Microstructural effects in breakage behavior of real and virtual agglomerates under compressive load[1]

Automated extraction of internal microstructures, their stochastic modeling and copula-based breakage models fitted to DEM data

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1. Introduction and overview

The discrete element method (DEM) is an effective computational technique that is used to investigate the mechanical behavior of various particle systems like, for example, agglomerates. In [1], we have presented a flexible stochastic model that can be used to generate agglomerates with various types of microstructures. However, in literature, the (two- or three-dimensional) structural input is almost always based only qualitatively on experimentally observed structures. Therefore, in [2], we have proposed a new bonded-particle extraction method for the automated approximation of agglomerate structures in tomographic data sets. Having derived such a simple description of complex tomographic data sets, one can perform DEM simulations with well-established models based on real microstructures. In particular, we show in [2] that the stochastic model presented in [1] can be used to generate statistically equivalent microstructures. Systematic variation of model parameters combined with DEM simulations reveals microstructural effects in the breakage behavior. For example, simple agglomerates (where only the mixing ratio of two fixed primary particle sizes is varied), are investigated in [1]. However, it is desirable to obtain more general functional relationships of microstructure/material parameters to breakage behavior. Therefore, we present a new and flexible approach for the modeling of particle breakage. It is based on the stochastic modeling of multivariate probability distributions using so-called copulas. Such an approximation model for agglomerate breakage is especially suitable for population balance modeling. In the present survey, the main ideas are summarized and linked together.

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2. Bonded-particle extraction

Three-dimensional microstructures used as input to DEM simulations should clearly be realistic. A direct approach is to approximate 3D structures of real agglomerates by (idealized) objects. In literature, experimentally obtained structures have been represented by, e.g., ellipsoids or clusters of spheres. Complementary, in [2], we consider the case of highly spherical primary particles. Fig. 1(left) shows a visualization of the microstructure of a maltodextrin agglomerate obtained by µCT, where the primary particles are sphere-like. This makes it possible to represent each particle by exactly one sphere. However, this kind of simplicity comes at a cost: it is hard to find a non-overlapping set of spheres without changing the structure too much - even for a packing of particles with high sphericities.

With this problem in mind, we propose a new automated method to extract bonded primary particle systems from tomographic data [2]. First, the particle system observed in image data is split up into particle regions, where each particle corresponds to one region. Solid bridges between particles contribute to the so-called “local volume” of a particle region – the simple reason is that the volume of solid bridges cannot be identified separately due to missing contrast in tomographic data. Then, an optimization problem is formulated to find a configuration of bonded particles such that (i) the particles are spherical and non-overlapping, (ii) the cylindrical bonds have diameters that correspond to the widths of solid bridges, (iii) the agglomerate volume is preserved, and (iv) the agglomerate shape is captured well. The optimization detects “optimal” sphere volumes and positions describing the particles, with the condition that the set of cylindrical bonds is plausible. This is a high-dimensional and multi-extremal optimization problem, and a stochastic optimization method is applied to solve it. Fig. 1(right) shows the bonded-particle representation corresponding to the experimental particle system shown in Fig. 1(left), where a very good agreement can be observed.

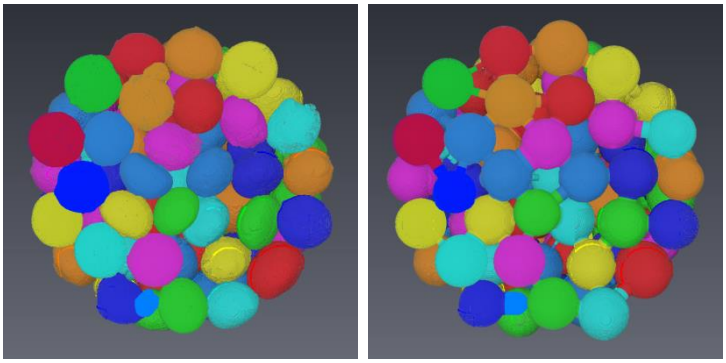

Fig. 1: 3D visualization of original tomographic data (left) and result of bonded-particle extraction (right), where colors of primary particles were chosen at random.

3. Stochastic microstructure modeling

A large data base of statistically equivalent microstructures and the possibility of systematic model parameter variation are useful for the analysis of structure–property relationships. The stochastic model introduced in [1] is based on the idea of a network of primary particles that are connected to each other directly or indirectly through a bond system. The primary particles are obtained from a sphere-packing algorithm that generates isotropic structures. The spheres follow a (predefined) radius distribution and they are packed with a certain packing density. The parameters for bond generation are the radius distribution for the cylindrical bonds and the total volume of bonds. The latter is defined relative to the total volume of primary particles. The bond radius is obtained as follows. For every possible bond, a (possibly random) factor is applied to the minimum radius of its primary particles to obtain the bond radius. Intuitively, primary particles with small distances are likely to be connected by a solid bridge. Tools from graph theory like the minimum-spanning tree are used to decide which particles should be connected by a bond, while at the same time guaranteeing connectivity of the agglomerate and targeting the desired total bond volume (for details, see [1]). Such a stochastic model is useful because of the high control over the microstructure; however, one should also take care to consider realistic scenarios for validation. For this reason, in [2] we have fitted the stochastic microstructure model to the bonded-particle approximations of real agglomerates (cf. Section 2). We observe that the stochastic model is able to capture the main features of the real agglomerates quite nicely.

4. Modeling of breakage behavior

The stochastic microstructure model presented in Section 3 is suitable to investigate

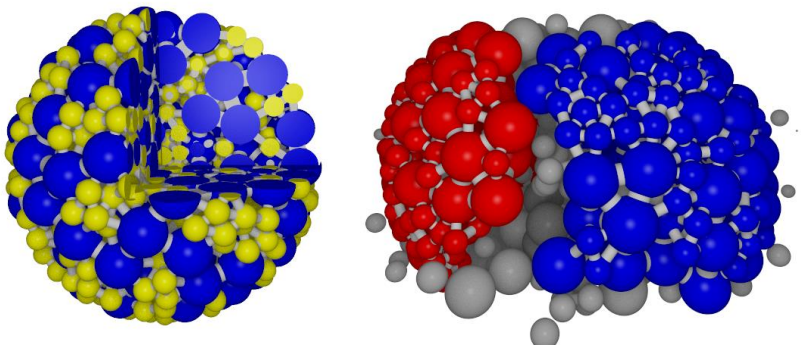

Fig. 2: 3D visualization of simulated agglomerate structure with mixing ratio 0.72 from [1] (left; one eight of the interior is cut-out for visualization purposes; large primary particles are drawn in blue) and microstructure of the same agglomerate after primary break (right; largest fragment in blue, second largest fragment in red).

structure–property relationships of agglomerates when combined with DEM simulations. As an example, in [1], the parameters of the stochastic model are all held fixed as constant values, with one exception: the primary particle radius distribution is a mixing of two different fixed particle sizes. Fig. 2 shows an agglomerate and its fragments after breakage simulated by DEM. In [1], it is shown that the mixing ratio influences the maximum force needed for breakage – and it is surprising that the breakage force is relatively large for both extreme mixing scenarios (i.e., mixing ratio near 0 or 1) in comparison to intermediate mixing ratios. A possible reason is the higher variability of the structure in the intermediate scenarios.

DEM is a powerful tool, but the computational effort is high. Therefore, there is often the need to describe breakage of agglomerates (or other particles) with sufficiently simple models. For example, a popular tool for the description of (dynamic) processes is population balance modeling (PBM). In PBM, the statistical distribution of particle properties and their evolution over time is modeled. If breakage occurs in a process, simple and fast breakage models are required. We present a new and flexible approach that provides a link from results obtained by DEM to breakage modeling suitable for PBM. It is based on the stochastic modeling of multivariate distributions using so-called copulas. For example, consider the agglomerates with different mixing ratios from above and their corresponding breakage energies observed in DEM simulations. Both variables can be understood as realizations of, say, random variables R_{mix} and E_{break}. By modeling the bivariate distribution of (R_{mix}, E_{break}), the critical breakage energy can be predicted by the conditional distribution of $E_{break} | \, R_{mix} = r_{mix}$ given any fixed mixing ratio r_{mix}. With this information, the breakage probability can be predicted (depending on mixing ratio and applied energy). In a forthcoming paper, we give a general definition of breakage models with a strict separation of material- and machine-dependent influences, and we show that copula-based approximations of breakage behavior are a practical choice to obtain such a breakage model.

[1] Spettl, A., Dosta, M., Antonyuk, S., Heinrich, S. and Schmidt, V.: Statistical investigation of agglomerate breakage based on combined stochastic microstructure modeling and DEM simulations. Adv. Powder Tech. 26 (2015), pp. 1021–1030

[2] Spettl, A., Bachstein, S., Dosta, M., Goslinska, M., Heinrich, S. and Schmidt, V.: Bonded-particle extraction and stochastic modeling of internal agglomerate structures. Preprint (available on personal homepage of A. Spettl)