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Original Research Paper

Bonded-particle extraction and stochastic modeling of internal agglomerate structures

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ABSTRACT

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. However, for systems of perfectly spherical and non-overlapping particles, the structural input is almost always based only qualitatively on experimentally observed structures. In this paper, we consider the case of agglomerates where particles are nearly spherical and connected by bonds. A novel bonded-particle extraction (BPE) method is proposed for the automated approximation of such agglomerate structures from tomographic data sets. This method can be effectively used in conjunction with various commercial or open-source DEM simulation systems. By BPE, sphere-like primary particles are represented each by exactly one (perfect) sphere, and the set of spheres is non-overlapping. Furthermore, the solid bridge bonds between primary particles are retained. Having derived such a simple description of complex tomographic data sets, one can perform DEM simulations with well-established models like the bonded-particle model. Moreover, it is shown that a larger data base of statistically equivalent microstructures can be generated by a stochastic modeling approach. This approach reduces the need for (time-consuming) experimental agglomerate production and characterization.

1. Introduction

The discrete element method (DEM) [1] is a modern and effective computational technique to simulate the mechanical behavior of granular systems on microscale. A common approach to the simulation-based investigation of agglomerates is the bonded-particle model [2]. The particles are specified as a dense packing of spheres that are bonded together. Usually, particles are spherical and bonds cylindrical. More complex geometries are possible, but they lead to higher computational effort. This is due to the need for more complex contact models or the description of complex objects as a cluster of spheres [3–7]. So far, very often agglomerate microstructures are obtained by generating packings of (bonded) particles, such that they have similar properties as observed experimentally in real agglomerates (see, *e.g.*, [8–10]). However, more realistic morphologies are desirable [7]. In the last few years, the microstructural characterization in 3D using μCT has become feasible and, therefore, more popular. For example, agglomerate microstructures have been studied [11,12] and, *e.g.*, their relationship to process variables has been investigated [13,14]. As a link to DEM, a direct approach is to approximate 3D structures of real agglomerates by (idealized) objects. Recently, experimentally obtained structures have been represented by different kinds of objects. For example, individual particles may be approximated by ellipsoids [15,16], clusters of (non-overlapping or overlapping) spheres [15,17,18], polyhedra [19] or splines [20]. In that case, DEM simulations and real experiments can be compared directly – the structures are not only statistically equivalent with respect to some characteristics, they are identical (under the restriction of having idealized objects).

In this paper, we consider the case of highly spherical primary particles. In contrast to the literature mentioned above, this allows us to represent each particle by exactly one sphere. However, this simplicity comes at a cost. Even for a packing of particles with high sphericities of about 0.9, it is hard to find a non-overlapping set of spheres without changing the structure too much. To the authors knowledge, volume-equivalent spheres with a subsequent DEM relaxation step have been used to obtain particle configurations from tomographic data; see, *e.g.*, [21]. However, the presence of solid bridges in agglomerates is a problem because mechanical equilibrium of the system is not a sufficient criterion for relaxation,

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and, of course, solid bridges have a volume as well. With these problems in mind, we propose a new automated method to extract bonded particle systems from tomographic data. We state an optimization problem to find a configuration of bonded particles such that (i) the spherical particles are non-overlapping, (ii) the cylindrical bonds match the thickness of solid bridges, (iii) the agglomerate mass does not change, and (iv) the shape and size of the agglomerate is captured well. A stochastic optimization method is applied to find a solution to this high-dimensional and multi-extremal optimization problem. We call this method the bonded-particle extraction (BPE) method.

In the second part of the paper, we show how statistically equivalent microstructures can be obtained by a parametric stochastic model for agglomerate microstructures. The model proposed in [22] is fitted to real agglomerate structures. There are several advantages of such an approach. First, one can reduce the number of real agglomerates that have to be produced and characterized experimentally. Second, realizations generated by a fitted stochastic model are more closely related to the real microstructures than packings generated with less information (*e.g.*, only based on aggregated characteristics like the mean coordination number). Third, parametric models allow the systematic variation of individual structural parameters in a realistic setting. As mentioned in [22], this is an important step to obtain reliable results by means of DEM, which leads to a better understanding of the relationship between microstructure and mechanical properties.

2. Experimental data

In this contribution, agglomerates consisting of maltodextrin (DE47) primary particles have been analyzed. Maltodextrin is a material which is widely used as a model substance for amorphous food powders and employed often as carrier or filler in the food industry. The production of agglomerates was performed in three subsequent steps: (1) creation of spherical primary particles; (2) storage of primary particles under specific conditions (temperature, humidity); (3) agglomeration of primary particles under high temperature.

To produce spherical maltodextrin particles, a solution consisting of 70 wt% maltodextrin and 30 wt% water was prepared. In order to decrease the water content, the solution was preheated in the microwave oven. Afterwards, it was dropped via separate droplets into an oil bath and primary particles were formed. For further decrease of the water content, the particles were placed in the oven at a temperature of 85 °C. This allows to get primary particles with a mean sphericity of 0.864 (standard deviation 0.026; sphericity as defined by Wadell [23]) and water content of 3 wt% (Fig. 1(a)). In the second step, in order to reproduce different storage conditions, the water content of primary particles was increased by placing them into a chamber with high air humidity and temperature. Finally, agglomerates were assembled by putting particles together into spherical (Fig. 1(b)) or cylindrical form and placing them in the oven at a temperature of 65 °C.

In total, 34 maltodextrin agglomerates were produced and characterized using a μCT 35 of SCANCO Medical AG. The tomographic reconstruction was performed based on 100 rotations, where each 2D cross-section was captured at a resolution of 2048 × 2048 pixels. A visualization is given in Fig. 2. There are 10 spherical agglomerates (diameter about 16 mm) and 24 cylindrical agglomerates (diameter about 16 mm, height about 11 mm). A dataset label is assigned to each agglomerate. The spherical agglomerates are labeled by elements of a certain set $\mathcal{L}_S$, the cylindrical agglomerates by $\mathcal{L}_C$, and $\mathcal{L} = \mathcal{L}_S \cup \mathcal{L}_C$ corresponds to all datasets. Furthermore, the mass of each agglomerate was measured. It is in the range of 1.8–2.25 g, where each agglomerate consists of about 130–170 primary particles.

3. Image processing

The tomographic data sets are denoted by $I_\ell = \{I_\ell(x,y,z) \in \{0,\dots,255\} : (x,y,z) \in W\}$, where $\ell \in \mathcal{L}$ denotes the considered dataset and $W \subset \mathbb{N}^3$ is a grid of voxel coordinates. Because of the high resolution, the original image data were (down) scaled by factor 0.5 in all three directions. The final grid of voxel coordinates has a size of $1024 \times 1024 \times 1024$ and the edge length of a voxel in the processed data corresponds to 0.02 mm.

In a first step, all images are preprocessed. As the sample holder is visible, it is removed from all data sets. This is easily possible by setting the affected voxels to black, *i.e.*, grayscale value zero, because the sample holder is located at the same position in all datasets. Furthermore, a median-filter [24] with a box size of $3 \times 3 \times 3$ voxels is applied, which reduces noise without losing much structural specifics. The resulting images are denoted by I'_ℓ.

Global thresholding is used to binarize all images I'_ℓ. For a threshold τ_ℓ, the resulting binary image $I_\ell^{\tau_\ell}$ is given by

$$I_\ell^{\tau_\ell}(x,y,z) = \begin{cases} 255 & \text{if } I'_\ell(x,y,z) \geqslant \tau_\ell, \\ 0 & \text{if } I'_\ell(x,y,z) < \tau_\ell, \end{cases}$$

where the value 255 corresponds to the solid (maltodextrin) phase, also called foreground phase. Because the mass of each agglomerate and the density $\rho = 1500\ \mathrm{kg/m^3}$ of maltodextrin are known, the threshold τ_ℓ can be chosen such that the "mass" of the foreground phase

$$\#\{(x,y,z) \in W : I_\ell^{\tau_\ell}(x,y,z) = 255\} \cdot (0.02\ \mathrm{mm})^3 \cdot \rho$$

corresponds to the experimentally measured mass as closely as possible ($\#A$ denotes the number of elements in a set A).

Having obtained the thresholds τ_ℓ and the corresponding thresholded images $I_\ell^{\tau_\ell}$, a further processing step is necessary to obtain the final binary image that will be used in all subsequent steps. One can observe that there are very small foreground or background clusters of voxels present in the thresholded images, which are obviously not relevant. The Hoshen–Kopelman algorithm [25] is applied to detect clusters in the foreground as well as in the background. Small clusters with a volume of at most 5^3 voxels are removed. The resulting binary images are denoted by I_ℓ^{bin}.

3.1. Agglomerate shape parameters

Later on, the position and exact shape of agglomerates is required. Therefore, it is necessary to detect the spheres or cylinders that match the agglomerates best. It is already known which agglomerate has a spherical or cylindrical shape. However, the exact coordinates and sizes of these spheres and cylinders have to be determined.

The Hough transform (HT) [26–28] is used to estimate the "best-fit" spheres or cylinders, respectively. The idea of the HT is to maximize the agreement between the boundary of an object observed in (binary) image data, and a simple geometric object that has one or several parameters. Essentially, the (discretized) parameter space is scanned and a so-called accumulator space is constructed, where a score is assigned to every parameter. The score is the number of voxels that belong to the object boundary in both the image and the parametric object. Then, the global maximum in this accumulator space identifies the object providing the best match. For example, for a sphere there are four parameters: