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Original Research Paper

DEM simulations of amorphous irregular shaped micrometer-sized titania agglomerates at compression

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ABSTRACT

Bulk solids are exposed to time-dependent mechanical stressing due to particle–particle and particle-apparatus contact interactions during various manufacturing processes and transportation steps. These interactions can be described by discrete element method (DEM) based on the contact models of particles. Usually in DEM simulations the particles are assumed to be spheres and as a consequence shape effects are neglected. However, most bulk solids processed in industry consist of irregular shaped particles. Therefore, in order to improve accuracy of numerical simulation the real shapes of particles must be considered in DEM. In this work, amorphous irregular shaped micrometer-sized titanium dioxide agglomerates were investigated. The force–displacement curves at compression were obtained with the help of a self-designed experimental setup. Based on the experimental data, several material parameters were determined and implemented in viscoelastic and elastic–plastic contact models. To consider the shape effect in the estimation of contact parameters the DEM simulation of studied agglomerates was performed by multi-sphere approach and bonded-particle model. The shape and position of the agglomerates on the loading pin were obtained by X-ray computer tomography and used in DEM simulations. From the obtained results it was pointed out that the bonded-particle model based on Maxwell viscoelastic model gives the best agreement with experimental data from compression tests with titania agglomerates.

1. Introduction

The dynamic behaviour of bulk solids during the various manufacturing processes and transportation steps is quite complicated due to time-dependent particle–particle, particle-apparatus and particle-gas/liquid interactions. In order to simulate the particle ensemble on the microscale, the discrete element method (DEM) is widely used. The DEM firstly introduced by Cundall and Strack [1] describes each particle of the bulk material as a separate entity by numerical calculation of the Newtonian/Eulerian equations of motion. By coupling of DEM with computational fluid dynamics (CFD), dynamic behaviour of particle collectives in a fluid can be studied [2–4]. The basis for accurate DEM simulations is a precise characterization of shape and material dependent properties of individual particles. The selection of inappropriate contact models of particle–particle/particle–wall interactions or wrong material parameters can lead to erroneous results. Therefore, to validate simulation results and to estimate material parameters experimental investigations should be performed. For example, the mechanical contact properties of particles can be effectively determined by single particle compression tests [5]. The particles, which are modelled with the DEM, are usually represented as ideally spherical objects. Such simplification significantly reduces computational effort and allows to simulate large particle assemblies with DEM method. However, solid particles processed in industrial fields often have irregular shapes. Since the contact interactions of complex shaped particles differ significantly from spherical one, the approximation with a spherical shape cannot be used for an accurate description of many bulk materials with DEM.

In the earliest DEM simulations two-dimensional circular elements were used [1]. For non-circular description of granular particle shape in two-dimensional case [6], the polygons [7], ellipses [8,9], superquadrics [10] as well as elements represented by discrete functions [11,12] can be employed. For the particle shape representation in three-dimensional simulations, the DEM was

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extended with spherical [13], elliptical [14] and polyhedral [15] bodies. Moreover, the representation of complex three-dimensional shapes by continuous [16,10] as well as discrete functions [6] was realised.

Nowadays, the multi-sphere method is widely used in the DEM community [17]. This method mimics the shape of an irregular particle with a set of overlapped non-interacting spheres [18–20]. Within a multi-spherical representation, the quality of the shape approximation is affected by number and radii of spheres inscribed into the original particle shape. The macroscopic response of a multi-spherical particle also depends on the shape approximation accuracy, even for such regular geometry like a spherical particle, which was represented as a cluster of spheres [20]. Especially, the strong effect of the particle shape complexity on bulk behaviour and mixing in a fluidized bed was observed in simulations with DEM/CFD models [21,22]. Moreover, the type of contact force model, including the cohesive forces and particle-air (fluid) interaction relationships used in DEM/CFD simulations, deeply influences the overall bulk behaviour [23].

Alternatively to the multi-sphere approach the bonded-particle model (BPM) can be employed to describe agglomerated structures and irregular shaped particles. By the BPM the investigated agglomerate is represented as clusters consisting of non-overlapping (primary) solid spheres, which are bonded together through solid bridges [24]. Each separate bond behaves like an elastic or an elastic–plastic beam and can transfer the forces and moments originated from the translational and rotational movement of connected particles. To describe the breakage of these solid bonds in an agglomerate, the different stress-based breakage criteria are employed. The bonds are destroyed and removed from the simulation when the equivalent stress exceeds either the tensile or the shear strength of the bond material [25–27]. The implementation of such bonded-particle model gives a possibility to simulate the agglomerate deformation as well as the breakage at static and dynamic loading on the micro-scale. However, the computational effort of the numerical studies, where complex particle shapes are described by multi-sphere or by BPM approach, is significantly larger compared to the DEM with ideally spherical particles. This is caused by the multicontact events, smaller size of primary particles and increased number of modelled objects.

Since the shape representation as well as inner structure of the agglomerate affects the contact behaviour and breakage mechanisms in DEM simulations, the shape of agglomerates used in simulations of industrial processes must coincide with real agglomerates. For this purpose, the irregular shape of the agglomerates can be obtained by X-ray microtomography (XRMT). The XRMT is a non-destructive imaging technique that permits to obtain a 3D image of a scanned object (single particles, agglomerates or a particle bed) from a series of X-ray slices [28]. A combination of data obtained from XRMT with DEM simulations enables the study of particle properties during mechanical loading [29]. More often XRMT is applied for investigation of granules behaviour during mixing, segregation, sintering as well as for the determination of bed porosity and moisture contents [28] For nano-scale particles, the three-dimensional transmission electron microscopy (3D TEM) [30] or plasmon tomography [31] can be successfully used to reconstruct their shape.

The aim of the present study is to numerically reproduce the compression test with irregular shaped titania agglomerates by means of discrete element method and to find the models and their parameters, which give the best agreement with the experimental results. For this purpose, the real size and shape of the particle was obtained from XRMT measurement and the compression test was carried out. Afterwards, the DEM simulation of the compression test was performed, where the agglomerate positioning on a loading pin was corresponded to the real experiment. For the irregular particle shape representation in numerical simulations, the multi-sphere approach and bonded-particle model were used and compared.

2. Experimental investigations

2.1. Tested material

Titania TiO_2 is the naturally occurring oxide of titanium. Titania can exist in three crystalline modifications (brookite, rutile and anatase) with three different crystal lattice structures and as an amorphous material [32]. In this study, amorphous irregular shaped titanium dioxide particles were used for the investigation. The particles were produced at the Institute of Mechanical Process Engineering (Otto von Guericke University of Magdeburg, Germany) via a sol–gel process without calcination [33]. The SEM images (Fig. 1) showed that the produced titanium dioxide particles had a typical agglomerate structure.

Titania was analysed by combined differential scanning calorimetry (DSC) (NETZSCH DSC 204 F1 Phoenix), and thermogravimetric analysis (TGA) (Q500, TA Instruments), which detect the heat flow and the mass loss as a function of temperature changes. The measurements showed a weight loss of approximately 17.74 ± 2.62% at a temperature of 170 °C (Table 1). As pointed out in [34], chemical bonding $TiO_2 \cdot H_2O$ can arise during a sol–gel process, whereby H_2O has a mass fraction of 18.4% and is evaporated at temperatures from 170 °C to 200 °C. In addition to water residue, the used sample can contain sodium dodecyl sulfate (SDS) due to the manufacturing process. The decomposition of SDS usually takes place in a range between 200 °C and 400 °C, so SDS plays a minor role in the mass loss at temperatures up to

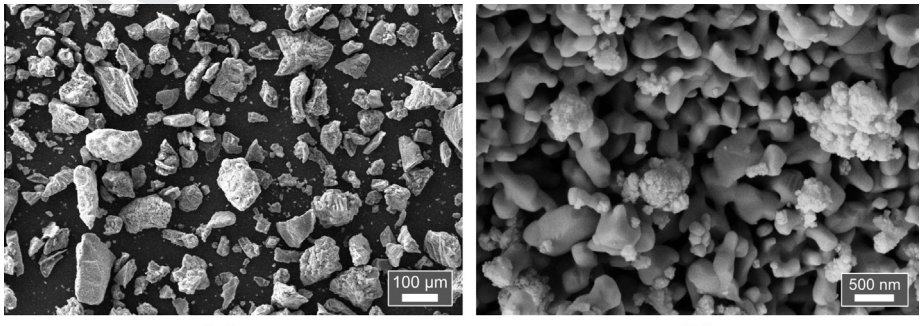

Fig. 1. SEM images: (a) titanium dioxide agglomerates; (b) image with higher magnification showing agglomerate inner structure.

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