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Simulation-based investigation of core-shell agglomerates: Influence of spatial heterogeneity in particle sizes on breakage characteristics

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ABSTRACT

The stability and breakage behavior of agglomerates is of interest in many applications. It is well known that the internal microstructure is of great influence thereupon. However, the precise relationship of structural properties and mechanical behavior is not yet known for many scenarios. In this paper, we consider a flexible stochastic model to analyze the strength of spherical agglomerates consisting of spherical primary particles, arranged as core and shell. Structural properties can be varied in core and shell independently. Applying the bonded-particle model (BPM), we investigate the influence of the primary particle size distributions in core and shell on the breakage behavior under uniaxial compressive load. To get more meaningful results, we perform numerical studies of the same agglomerate with different directions of force and investigate the variation in breakage behavior.

1. Introduction

The mechanical stability of agglomerates consisting of spherical primary particles is of interest in various applications. As computational resources have become cheap and readily available, many mechanical properties can be evaluated using simulation methods. This has been done for several applications and agglomerate parameters. For instance, the effect of the agglomerate's shape on the mechanical behavior under impact load has been examined [1,2].

The mechanical behavior under compressive load is of interest for many applications [3,4]. Different models [5–8] have been proposed for the description of forces occurring inside the agglomerate, when primary particles are in contact with each other. An overview of different models for the contact force-displacement behavior can be found in [9].

Often, this is computationally studied by applying the discrete element method (DEM) extended with a bonded-particle model (BPM) [10–12], where the investigated material is represented as a set of densely packed spheres connected with ideally elastic or viscoelastic [13,14] bonds. Opposed to experimental measurements, computational studies can give detailed information about stresses within the agglomerate. DEM simulations have been used to investigate the agglomerate breakage under impact load [2,15–18] as well as under compression [3,19].

In [14], a flexible stochastic microstructure model for the generation of homogeneous agglomerates consisting of primary particles of two different sizes has been presented. This model has been applied to study the effect of the primary particle size distribution on the breakage behavior. But for some applications, agglomerates with a core-shell structure need to be examined [20,21]. Current microstructure models do not cover this type of agglomerates. In this paper, we therefore extend the model presented in [14] to core-shell scenarios and evaluate the influence of spatial inhomogeneity on the breakage behavior by comparing our results to previously obtained data. Moreover, we investigate the variation of breakage behavior considering varied directions of compression. This is an important influencing factor since the investigated agglomerates are strongly anisotropic.

We investigate spherical glass agglomerates with a diameter of 8 mm which can be spatially divided into core and shell. Both, core and shell, consist of spherical primary particles of two different sizes which are bonded with hydroxypropyl methylcellulose (HPMC) binder. Main material parameters, which are used in the simulations, are listed in Table 1.

The overall packing density of primary particles is kept constant at 56% and the mixing ratio of small and large particles is varied in core and shell. Cylindrical bonds consisting of binder material are placed between particles such that the total binder volume is

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Table 1
Main material parameters of primary particles and bonds [14].

Parameter	Value
Primary particles (glass)	
Density	2500 kg/m^3
Young's modulus	$6 \cdot 10^{10}$ Pa
Poisson ratio	0.21
Binder (HPMC)	
Young's modulus	$4 \cdot 10^{8}$ Pa
Normal and tangential strength	$5 \cdot 10^{7}$ Pa

10% of the total volume of primary particles and the ratio of the bond radius to the radius of the smallest adjacent particle is 0.4.

The rest of this paper is organized as follows. The stochastic model for generating the core-shell agglomerates is explained in Section 2, whereas the compression experiments are described in Section 3. Breakage detection and statistical analysis of the results is done in Section 4. Section 5 concludes and gives a short outlook to possible future research.

2. Stochastic microstructure model

In the following, we describe the stochastic model used to generate the microstructure of core-shell agglomerates. Similarly to [14] the model is given by an isotropic random set. This means the agglomerate's microstructure is represented as a random set of non-overlapping (spherical) primary particles connected by cylindrical bonds, where the structure has no preferred orientation.

As we want to investigate the influence of spatial heterogeneity in particle sizes on the breakage behavior, we consider different sizes for spherical primary particles. While in general the model is suitable for any particle size distribution, for simplicity we only take into account two different sizes for primary particles, namely large particles with radius r_1 and small particles with radius $r_2 < r_1$. Furthermore we split the volume of the spherical agglomerate of radius r into a core with radius $r_C < r$ and a shell. For each part of the agglomerate, a mixing ratio m_C (m_S) specifies the volume fraction of large particles with respect to the overall particle volume for the core and shell, respectively. Furthermore we specify an overall packing density.

The primary particles are generated by a packing algorithm described in Section 2.1 and connected by a network of cylindrical bonds described in Section 2.2.

2.1. Core-shell primary particle model

In this section, we extend the stochastic model introduced in [14] to generate the primary particle's structure.

Using the parameters r, r_C, m_C, m_S, r_1 and r_2 from above, we transform the volumetric mixing ratios m_C and m_S into ratios of particle numbers. If large particles contribute a fraction m to the overall particle's volume, the fraction a of large particles in the overall particle count is given by

$$a = \frac{m \cdot r_2^3}{m \cdot r_2^3 + (1-m) \cdot r_1^3},$$

see [14]. We use this formula to compute the ratios of large particle numbers a_C and a_S for core and shell.

In the following steps we describe the procedure of primary particle configuration.

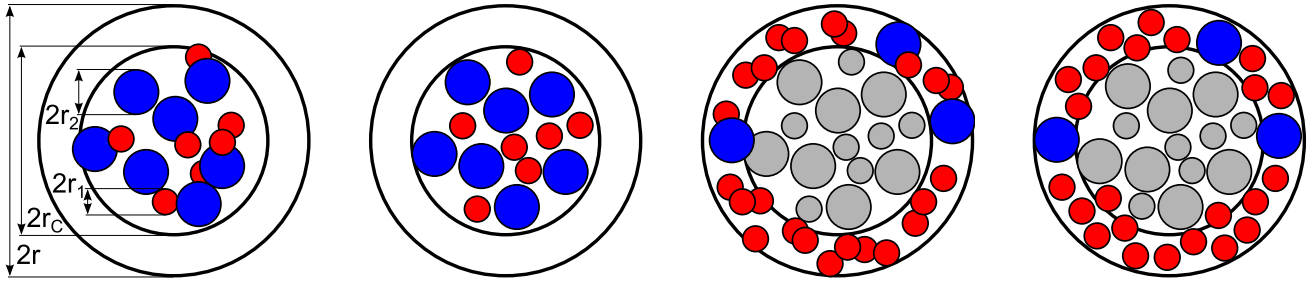
Step 1 First, we generate an initial configuration of possibly overlapping primary particles for the core. We draw points from the uniform distribution on the core and independently mark each point with a random radius R_C where $\mathbb{P}(R_C = r_1) = a_C$ and $\mathbb{P}(R_C = r_2) = 1 - a_C$. Each marked point corresponds to one particle. When the total volume of all particles divided by the core volume exceeds the packing density η, we discard the last particle and proceed with step 2. This results in a packing density slightly smaller than η.

Step 2 The force-biased packing algorithm [22,23] is applied to transform the initial particle configuration into a set of non-overlapping particles inside the core.

Step 3 Similarly we generate an initial configuration of primary particles for the shell where the particles' positions are drawn from the uniform distribution on the shell and the radii are drawn from R_S with $\mathbb{P}(R_S = r_1) = a_S$ and $\mathbb{P}(R_S = r_2) = 1 - a_S$. Again, we stop generating new particles when the total volume of all particles in the shell divided by the shell volume would exceed η.

Step 4 Then we combine the already packed core particles and the (not yet packed) shell particles and apply the force-biased packing algorithm to all particles inside the agglomerate. This results in a random packing of small and large particles where the mixing ratios in core and shell can be specified separately.

An illustration of this procedure in 2D is shown in Fig. 1.



(a) Initial arrangement of core particles together with the radii r, r_C, r_1, r_2.

(b) Non-overlapping core particles after re-arrangement.

(c) Initial arrangement of shell particles, core particles in grey.

(d) Final configuration of non-overlapping particles.

Fig. 1. Configuration of non-overlapping primary particles. Here, $m_C > 0.5 > m_S$, resulting in a large fraction of large particles in the core and, vice versa, in a small fraction of large particles in the shell.