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Numerical and analytical description of the mechanical properties of quasi tetrahedral agglomerates

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ABSTRACT

Quasi tetrahedral agglomerates consist of four spherical primary particles, of which three primary particles generally form a mechanically stable base on which the fourth primary particle is arranged centrally (as in the regular case, where the primary particles have equal radii) forming an apparent trigonal pyramid.
The coordinates of the centers of the primary particles are derived for agglomerates composed of monodisperse spherical primary particles (regular tetrahedron) and polydisperse spherical primary particles (skewed tetrahedron). Moreover, the force distribution within the agglomerates at compression is described and an analytical model for elastic contact deformation is derived on the basis of the Hertz model [1].
Following, the regular structure of the agglomerates is experimentally analyzed using compression tests and the recorded force–displacement curves are evaluated with the new analytical model. Additionally, mechanical properties like the modulus of elasticity and the yield point of the primary particles as well that as of the tetrahedral agglomerates are also derived.
Subsequently, tetrahedral agglomerates are modeled using the discrete element method (DEM) and their compression behavior between two rigid plates is simulated. The received numerical force–displacement curves are compared with the model-based approximated analytical force–displacement curves. Force–displacement curves of agglomerates composed of poly-disperse spherical primary particles are recorded and evaluated as well. It was found that the regular tetrahedron represents the most stable configuration, with an upper threshold force–displacement curve on varying the upper primary particle size and limiting curves on varying the size of one of the lower primary particles.

1. Introduction

Agglomeration is the generic term for processes of mechanical particle size enlargement, whereby fine primary particles are bonded together to form particle collectives, using different binding mechanisms and forces. The primary agglomeration processes are pelletizing, press agglomeration and sintering.

The problems faced in the experimental investigation and theoretical description of the microscopic binding mechanisms and binding forces between primary particles, the micro-mechanical properties and the resulting macroscopic product properties have so far only been insufficiently investigated empirically. Besides, an adequate quantification is not yet established due to the substantial difficulties that hinder the necessary physical description of micro-mechanical properties of the primary particles, fundamental interactions between them and stochastic micro-process dynamics (at stressing) in terms of a desired and guaranteed mechanical product quality.

Established experimental methods for measuring the mechanical properties of agglomerates are tension, compression and impact tests. In this context, the strength and fracture behavior are often studied as this knowledge is of vital interest for many industrial applications which strive to minimize comminution effects at processing, transportation and storage. Bika et al. [2] describe in detail the experimental measuring methods to determinate tensile strength, yield strength, hardness and fracture strength. Moreover, the authors describe the effects of moisture from their tests on dry and moist agglomerates.

For the investigation of macro-voids and interparticle bond strength on the agglomerate breakage, Subero et al. [3] studied the impact of single glass ballotini agglomerates adhered together by an epoxy resin binder. The effects of the curing procedure of the binder and the amount of binder on the agglomerate strength are reported. The authors concluded that very small changes in the solid fraction, obtained by generating large cavities into the assembly i.e. macro-voids, drastically affect the extent of breakage of the agglomerates upon impact.

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Furthermore, the compressive strength and fracture behavior of cylindrical agglomerates consisting of macroscopic γ-Al_2O_3 granules and hydroxypropylmethylcellulose (HPMC) as binder have been studied by Antonyuk et al. [4]. The agglomerates had been uniaxially compressed until primary breakage. As expected, the mechanical properties like stiffness and strength of the agglomerates were found to be directly proportional to the binder content and agglomerate size (height).

Machii and Nakamura [5] experimentally analyzed sintered agglomerates of coarse glass beads ($d = 5$ mm) by tension, bending and impact tests ($v = 40$–280 m/s). When the surface roughness of the primary particles begins to get layered by the sintered material, then the tensile strength of the agglomerates was found to be proportional to the cross-section of the sinter neck (i.e. sinter bridge) connecting the primary particles. Furthermore, smaller forces are required to break a neck over its diameter, in comparison to breakage over its length. At impact, the energy required to catastrophically break an agglomerate is a few multiples of the total energy required to break all of the necks in the agglomerate connecting the primary particles.

In addition, agglomerates and their micro–macro-interactions are increasingly studied using numerical methods like the finite element method (FEM) and the discrete element method (DEM).

For that purpose, the group of Thornton [6–8] had carried out extensive numerical studies. Among other things, influences of material properties and processing conditions like impact velocity, solid fraction, contact density, local arrangement of particles near the impact zone and interparticle bond strength on the fracture behavior of agglomerates at impact had been investigated. Results of the simulations showed distinct fracture patterns for dense agglomerates (above a critical impact velocity), whereas for loose agglomerates, disintegration occurs under identical testing conditions.

Following, Moreno et al. [9] had studied the influence of impact angle (at oblique impact) on the fracture behavior of spherical agglomerates. The effect of interparticle bond strength had been analyzed as well.

Khanal and Tomas [10] had modeled the oblique impact of coarse concrete agglomerates using two dimensional FEM to understand the stress distributions before crack initiation and two dimensional DEM to study the fracture behavior. Different impact angles in the range of $\Theta_A = 30$–$60°$ and different impact velocities in the range of $v = 7.7$–180 m/s had been chosen. It was shown that at high impact velocities, fragment size distributions are almost independent of the impact angle. Furthermore, it was established that increasing impact velocities do not necessarily produce more new surfaces after a certain critical velocity limit.

To study the micro-mechanics of agglomerate breakage, Liu et al. [11] carried out DEM simulations of spherical, cuboidal and cylindrical agglomerates (consisting of 10,000 auto-adhesive primary particles) impacting on a target wall. It was found from the simulations that during impact of cuboidal edges, cylindrical rims and cuboidal corners, lesser damage is realized than during impact of a spherical curvature. The cuboidal face, cylindrical side and cylindrical end impacts fracture the agglomerates into several fragments. Detailed examinations of the damage ratio, number of wall contacts and total wall force indicate that the area of the contact zone and the rate of change of the contact area play important roles in agglomerate breakage behavior. As a summary, it is clear that the larger the contact zone and the rate of its change (with increasing load), the larger is the deformation and higher is the breakage probability.

2. Composition and coordinates of quasi tetrahedral agglomerates

Quasi tetrahedral agglomerates, as shown in Fig. 1a, consist of four spherical primary particles. Three of these primary particles generally form the base area on which the fourth primary particle is arranged centrally (as in the regular case of equal sized primary particles where $R_A = R_B = R_C = R_D$). The center of the four primary particles always span a tetrahedron $\overline{ABCD}$, see Fig. 1b.

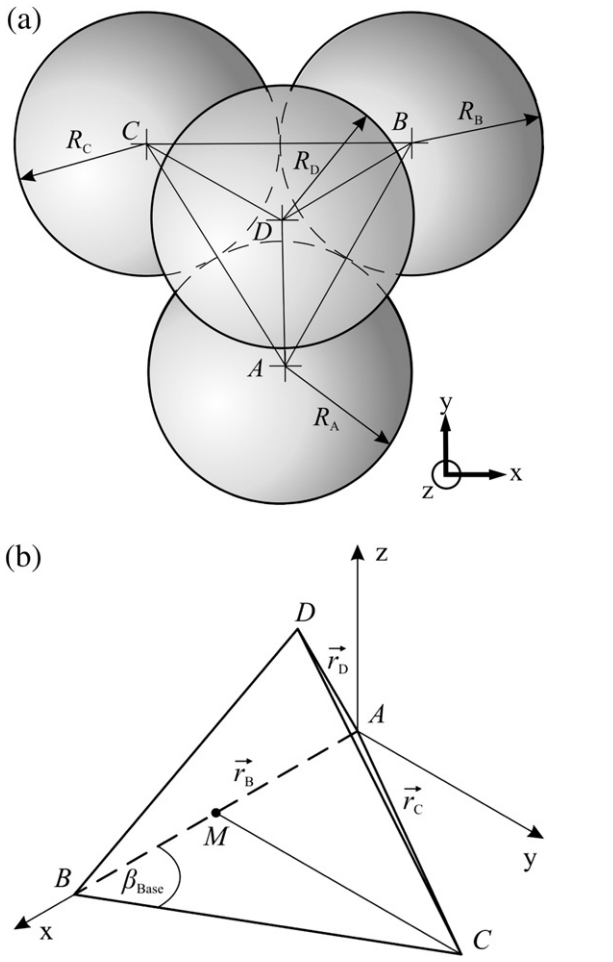

Fig. 1. Structural orientation of a regular quasi tetrahedral agglomerate. (a) Top view and inner tetrahedron. (b) Inner tetrahedron spanned by the centers of the primary particles.

2.1. Composition of the skewed tetrahedron

A skewed tetrahedral spanning results when the primary particles exhibit different radii (R_A, R_B, R_C, R_D). The side lengths of the inner tetrahedron, summarized in Table 1, arise from the radii of each of the contacting adjacent primary particles.

The coordinates of the centers of the primary particles are represented by the following vectors $\vec{r}_A$, $\vec{r}_B$, $\vec{r}_C$, $\vec{r}_D$, see Fig. 1b, where a regular tetrahedron is shown.

To derive the vectors for the composition of the skewed tetrahedron, the base area $\overline{ABC}$ is considered at first. Point A is considered as the origin

$$\vec{r}_A = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \tag{1}$$

Table 1
Edge lengths of the tetrahedron.

Edge	Edge length
$\overline{AB}$	$R_A + R_B$
$\overline{AC}$	$R_A + R_C$
$\overline{AD}$	$R_A + R_D$
$\overline{BC}$	$R_B + R_C$
$\overline{BD}$	$R_B + R_D$
$\overline{CD}$	$R_C + R_D$