity can result in significantly different fracture patterns in non-spherical agglomerates.

1. Introduction

In mining technology, impact crushing is a primary fragmentation method for crushing mineral materials. Currently, experimental studies of the impact breakage of agglomerates have been carried out [1–7]. However, the problem of such experiments is that the effective information gained is restricted to examining the particle size distribution after breakage; thus, it is difficult to describe the agglomerate's breakage mechanism.

In the last two decades, DEM has been used to explore the detailed evolution of agglomerate breakage due to impact. However, these studies primarily investigated normal impacts between spherical agglomerates and a target wall. Granular dynamics simulations of dense spherical agglomerate impacting orthogonally with target wall were studied by C. Thornton [8]. They have also found that fracture is the result of the manner in which strong inter-particle forces are transmitted into the agglomerate and the consequent development of a heterogeneous distribution of primary particle velocities [9]. Numerical simulations of spherical agglomerates impacting orthogonally on a target wall have been performed to study the effects of mainly factors (impact velocity, solid fraction, and contact density), and it was confirmed that all these factors have great influence on agglomerate breakage behavior [10,11]. Numerical simulations have been performed to study the breakage and captured behavior of loose fine-particle agglomerates on impact with a target particle, it has been found that impact velocity is a significant parameter not only for the adhesion strength but also for the structure of the particles captured on the target [12]. The numerical results of sphere agglomerate impact simulations were presented in these papers to describe the breakage behaviors occurring. However, the collision behaviors of non-spherical bodies are relatively more complex compared with those of spherical agglomerates. The study of non-spherical bodies has significant implications for the potential impact breakage of non-spherical agglomerates.

A simple and fast original method to create agglomerates with irregular shape by assembling spheres together was described by Ferellec J F, the method showed its ability to reproduce a shape, its degree of resolution and the number of spheres required [13,14]. The influence of clump shape on the heterogeneous stresses within an aggregate has been investigated by Lu M., and it has been found that more angular

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clumps lead to a greater degree of homogeneity [15]. 3D laser ranging (LADAR) has been used to capture astonishingly realistic rock aggregate geometries, and a suggested procedure has been developed to establish FEM or DEM models by Latham J. P. [16]. An automatic method to generate sphere clump models of real agglomerates was presented by Price M., and quantitative tests conducted on a sample of diamond particle showed that approximate particle shape can be achieved with spheres by the method [17,18]. New methodologies for individual particle representation, particle kinematics, and local strain quantification were developed by Wang L for analyzing a compression test by using X-ray tomography imaging. By comparing the simulations based on spherical particles and irregular particles, it was concluded that particle shapes have a significant effect on both micro-properties and macro-properties of granular materials [19,20]. The combination of X-ray tomography and spherical harmonic analysis allows the routine 3D analysis of agglomerate shapes, completing the multiscale picture of “particle” shape for a very wide range of length scales [21,22]. The application of spherical harmonic series to analyze 3D X-ray CT images can be used to construct accurate 3-D representations of actual particles, which can be used in 3-D microstructure simulation models [23,24].

However, irregular agglomerates using a DEM model are all considered to be rigid bodies. Fragments after breakage cannot typically be generated in numerical models. For non-spherical agglomerates, their breakage not only depends on the impact speed and angle but is also related to the impact mode. The breakage behaviors of three different shape agglomerates (spherical, cuboidal and cylindrical) impacting with a target wall have also been examined based on discrete element simulations [25]. However, the breakage of non-spherical agglomerates is typically much more complex than that of spherical agglomerates. The breakage behavior of non-spherical agglomerates with different sphericities under different impact modes are not considered in the previous studies.

In this study, the common non-spherical objects considered are restricted to regular polyhedra (regular tetrahedron, cuboidal, regular octahedron, regular dodecahedron and regular icosahedrons). This study examines the impact breakage of non-spherical agglomerates during an impact with a target wall in different impact modes. Finally, the influence of different impact modes on the breakage behavior of non-spherical agglomerates is studied, and the relationship between the sphericity of the non-sphere agglomerate and the impact mode is analyzed.

2. Simulation procedure and experimental verification

In the study of particle breakage, experimentation and simulation studies have focused on sphere agglomerates. C. Thornton, Mishra B. K., Nguyen D. and Kafui K. D. have adequately studied normal impacts between sphere agglomerates and a target wall [8–12]. Numerical results have been presented to describe the breakage behavior of agglomerates; however, agglomerates in real mining applications are all different shapes with different surface areas. Ferellec J. F., Lu M. and Latham J. P. described the feasibility of different methods to create irregular particles using DEM [14–16]; however, the internal fragmentation of non-spherical agglomerates was not considered in these models.

Common non-spherical objects are investigated in this study. Six agglomerates with different shapes are examined: regular tetrahedron, cuboidal, regular octahedron, regular dodecahedron, regular icosahedrons and spherical. As one of the primary parameters used to describe the morphology of a non-spherical particle, sphericity has become widely applied in various research fields. Particle sphericity is a measure of the degree to which a particle's shape approaches the shape of a sphere [26]. The sphericity φ of a particle is defined as the ratio of the surface area of a sphere with the same volume as the given particle to the surface area of the particle [27,28]. As shown in Eq. (1), S_{sphere} represents the surface area of sphere, and $S_{particle}$ represents the surface area of the given particle:

$$\varphi = \frac{S_{sphere}}{S_{particle}}. \quad (1)$$

The sphericities of the six agglomerates investigated in this study are determined to be 0.671, 0.806, 0.846, 0.910, 0.939, and 1.000, respectively. Fig. 1 shows a comparison of these sphericities and indicates that sphericity grows as the number of edges and faces on a polyhedron increases because the shape of polyhedron approximates a sphere as more faces are added.

2.1. Parameter calibration

Parameter calibration is used to determine the correct numerical representation of a given specimen. The appropriate micro-parameters of a coal specimen is critical to establish an accurate numerical model. To determine the appropriate micro-parameters for a given numerical model, a series of uniaxial compressive simulations are performed. The flowchart used to establish a discrete element model of coal is shown in Fig. 2. In the DEM simulation, the primary particles in agglomerate are all treated as discrete elements, which are rigid bodies, and are connected to each other by parallel bonds. Parallel bonds can transmit both force and moment between particles. In the numerical model, parallel bonds establish an elastic interaction between particles that acts in parallel with the slip or contact-bond constitutive models [29]. The optimization steps used to establish an accurate discrete element model could be divided as follows:

(1): Conduct uniaxial compressive experiments on coal rock materials to determine the macro-physical and mechanical simulation parameters (e.g., elastic modulus, Poisson's ratio and compressive strength).
(2): Establish a discrete element model for coal rock based on the preliminary set of microscopic characteristic parameters in PFC3D.
(3): Conduct uniaxial compression simulations on coal specimens to determine the macro-physical and mechanical simulation parameters.

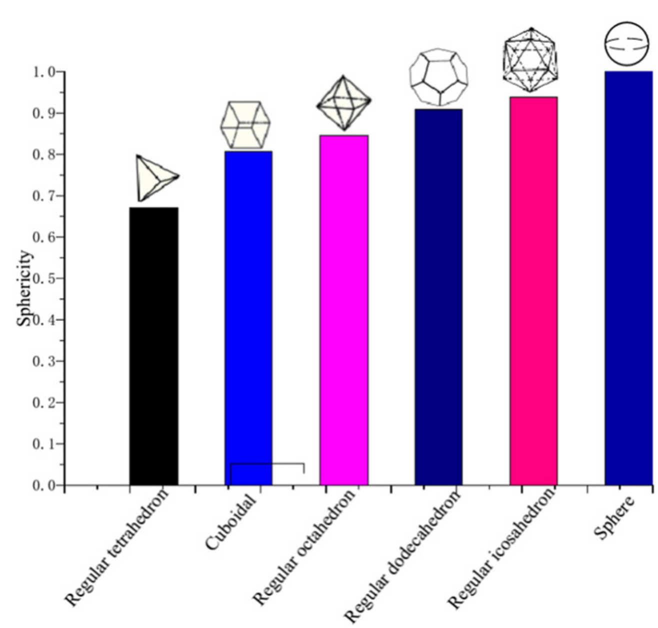

Fig. 1. Sphericity of common 3D objects.