Predicting Breakage of High Aspect Ratio Particles in an Agitated Bed Using the Discrete Element Method

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Abstract

Predicting particle breakage is critical for the control of particle size in some bulk solids handling processes, such as those found in the pharmaceutical, food, consumer product, and mineral processing industries. This article presents a computational study of the breakage of high aspect ratio particles subject to mechanical agitation using the Discrete Element Method (DEM), in which a particle, represented by a string of bonded spheres, breaks at the center of a bond where the tensile or shear stress exceeds the material strength. The numerical model is validated using experimental results from the breakage of blackboard chalk sticks subject to uniaxial compression in a cylindrical container. The validated model is used to investigate particle breakage when agitated by rotating blades, which is encountered in a range of pharmaceutical processes, such as agitated filter drying, rotary tablet press feeding, and powder blending. The simulation results show that the breakage rate, that is the rate of particle size reduction (or the rate of fragment mass increase), increases as the applied pressure, impeller rotational speed, particle-particle friction, or particle-equipment friction increases. However, the extent of breakage per impeller revolution is independent of impeller rotational speed. Most importantly, it is found that the extent of particle breakage is a function of the work performed on the material, and the parameters in this function depend on the particle-particle and particle-wall friction coefficients. Large friction coefficients enable the input energy to break the particles more efficiently.

Keywords: Particle breakage; High aspect ratio particle; Agitated filter dryer; Discrete Element Method

1. Introduction

Particle breakage and degradation can be problematic in the processing of granular materials in pharmaceutical and consumer product industries, causing hazardous dust, handling problems in subsequent processes, and product quality problems. On the other hand, in mineral processing, large rocks need to be crushed into smaller ones for the extraction of mineral materials. In this process, the energy required for comminution needs to be predicted for proper equipment design. As a result, the prediction and control of particle breakage is crucial to many industries. Achieving this goal depends on the understanding of particle breakage in a bulk material and the effects of critical controlling parameters. From a single particle point of view, particle breakage is usually caused by the propagation of cracks, which is driven by stresses concentrated at the crack tips. Smaller particles are more difficult to break than larger ones because a small particle size can limit the length of cracks and allow little room for the stress distribution patterns to develop. As a result, smaller stress concentrations occur at the crack tips and larger external forces are required to drive crack propagation. Rather than single particle breakage, it is the overall particle size reduction and energy consumption of a bulk system that is of interest in most industrial situations. In these bulk systems, concurrent and continuous breakage of the particles depends on the particle properties and particle-particle and particle-equipment interactions.

A number of empirical models have been proposed to predict particle size reduction based on experimental data. However, these models have very specific applications (Rhodes, 1998). If the material or process is changed, the parameters in the models must be re-calibrated or may not be applicable. In recent years, computational modeling based on the Discrete Element Method (DEM) has been utilized to investigate particle breakage in many applications, such as in mineral processing (Weerasekara et al., 2013). The advantage of computational modeling of particle breakage is the ease with which material properties can be specified and operating processes adjusted. Nevertheless, high computational cost and the need for validated particle breakage models make model development challenging. The current work focuses primarily on this latter topic: the development and validation of a particle breakage model for high aspect ratio particles.

1.1 Prediction of Particle Size Reduction

From a population balance of a granular system (Rhodes, 1998), the rate of mass change of particle size interval i can be expressed as,

$$\frac{dm_i}{dt} = \sum_{j=1}^{j=i-1} \{b(i, j)S_j m_j\} - S_i m_i, \quad (1)$$

where m_i is the mass of particles of size interval i and S_i is the probability of particles of size interval i being broken in unit time. The quantities m_j and S_j are for particles of size interval j . Assuming that the particle size decreases as the size interval level increases, the breakage distribution function $b(i, j)$ represents the fraction of breakage product from size interval j that falls into size interval i . On the right hand side of Eq. (1), the first term represents the birth rate, which is the generation rate of new particles of size interval i due to the breakage of larger particles while the second term represents the death rate, which is the breakage rate of particles of size interval i . In practice, the values of S_i and $b(i, j)$ are determined from small scale tests and then Eq. (1) is used to predict the particle size distribution at a larger scale. Population balances have been widely employed for the prediction of particle breakage in various granular systems. For example, Sato et al. (2008) developed a population balance model for their experiments involving the breakage of high aspect ratio crystals in an agitated crystal bed in a thermostatic glass vessel. Grof et al. (2011) also developed a population balance model for needle-shaped crystals under uni-axial compaction, but determined the breakage probability and breakage distribution functions using a combination of computational and experimental methods.

Particle size reduction can also be caused by particle attrition, in which a small amount of mass is worn down from the particle surface. Neil and Bridgwater (1994) and Ghadiri et al. (2000) found that the extent of attrition is a function of the applied normal stress and shear strain and can be described by,

$$M = k_N \left[\left(\frac{\sigma}{\sigma_{SCS}} \right) \Gamma \phi \right]^\beta, \quad (2)$$

where M is the mass of the lost material due to attrition, σ is the normal stress, and Γ is the shear strain. The side-crushing strength of the material, σ_{SCS} , is used to normalize σ . Three parameters k_N , β , and ϕ can be obtained by fitting the formula with experimental data. Using numerical modeling, Potapov and Campbell (1997) observed a different relationship between the extent of attrition, M , and the work exerted by an external force on the sheared particle system, W ,

$$M = k_w W^\alpha, \quad (3)$$

where k_w and α are fitting parameters.

1.2 Computational Modeling of Particle Breakage

Several DEM-based computational methods have been developed to simulate particle breakage including the bonded-particle method, the combined Finite-Discrete Element Method (FDEM),

the fragment spawning method or particle replacement method, and the particle attrition prediction method. These techniques are discussed in the following paragraphs.

In the bonded-particle method, a particle is formed by bonding a finite number of sub-particles, which can be spheres (Potyondy and Cundall, 2004; Grof et al. 2007), triangles (Potapov and Campbell, 1997), or polygons (Hosseini and Mirghasemi, 2006). A particle breaks at the bond position where the stress exceeds the prescribed material strength. In the FDEM method (Munjiza, 2004; Ma et al., 2014), a particle is partitioned into a finite number of elements. Breakage occurs at the boundaries between the elements. A significant advantage of the bonded-particle method and FDEM method is that the stress distribution and fracture propagation within a particle can be modeled. The drawback of these two methods is that the size distribution after breakage is limited, considering that breakage has to occur at the bond positions or element boundaries. To increase the fragment size distribution, one may use additional sub-particles or elements to discretize a parent particle. However, the computational expense may be significantly increased. As a result, using the bonded-particle method is challenging for modeling an attrition process where only small fragments are broken off a particle.

To address the limited fragment size distribution and high computational cost in modeling stress and crack propagation, the fragment spawning method or particle replacement method was proposed (Kalman et al., 2009; Brosh et al., 2011; Bruchmüller et al., 2011). In this model, if the stress acting on a particle is smaller than the strength of the particle, a fatigue function is called and a reduced strength is assigned to the particle. Otherwise, if the operating stress is greater than the particle strength, a breakage function is called and a mother spherical particle is then replaced by child spheres having a wide size distribution. The generation of the child particles after breakage is governed by the specified fragment spawning, seeding, and interaction algorithms, which lead to an empirical size distribution obtained from experiments. Mass, momentum, and energy are all conserved in the replacement of the parent sphere with child spheres. This method has been successfully used to predict particle comminution in jet milling and pneumatic conveying (Brosh et al., 2011). Delaney et al. (2010) applied this approach to non-spherical particles breaking into many smaller non-spherical particles. In the fragments spawning or particle replacement method, the process of particle breakage is assumed to be transient, and the stress distribution and crack propagation within a particle are not resolved.

Hare et al. (2011) introduced a DEM approach for predicting the extent of particle attrition in agitated particle beds. In their method, the distributions of bulk stresses and strains in the bed are estimated from the DEM model. Next, the extent of particle attrition is predicted from an empirical correlation between attrition and particle-phase stresses and strains. This correlation

can be obtained experimentally from shear cell tests (Neil & Bridgewater, 1994). In this approach, the particle size change due to breakage and attrition is not considered directly in the DEM model, but the attrited mass is computed based on the DEM outputs (i.e., stresses and strains). Therefore, this particle attrition prediction method may be applicable only to a system with a small extent of breakage and negligible particle size change during the agitation process.

In their DEM simulations, Hua et al. (2015) investigated the internal load and moment distributions within rod-like particles in a blade-agitated mixer. The rod-like particles were modeled using sphero-cylinders, each of which has a cylindrical body and two hemispherical ends. With the assumption of small particle deformation, the stress distribution in a cross sectional area of a rod-like particle, which is perpendicular to the major axis of the particle, can be determined. They observed that the maximum absolute principal stress occurs along the particle circumference at the center-plane of the particle, indicating that high aspect ratio, rod-like particles are more likely to break in the center with the failure beginning from the circumference. This finding is consistent with previous results by Grof et al. (2007).

1.3 Layout of This Article

In this article, we use a bonded-particle method to model the breakage of high aspect ratio particles. Unlike the bonded-particle method employed in the work of Grof et al. (2007), for which the spheres are rigidly connected to form a non-deformable, needle-like particle, the current high aspect ratio particle model uses spheres that are connected using elastic bonds, allowing bending, twisting, and axial stretching deformation of an elongated rod-like particle (Guo et al., 2013b). A breakage criterion is implemented in the particle model so that the particle breaks when the tensile or shear stress in a bond exceeds the prescribed material strengths. The bonded-particle model used in this work is described in Sec. 2. In Sec. 3, we validate our numerical model by comparing simulation and experimental results for the breakage of blackboard chalk sticks under uni-axial compression in a cylindrical container. In the Sec. 4, the numerical model is applied to investigate the breakage of high aspect ratio particles in an agitated bed. This type of breakage phenomenon is observed in the crystallization and drying processes of active pharmaceutical ingredients (APIs). The effects of the stress environment, agitation rate, particle-particle friction, and particle-equipment friction on the extent of breakage are explored. Concluding remarks are made in Sec. 5.

2. DEM Modeling of High Aspect Ratio Particle Breakage

2.1 Bonded-Particle Model

The bonded-particle model used in this study has been described in our recent work (Guo et al., 2013b; Guo et al., 2015). In addition, a comprehensive verification of the mechanical responses of a single fiber, including bending, stretching/compressing, and twisting deformation, has been made by comparing the model with analytical solutions (Guo et al., 2013b). For convenience, the model is also summarized here.

A rod-like particle is formed by connecting a number of identical spheres in a straight line using virtual elastic bonds. Two ends of a single bond, which are fixed at the centers of two neighboring spheres, translate and rotate with the spheres. Thus, the relative movement of constituent spheres leads to the deformation of the bonds and also the fiber. A DEM simulation of the collision of two flexible fibers has been performed in our recent work, as shown in Figure 1. The bond forces/moments are generated and exerted on the spheres to resist the deformation. According to the bonded-particle model by Potyondy and Cundall (2004), the bond forces and moments can be calculated incrementally as follows:

$$dF_n^b = K_n^b d\delta_n^b = \frac{E_b A}{l_b} d\delta_n^b = \frac{E_b A}{l_b} v_n^r dt, \quad (4)$$

$$dF_t^b = K_t^b d\delta_t^b = \frac{G_b A}{l_b} d\delta_t^b = \frac{G_b A}{l_b} v_t^r dt, \quad (5)$$

$$dM_n^b = K_{tor}^b d\theta_n^b = \frac{G_b I_p}{l_b} d\theta_n^b = \frac{G_b I_p}{l_b} \omega_n^r dt, \quad (6)$$

$$dM_t^b = K_{ben}^b d\theta_t^b = \frac{E_b I}{l_b} d\theta_t^b = \frac{E_b I}{l_b} \omega_t^r dt, \quad (7)$$

in which dF_n^b , dF_t^b , dM_n^b , and dM_t^b are the incremental bond normal force, shear force, torsional moment, and bending moment, respectively, and $d\delta_n^b$, $d\delta_t^b$, $d\theta_n^b$, and $d\theta_t^b$ are the incremental normal deformation, shear deformation, torsional (normal) angular deformation, and bending (tangential) angular deformation, respectively, of the bond. Thus, K_n^b , K_t^b , K_{tor}^b , and K_{ben}^b represent the normal, shear, torsional, and bending stiffnesses, respectively, of the bond. The cylindrical bond of Young's modulus E_b and shear modulus G_b has a radius r_b , a length l_b , a cross sectional area $A = \pi r_b^2$, an area moment of inertia $I = \pi r_b^4/4$, and a polar area moment of inertia $I_p = \pi r_b^4/2$. In the present model, the bond radius r_b is assumed to be

the same as the constituent sphere radius r_s , and the bond Young's modulus E_b and shear modulus G_b are correlated through the Poisson's ratio ζ : $E_b = 2(1 + \zeta)G_b$. The virtual bond has no mass. The incremental bond deformation can be obtained from the product of the corresponding relative velocity between two bonded spheres (v_n^r , v_t^r , ω_n^r , or ω_t^r) and the time step dt .

The movement of individual constituent spheres in each fiber is governed by Newton's second law of motion, i.e.,

$$m_s \frac{d^2 \mathbf{x}_s}{dt^2} = \mathbf{F}^c + \mathbf{F}^b + m_s \mathbf{g} + \mathbf{F}_d^c + \mathbf{F}_d^b, \quad (8)$$

$$J_s \frac{d^2 \boldsymbol{\theta}_s}{dt^2} = \mathbf{M}^c + \mathbf{M}^b + \mathbf{M}_d^c + \mathbf{M}_d^b, \quad (9)$$

in which $\mathbf{x}_s$ and $\boldsymbol{\theta}_s$ are the translational displacement and angular displacement, respectively, of the sphere of mass m_s and moment of inertia $J_s = \frac{2}{5}m_s r_s^2$. The translational motion of the sphere is driven by the contact force $\mathbf{F}^c$ exerted by the spheres that are not bonded to it or come from a different composite particle, the bond force $\mathbf{F}^b$ exerted by the bonds connecting to it, and the gravitational force $m_s \mathbf{g}$. The bond force $\mathbf{F}^b$ is calculated incrementally based on Eqs. (4) and (5). The moment $\mathbf{M}^c$ arises from the tangential component of contact forces $\mathbf{F}^c$, and $\mathbf{M}^b$ represents the bond moment induced by the shearing, bending, and twisting deformation of the bond. A contact force $\mathbf{F}^c$ can be decomposed into a normal force and a tangential force. The elastic normal force is computed based on the current normal overlap between two spheres using the Hertz model (Johnson, 1985). The tangential interaction consists of static and sliding friction processes. For static friction, the tangential force depends on the current normal force and the tangential loading path according to the Mindlin-Deresiewicz theory (Thornton and Yin, 1991). When the tangential force exceeds the product of the friction coefficient μ and current normal contact force F_n^c , sliding friction occurs. The tangential force during sliding is equal to μF_n^c , according to Coulombic sliding friction theory.

In Eq. (8), a contact damping force $\mathbf{F}_d^c$ is introduced to account for the energy dissipation when two spheres collide. The normal and tangential contact damping forces can be written as,

$$F_{dn}^c = \beta_c \sqrt{\frac{5}{6}} \sqrt{2m_p K_n^c} v_n^c, \quad (10)$$

$$F_{dt}^c = \beta_c \sqrt{\frac{5}{6}} \sqrt{2m_p K_t^c} v_t^c, \quad (11)$$

in which m_p is the mass of a bonded particle or fiber. The symbols K_n^c and K_t^c represent the contact normal stiffness and the contact tangential stiffness, respectively. The expressions of K_n^c and K_t^c are given by Thornton and Yin (1991) and are also summarized in Guo (2010). The variables v_n^c and v_t^c represent the normal and tangential components, respectively, of the relative velocity at the contact point. The contact damping coefficient β_c is related to the coefficient of restitution e , which is defined as the ratio of the post-collisional to pre-collisional relative velocity at the contact point. The correlation between β_c and coefficient of restitution e is provided in Guo et al. (2013a) and is expressed as,

$$\beta_c = -\frac{\ln e}{\sqrt{\pi^2 + \ln^2 e}}.$$

In this study, the coefficients β_c are chosen to give $e = 0.95$ for particle-particle contacts and $e = 0.90$ for particle-wall contacts. In Eq. (9), $\mathbf{M}_d^c$ is the moment arising from the contact damping force $\mathbf{F}_d^c$:

$$\mathbf{M}_d^c = \mathbf{r} \times \mathbf{F}_d^c,$$

in which $\mathbf{r}$ is the vector from the center of the sphere to the contact point.

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Analogous to contact damping, bond damping is proposed to take into account energy dissipation due to elastic wave propagation within a particle. Thus, the bond damping forces and moments are assumed to follow,

$$F_{dn}^b = \beta_b \sqrt{2m_s K_n^b} v_n^r, \quad (12)$$

$$F_{dt}^b = \beta_b \sqrt{2m_s K_t^b} v_t^r, \quad (13)$$

$$M_{dn}^b = \beta_b \sqrt{2J_s K_{tor}^b} \omega_n^r, \quad (14)$$

$$M_{dt}^b = \beta_b \sqrt{2J_s K_{ben}^b} \omega_t^r. \quad (15)$$

The bond damping coefficient β_b varies in the range 0-1 and determines the energy dissipation rate as the bond deforms. Similar to the contact damping coefficient β_c , the bond damping coefficient is given by,

$$\beta_b = -\frac{\ln e_b}{\sqrt{\pi^2 + \ln^2 e_b}},$$

in which e_b reflects the reduction in the relative velocity between two bonded spheres due to the bond damping. In this study, the values of e_b were assigned to be 0.88, 0.76, and 0.64 to give β_b values of 4.20 e-2, 8.87 e-2, and 1.41 e-1, respectively. The bond damping force F_d^b and bond damping moment M_d^b (based on Eqs. (12)-(15)) are inputted to Eqs. (8) and (9).

2.2 Breakage Criterion

In this work, the breakage of a particle is modeled as the failure of bonds and the disconnection of two bonded constituent spheres. As proposed by Potyondy and Cundall (2004), a bond fails when the maximum normal stress, $\sigma_{\max}^b$, or the maximum shear stress, $\tau_{\max}^b$, exceeds the corresponding tensile strength, σ_{ten} , or shear strength, τ_{sh} ,

$$\sigma_{\max}^b = \frac{F_n^b}{A} + \frac{|M_t^b| r_b}{I} > \sigma_{\text{ten}} \quad (16)$$

$$\text{or} \quad \tau_{\max}^b = \frac{|F_t^b|}{A} + \frac{|M_n^b| r_b}{I_p} > \tau_{\text{sh}}. \quad (17)$$

3. Validation of Particle Breakage Model by Uniaxial Compression Tests

Validation of the implemented particle breakage model was examined by conducting experiments and performing numerical simulations of particle breakage under uniaxial compression. The uniaxial compression experiment is shown in Figure 2. A bed of 300 identical blackboard chalks was gently deposited in a cylindrical container of diameter 200 mm. The cylindrical chalks have a length of $L = 80$ mm and a diameter of $D = 10$ mm. Using a three point bending test, the Young's modulus of the chalk sticks was measured as $E = 527.6 \pm 18.1$ MPa and the tensile strength as $\sigma_{\text{ten}} = 3.99 \pm 0.06$ MPa. The experimental setup and procedure for performing three-point bending tests are provided in the supplementary material for this article. The shear strength is assumed to be the same as the tensile strength: $\tau_{\text{sh}} = \sigma_{\text{ten}}$. Five tests were performed for this measurement. The friction coefficient between the chalks was measured as $\mu_{\text{pp}} = 0.624 \pm 0.024$ (obtained from six tests) using the "tilted plane" method in

which the angle of the tilted plane from the horizontal is recorded when a chalk starts sliding on the surface of a pack of chalks fixed on the top of the plane. The mass of a chalk stick is measured using a scale and the volume is computed from its diameter and length. The chalk density, which is equal to the mass divided by the volume, was measured as $1570 \pm 12 \text{ kg/m}^3$ (from ten tests). The bed of chalks in the container was compressed as the punch moved downwards at a speed in the range 5-10 mm/s. During compression, the load applied to the punch was recorded as a function of the displacement of the punch. After compression, the chalks, which underwent significant breakage, were carefully taken out of the container. The length distribution of the resulting chalk fragments was analyzed using the free image analysis software *ImageJ*.

The parameters used in the DEM simulations are provided in Table 1. The measured values of chalk material properties were used as the input parameters for the base case simulations. The particle-cylindrical wall friction coefficient, particle-flat wall friction coefficient, and particle bond damping coefficient were not measured experimentally. However, the friction between a chalk stick and a piece of plate, which has similar surface roughness to the walls in the compression tests, was estimated to be in the range 0.4-0.6. Thus, the sensitivity to the particle-wall friction coefficient has been examined in a wider range 0.1-0.6 in the simulations. A chalk stick was represented using eight identical spheres with 10 mm diameter that were bonded in a straight line, leading to a stick 80 mm long. As shown in Figure 3, 300 modeled chalk sticks settled in a cylindrical container of diameter 200 mm before compression. A constant speed of $v_p = 6.18 \text{ mm/s}$ was assigned to the punch, corresponding to the average value of the punch speed measured in the experiment. The sticks were compressed by the punch in the container. After compression, a large number of sticks were broken. In Figure 3b, the fragments after breakage were colored differently according to their aspect ratios (*AR*).

The results of base simulations were subsequently compared with the experimental results. The load applied to the top of the bulk material is plotted as a function of the displacement of the punch or upper wall in Figure 4. In the experiment, the load increased to 1023 N (230 lbf) at which point the punch moved upwards and the load was rapidly removed. In the simulation, only the loading process was simulated. It can be seen that the loading curve obtained from the simulation is generally in good agreement with that from the experiment. A comparison of the fragment length distributions between the simulation and experiment under the compression load of 1023 N is shown in Figure 5. The compression tests were repeated three times with different initial particle spatial configurations for both experimental and simulation studies. Ignoring the unbroken sticks with a ratio of fragment length to initial particle length equal to one, a normal distribution is observed with the peak value occurring at a length ratio equal to 0.5. This observation indicates that the high aspect ratio particles are more likely to break in the

center, which was also found in previous work by Hua et al. (2015) and Grof et al. (2007). Also, similar distribution profiles are observed for the simulation and experiment.

The effects of particle-cylindrical wall friction and particle-flat wall friction on the fragment length distribution are shown in Figure 6. In general, the particle-wall friction coefficients have a limited impact on the particle breakage in the ranges considered. It is observed that the fraction of middle size fragments increases slightly with an increase in the friction coefficient between the particles and the flat punch surface and container base wall, μ_{pw} . As shown in Figure 7, the particle bond damping has a negligible influence on the particle breakage in the process considered. A high aspect ratio particle, which is represented as a string of bonded spheres, has a bumpy surface (see Figure 1). This bumpy surface structure increases the chance for particle interlocking, making it more difficult for particles to slide past each other. It appears that the effect of a bumpy particle surface on compression and particle breakage is minimal, as demonstrated by the good agreement between the simulation and experimental results observed in Figures 4-7.

4. Breakage in an Agitated Bed

Particle breakage due to blade agitation has been frequently encountered in bulk solids handling processes, such as agitated filter drying of active pharmaceutical ingredients (API) (am Ende et al., 2013). Lamberto et al. (2011) developed a laboratory agitation cell to study the breakage of API particles subject to mechanical agitation. In the cylindrical cell, a bed of granular material is stirred by a rotating impeller comprised of several blades and a shaft. A weight is applied to compress the material from the top in order to account for the effect of the larger bed depth in the real operation. Based on the difference in the mean particle size before and after agitation, the materials are classified as hard, medium, or easy to break. Using a similar experimental setup to that used by Lamberto et al. (2011), Remy et al. (2015) investigated the effects of shear stress and hydrostatic pressure on the API attrition. Subsequently, they proposed a workflow for scale-up of agitated drying of API materials.

Particle breakage is determined by particle flow and contacts. The kinematics and internal stresses of elongated, rod-like particles in a blade-agitated mixer have been computationally investigated by Hua et al. (2013; 2015). It was found that as the particle aspect ratio increases, the particle velocity and average solid volume fraction decrease and the internal stresses within a particle increase. The computational simulations of granular shear flows by Guo et al. (2012; 2013a) show that the inter-particle contact forces and solid phase stresses increase with increasing particle friction coefficient and particle aspect ratio in dense flows.

In this study, the previously described and validated particle breakage model is employed to simulate the breakage of high aspect ratio particles in an agitation cell. High aspect ratio particle breakage in uniaxial compression tests is mainly caused by bending deformation, which is driven by the external forces from particle-particle contacts and particle-boundary wall contacts. Particle breakage in the agitated bed occurs for the same mechanism. As a result, validation of particle breakage under uniaxial compression gives confidence in predicting particle breakage in an agitated bed. However, the effects of significant particle motion and particle-blade interaction have not been taken into account in the uniaxial compression tests. In the following subsections, the present agitated bed simulation results will be compared with previous experimental and simulation work.

The simulations are designed to explore the major factors that govern particle breakage. The modeled agitation cell is illustrated in Figure 8. The impeller in the cylindrical cell has three blades with a pitch angle of 60° from the horizontal. A number of particles of a specified aspect ratio (10 in the present study) are initially generated in random positions and with random orientation inside the agitation cell. After the initial generation, the particles are allowed to settle under gravity in the cell. Next, the particle bed is compressed by applying a weight to the top wall. When a balance is achieved between the weight of the top wall and the resultant particle-wall contact force, agitation is started by rotating the impeller about the central shaft at a constant angular velocity. During agitation, the applied weight on the top remains constant. The agitation cell size, particle properties, bond properties, blade properties, and operating parameters are shown in Table 2. The Young's modulus, density and material strength of the particles and bonds are the same as those of pregelatinized starch compacts, which are pharmaceutical materials, as reported by van Veen et al. (2004).

During the agitation process, the mass of small fragments increases due to particle breakage. This mass fraction of fragments with the aspect ratio (AR) less than or equal to a specified sieve cut AR is plotted as a function of the impeller angular displacement, ωt , for the normalized pressures $\frac{P}{\sigma_{ten}} = 1.69\text{e-}3$ and $3.38\text{e-}3$ in Figure 9, in which P is the applied pressure to the top of the particle bed and σ_{ten} is the material tensile strength. As shown in Figure 9, the fragment mass fraction initially increases with the impeller angular displacement and eventually approaches an asymptotic value for various sieve cut aspect ratios (AR). The particle aspect ratio distributions at various impeller angular displacements are plotted in Figure 10. It can be seen that most of the fragments have aspect ratios smaller than six indicating that the longer particles are easier to break than shorter ones, and they tend to break near the center.

4.1 Agitation under Various Applied Pressures and with different cell sizes

As shown in Figure 11a, a larger fragment mass fraction with the sieve cut aspect ratio of $AR \leq 5$ is obtained with larger applied pressure, $\frac{P}{\sigma_{ten}}$. Particle breakage is promoted as larger pressures are applied to compress the material since larger internal particle stresses are induced by larger external forces. The slopes of the fragment mass fraction curves decrease as the impeller angular displacement, ωt , increases. The fragment mass fraction tends to approach a maximum limit as the agitation proceeds, and the limit is reached sooner with a larger applied pressure. In addition, a small agitation cell of diameter $D_c = 122$ mm and a large one of diameter $D_c = 244$ mm have been considered. With the same applied pressure, similar curves are obtained for the fragment mass fraction as a function of ωt for both small and large cells. The mean particle aspect ratio, AR_m , normalized by the initial mean particle aspect ratio before agitation occurs, AR_m^0 , is plotted as a function of impeller angular displacement in Figure 11b. The mean particle aspect ratio decreases as the impeller angular displacement increases. Smaller mean particle aspect ratios are observed with larger applied pressures. With the same applied pressure, similar results for particle aspect ratio reduction are obtained with the two different agitation cell sizes.

4.2 Effect of Impeller Rotational Speed

The effect of impeller rotational speed on the particle breakage results has also been explored. The variation of fragment mass fraction with $AR \leq 5$ and normalized mean particle aspect ratio with elapsed time, t , for various impeller rotational speeds is shown in Figure 12. At a given time instant, larger fragment mass fraction and smaller mean particle aspect ratio are observed with larger impeller rotational speed. The variation of fragment mass fraction and normalized mean particle aspect ratio with impeller angular displacement, ωt , is plotted in Figure 13. Interestingly, subject to a given applied pressure, the variation of fragment mass fraction and normalized mean particle aspect ratio with impeller angular displacement is independent of the impeller angular speed, ω , after an initial short period ($\omega t < 1$ rad or 60 degrees). Thus, the extent of particle breakage in an agitation cell is essentially determined by the impeller angular displacement rather than the impeller rotational speed. The same observation, that attrition is a function of displacement as opposed to speed, was obtained for the attrition of spherical particles in shear flows (Hare et al., 2011).

Considering that the particle breakage is significantly affected by normalized applied pressure, P/σ_{ten} , and impeller angular displacement, ωt , the fragment mass fraction and normalized mean particle aspect ratio are plotted as a function of $\omega t(P/\sigma_{ten})$ in Figure 14. The resulting curves tend to collapse for both the small and large cells, various impeller angular speeds, and various applied pressures.

Figure 15a shows the torque acting on the impeller, T , as a function of impeller angular displacement, ωt . For a given applied pressure, the torque rapidly increases then fluctuates around a constant value as the impeller rotates. It can be seen that the torque increases as the applied pressure increases. A linear relationship between the mean torque, T_{mean} , and the applied pressure, P/σ_{ten} , is observed in Figure 15b. Therefore, for a given agitation cell, the mean torque acting on the impeller, T_{mean} , is proportional to the applied pressure, P/σ_{ten} . This dependence of the torque on the pressure was also observed in the API agitated drying experiments by Remy et al. (2015). Therefore, we have

$$W = \omega t T_{mean} \propto \omega t (P/\sigma_{ten}). \quad (18)$$

The work performed by the impeller, W , is proportional to the dimensionless term, $\omega t (P/\sigma_{ten})$. The data collapse in Figure 14 indicates that the particle breakage results are governed by the work input from the impeller. This result is consistent with the previous finding by Potapov and Campbell (1997) in their 2D simulations of square particle breakage in shear flow. Also, Remy et al. (2015) obtained a similar correlation between the work done by the impeller and the degree of particle attrition in their experiments.

4.3 Effect of Inter-Particle Friction

The inter-particle friction coefficient determines how easily a particle slides past its neighbors, and also has a significant influence on the contact forces between particles. The effect of inter-particle friction on particle breakage in an agitation cell is shown in Figure 16, in which the fragment mass fraction (sieve cut $AR \leq 5$) and normalized mean particle aspect ratio are plotted as a function of the dimensionless term, $\omega t (\frac{P}{\sigma_{ten}})$. It can be seen that larger fragment mass fractions and smaller mean particle aspect ratios are obtained with larger inter-particle frictions, μ_{pp} . This result is due to the fact that larger inter-particle friction coefficients lead to larger contact forces, which promotes particle breakage.

In an effort to collapse the curves for different inter-particle frictions in Figure 16, the following correlations are assumed:

$$\text{Fragment Mass Fraction} = \text{function1} (K_1(\mu_{pp}) [\omega t (P/\sigma_{ten})]^{f_1(\mu_{pp})}), \quad (19)$$

and,

$$AR_m/AR_m^0 = \text{function2} (K_1(\mu_{pp}) [\omega t (P/\sigma_{ten})]^{f_1(\mu_{pp})}), \quad (20)$$

where K_1 and f_1 are empirically determined fitting functions of μ_{pp} . As shown in Figure 17, the collapse of particle breakage data with various inter-particle friction coefficients is achieved in the plots of fragment mass fraction and normalized mean particle aspect ratio as a function of the dimensionless term, $K_1(\mu_{pp})[\omega t(P/\sigma_{ten})]^{f_1(\mu_{pp})}$, in which

$$K_1(\mu_{pp}) = e^{8.5 \cdot (\mu_{pp} - 0.2)}, \quad (21)$$

and,

$$f_1(\mu_{pp}) = 0.75 \cdot e^{1.2 \cdot (\mu_{pp} - 0.2)}. \quad (22)$$

The exponential form for these functions is chosen based on the shape of the data curve. The constants in these functions are determined by a best fit to the data points using the least squares method.

4.4 Effect of Particle-Wall Friction

The particle-wall friction coefficient affects particle flow and interaction, and therefore also affects particle breakage. The impact of particle-wall friction coefficient, μ_{pw} , on fragment mass fraction (sieve cut $AR \leq 5$) and normalized mean particle aspect ratio is shown in Figure 18. With a small particle-wall friction coefficient of $\mu_{pw} = 0.2$, the whole particle bed rotates like a single solid body with the impeller and no particle breakage occurs after an initial transient. Thus, fragment mass fraction and mean particle aspect ratio remain constant when $\omega t(P/\sigma_{ten}) > 0.001$ for $\mu_{pw} = 0.2$. With larger wall-particle friction coefficients, the tangential contact forces between particles and walls are increased and it is more difficult for the particles to slide on the wall surfaces. As a result, retarded flow zones are obtained close to the base and top walls, and the material is significantly sheared in the cell by the rotating blades. The fragment mass fraction increases and mean particle aspect ratio decreases with an increase in μ_{pw} .

Similar to what was done for the particle-particle friction coefficients, to collapse the curves for different particle-wall friction coefficients in Figure 18, the following correlations are assumed,

$$\text{Fragment Mass Fraction} = \text{function3} (K_2(\mu_{pw})[\omega t(P/\sigma_{ten})]^{f_2(\mu_{pw})}), \quad (23)$$

And,

$$AR_m/AR_m^0 = \text{function4} (K_2(\mu_{pw})[\omega t(P/\sigma_{ten})]^{f_2(\mu_{pw})}). \quad (24)$$

As shown in Figure 19, the collapse of particle breakage data with various particle-wall friction coefficients is achieved in the plots of fragment mass fraction and normalized mean particle aspect ratio as a function of the dimensionless term, $K_2(\mu_{pw})[\omega t(P/\sigma_{ten})]^{f_2(\mu_{pw})}$, in which,

$$K_2(\mu_{pw}) = e^{18.1 \cdot (\mu_{pw} - 0.7)}, \quad (25)$$

and,

$$f_2(\mu_{pw}) = 1.28 \cdot e^{2.5 \cdot (\mu_{pw} - 0.7)}, \quad (26)$$

where, again, the form of the functions is proposed based on the shape of data curves and the constants in the functions are determined by a least-squares best fit.

Finally, the effects of inter-particle friction and particle-wall friction may be combined in the form

$$\text{Fragment Mass Fraction} = \text{function5}(K(\mu_{pp}, \mu_{pw})[\omega t(P/\sigma_{ten})]^{f(\mu_{pp}, \mu_{pw})}), \quad (27)$$

and,

$$AR_m/AR_m^0 = \text{function6}(K(\mu_{pp}, \mu_{pw})[\omega t(P/\sigma_{ten})]^{f(\mu_{pp}, \mu_{pw})}), \quad (28)$$

in which,

$$K(\mu_{pp}, \mu_{pw}) = K_1(\mu_{pp})^{f_2(\mu_{pw})} K_2(\mu_{pw})^{f_1(\mu_{pp})}, \quad (29)$$

and,

$$f(\mu_{pp}, \mu_{pw}) = f_1(\mu_{pp})f_2(\mu_{pw}). \quad (30)$$

The fragment mass fraction and normalized mean particle aspect ratio are plotted as a function of $K(\mu_{pp}, \mu_{pw})[\omega t(P/\sigma_{ten})]^{f(\mu_{pp}, \mu_{pw})}$ in Figure 20. The curves of particle breakage results with various inter-particle and particle-wall friction coefficients collapse reasonably well using the chosen fitting functions.

The total work performed on the material is partially converted to particle kinetic energy, partially dissipated through particle-particle and particle-wall frictional contacts, and partially used to break the particles. The term inside the *function5*() and *function6*() in Eqs. (27) and (28) may be treated as effective work terms that contribute to particle breakage. Thus, the extent of particle breakage is a function of the effective work term, which is strongly dependent on the exponent term, i.e. the term involving particle-particle and particle-wall friction coefficients. Larger particle-particle and/or particle-wall friction coefficients lead to larger

exponent terms and, therefore, larger effective work terms. As a result, a larger extent of breakage is obtained. In other words, larger friction coefficients enable the input energy to break the particles more efficiently.

It should be noted that the correlations obtained from Eqs. (27)-(30) are valid for particle-particle friction coefficients between 0.2 and 0.5 and particle-wall friction coefficients between 0.2 and 1. In addition, these correlations were developed by varying a single parameter at a time from baseline values. They may not be valid when multiple parameters are varied simultaneously. The interaction of multiple parameters, including particle-particle friction and particle-wall friction, needs to be investigated in the future.

5. Concluding remarks

In this work, a particle breakage model based on the Discrete Element Method (DEM) is employed to numerically model high aspect ratio particle breakage. A particle in the DEM is represented by a string of spheres connected in a straight line using elastic bonds. Particle breakage is modeled by eliminating a bond if the tensile or shear stresses exceed the material strengths. Validation of the particle breakage model is performed against experimental tests of the breakage of blackboard chalk sticks subject to uniaxial compression. Good agreement is achieved between simulation and experimental results of the applied load and particle size distribution profile.

The validated model is thereafter applied to investigate particle breakage due to agitation by rotating blades. Using the numerical model, the evolutions of fragment mass fraction and average particle size are explored. The DEM simulation results show that particle breakage rate depends on the applied pressure, blade rotational speed, inter-particle friction, and wall-particle friction. As a larger weight is applied to compress the bulk solid bed, the particle-particle and particle-wall contact forces increase, leading to an increase in breakage rate. The breakage rate increases as the rotational speed of blades increases due to increased frequency of particle-blade interaction. However, the extent of breakage per blade revolution is independent of rotational speed. With a small particle-wall friction coefficient, the particle bed rotates like a solid body along with the agitation blades and particle breakage is minimal. With large particle-wall friction coefficients, however, retarded flow zones are obtained close to the base and top walls, and more particles are broken due to the large shear forces as the blades rotate. One of the most important findings from this work is that the fragment mass fraction and the average particle size can be expressed as functions of the input work performed by the blades, particle-particle friction, and particle-wall friction. The input work performed by the

blades is linearly proportional to the blade rotational speed, agitation time, and the applied pressure.

Some recommendations are made based on the present work for controlling particle breakage in industry. Particle breakage, at least in agitated filter dryers, generally needs to be avoided during pharmaceutical processing. Reducing pressure (by reducing the bed depth for example), particle-particle friction, and/or particle-wall friction can decrease the forces acting on particles and therefore reduce particle breakage. Using a smaller number of blade revolutions during drying and blending processes leads to less work done on the particles and can also reduce particle breakage. In contrast, efficient breakage or milling of large solids is desirable in the mineral processing. Increasing the applied stresses can increase particle breakage. Increasing the particle-equipment surface friction can promote shear flow of the material, rather than rigid-body-like flow, which also leads to an increase in contact forces and particle breakage.

Appendix A. Supporting information

The experimental setup and procedure for performing the three-point bending tests are included as supplementary material for the measurement of Young's modulus and tensile yield strength of blackboard chalk sticks.

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Figure 1. DEM simulation of collision of two flexible fibers with their major axes perpendicular to each other using the bonded particle model (Guo et al., 2015).

Figure 2. Experimental set-up of uniaxial compression of blackboard chalk sticks in a cylindrical container.

Figure 3. DEM simulation of the uniaxial compression of chalk sticks. The chalk sticks with aspect ratios (AR) greater or equal to six are colored in blue and the shorter ones are differently colored based on their aspect ratios.

Figure 4. Load applied to the punch or the top of the bulk material as a function of displacement of the punch or upper wall. The base case parameters in Table 1 are used in the DEM simulation presented in this figure.

Figure 5. Fragment length distribution under the compression load of 1023 N (230 lbf). The integral of probability density across an interval of fragment length gives the number fraction of the fragments within the same interval. The error bars represent the standard deviation of three separate tests with different initial configurations of particle bed in the container.

Figure 6 Effects of (a) particle-cylindrical wall friction, μ_{pc} , and (b) particle-flat wall friction, μ_{pw} on the fragment length distribution after compression.

Figure 7 Effect of particle bond damping coefficient, β_b , on the fragment length distribution after compression. The error bars represent the standard deviation of three separate tests with different initial configurations of the particle bed in the container.

Figure 8 Simulation of elongated particle breakage in an agitation cell: (a) cylindrical agitation cell with three rotating blades, (b) a number of elongated particles generated and deposited in the cell, (c) the particle bed is compressed by specifying a weight for the top wall, and (d) agitation occurs by rotating the blades about the central shaft at a constant angular velocity.

(a) $\frac{P}{\sigma_{ten}} = 1.69e-3$

(b) $\frac{P}{\sigma_{ten}} = 3.38e-3$

Figure 9 The evolution (in terms of impeller angular displacement ωt) of fragment mass fraction with various sieve cut particle aspect ratios (AR) under the normalized pressure $\frac{P}{\sigma_{ten}} = 1.69e-3$ (a) and $\frac{P}{\sigma_{ten}} = 3.38e-3$ (b). (small cell, $\mu_{pp} = 0.2$, $\mu_{pw} = 0.7$, $\omega = 60$ rpm)

(a) $\frac{P}{\sigma_{ten}} = 1.69e-3$

(b) $\frac{P}{\sigma_{ten}} = 3.38e-3$

Figure 10 Particle aspect ratio distributions under the normalized pressure $\frac{P}{\sigma_{ten}} = 1.69e-3$ (a) and $\frac{P}{\sigma_{ten}} = 3.38e-3$ (b). (small cell, $\mu_{pp} = 0.2$, $\mu_{pw} = 0.7$, $\omega = 60$ rpm)

Figure 11 The evolution (in terms of impeller angular displacement ωt) of (a) fragment mass fraction (sieve cut AR ≤ 5) and (b) normalized mean particle aspect ratio with the small and large cells under various applied pressures. ($\mu_{pp} = 0.2$, $\mu_{pw} = 0.7$, $\omega = 60$ rpm)

Figure 12 The variation of (a) fragment mass fraction (sieve cut $AR \leq 5$) and (b) normalized mean particle aspect ratio with elapsed time, t , for various impeller rotational speeds. (small cell, $\mu_{pp} = 0.2$, $\mu_{pw} = 0.7$)

Figure 13 The variation of (a) fragment mass fraction (sieve cut $AR \leq 5$) and (b) normalized mean particle aspect ratio with the impeller angular displacement, ωt , for various impeller rotational speeds. (small cell, $\mu_{pp} = 0.2$, $\mu_{pw} = 0.7$)

Figure 14 Collapse of particle breakage results with the small and large cells, various impeller angular speeds, and various applied pressures. The unit of ωt is rad. ($\mu_{pp} = 0.2$, $\mu_{pw} = 0.7$)

Figure 15 Torque acting on the impeller, T , as a function of impeller angular displacement, ωt , for different applied pressures (a) and change of the mean torque, T_{mean} , with the applied pressure, P/σ_{ten} . The line in this figure is a linear curve fit. (small cell, $\mu_{pp} = 0.2$, $\mu_{pw} = 0.7$, $\omega = 60$ rpm)

Figure 16 The variation of (a) fragment mass fraction (sieve cut AR ≤ 5) and (b) normalized mean particle aspect ratio with $\omega t(\frac{P}{\sigma_{ten}})$ for various inter-particle friction coefficients, μ_{pp} . The unit of ωt is rad. (small cell, $\mu_{pw} = 0.7$, $\omega = 60$ rpm, $\frac{P}{\sigma_{ten}} = 1.69e-3$)

Figure 17 Collapse of particle breakage data with various inter-particle friction coefficients, μ_{pp} . The functions K_1 and f_1 are given in the text. The unit of ωt is rad. (small cell, $\mu_{pw} = 0.7$, $\omega = 60$ rpm, $\frac{P}{\sigma_{ten}} = 1.69e-3$)

Figure 18 The variation of (a) fragment mass fraction (sieve cut $AR \leq 5$) and (b) normalized mean particle aspect ratio with impeller angular displacement, $\omega t(\frac{P}{\sigma_{ten}})$, for various wall-particle friction coefficients, μ_{pw} . The unit of ωt is rad. (small cell, $\mu_{pp} = 0.2$, $\omega = 60$ rpm, $\frac{P}{\sigma_{ten}} = 1.69e-3$)

Figure 19 Collapse of particle breakage data with various wall-particle friction coefficients, μ_{pw} . The functions K_2 and f_2 are given in the text. The unit of ωt is rad. (small cell, $\mu_{pp} = 0.2$, $\omega = 60$ rpm, $\frac{P}{\sigma_{ten}} = 1.69\text{e-}3$)

Figure 20 Collapse of particle breakage data with various inter-particle frictions, μ_{pp} , and various wall-particle friction coefficients, μ_{pw} . The form of the fitting functions K and f are provided in the text. The unit of ωt is rad. (small cell, $\omega = 60$ rpm, $\frac{P}{\sigma_{ten}} = 1.69\text{e-}3$)

Table 1 Parameters used in the uniaxial compression simulations

	High Aspect Ratio Particle Properties									Wall
	Sphere Diameter D_s (mm)	Particle Aspect Ratio AR	Particle Young's Modulus E_p (Pa)	Contact Damping Coefficient β_c	Particle Poisson's Ratio ν_p	Particle Density ρ_p (Kg/m ³)	Particle-Particle Friction (μ_{pp})	Particle-Cylindrical Wall Friction (μ_{pc})	Particle-Flat Wall Friction (μ_{pw})	Cylindrical and Flat Wall Young's Modulus E_w (Pa)
Base Case	10	8	527.6 e6	1.59 e-2 (for particle- particle contact); 3.18 e-2 (for particle- wall contact);	0.3	1570	0.624	0.35	0.4	1.0 e9
Other Values Used	NONE	NONE	NONE	NONE	NONE	NONE	NONE	0.1, 0.5	0.1, 0.6	NONE

	Bond Properties					
	Diameter D_b (mm)	Length l_b (mm)	Bond Young's Modulus E_b (Pa)	Bond Damping Coefficient β_b	Bond Poisson's Ratio ν_b	Tensile Strength σ_{ten} and Shear Strength τ_{sh} (Pa)
Base Case	10	10	527.6 e6	4.20 e-2	0.3	3.99 e6
Other Values Used	NONE	NONE	NONE	8.87 e-2, 1.41 e-1	NONE	NONE

Table 2 Parameters used in the agitated bed simulations

	Agitation Cell	High Aspect Ratio Particle Properties							
	Diameter D_c (mm)	Sphere Diameter D_s (mm)	Particle Aspect Ratio AR	Particle Young's Modulus E_p (Pa)	Contact damping coefficient β_c	Particle Poisson's Ratio ν_p	Particle Density ρ_p (Kg/m ³)	Particle-Particle Friction (μ_{pp}) and Particle-Cylindrical Wall Friction (μ_{pc})	Particle-Flat Wall Friction (μ_{pw}) and Particle-Blade Friction (μ_{pb})
Base Case	122 (small cell)	5	10	2.68e9	1.59 e-2 (for particle-particle contact); 3.18 e-2 (for particle-wall contact);	0.3	1500	0.2	0.7
Other Values Used	244 (large cell)	NONE	NONE	NONE	NONE	NONE	NONE	0, 0.05, 0.1, 0.15, 0.3, 0.4, 0.5	0.2, 0.3, 0.4, 0.5, 0.6, 0.65, 0.75, 0.85, 1.0

	Bond Properties					
	Diameter D_b (mm)	Length l_b (mm)	Bond Young's Modulus E_b (Pa)	Bond Damping Coefficient β_b	Bond Poisson's Ratio ν_b	Tensile Strength σ_{ten} and Shear Strength τ_{sh} (Pa)
Base Case	5	5	2.68e9	4.2 e-2	0.3	12.3e6
Other Values Used	NONE	NONE	NONE	NONE	NONE	NONE

	Blade Properties				Operating Parameters					
	Blade Length L_{bl} (mm)	Blade Width W_{bl} (mm)	Blade Young's Modulus E_{bl} (Pa)	Blade Poisson's Ratio ν_{bl}	Number of Initial Elongated Particles	Normalized Applied Pressure P/σ_{ten}	Angular Velocity of Blades ω (rpm)	Position of Blades from the Base h_{bl} (mm)	Number of Blades	Pitch Angle of Blades θ (degree)
Base Case	61 (small cell)	10	2.68e9	0.3	250	1.69e-3	60	15	3	60
Other Values Used	122 (large cell)	NONE	NONE	NONE	750, 1500	8.45e-4, 3.38e-3	30, 120	NONE	NONE	NONE

Graphical Abstract

This article presents a computational study of the breakage of high aspect ratio particles subject to mechanical agitation using the Discrete Element Method (DEM), in which a particle, represented by a string of bonded spheres, breaks at the center of a bond where the tensile or shear stress exceeds the material strength. The model is validated and used to investigate particle breakage when agitated by rotating blades, which is encountered in a range of pharmaceutical processes. The simulation results show that the breakage rate, that is the rate of particle size reduction (or the rate of fragment mass increase), increases as the applied pressure, impeller rotational speed, particle-particle friction, or particle-equipment friction increases. It is found that the extent of particle breakage is a function of the work performed on the material, and the parameters in this function depend on the particle-particle and particle-wall friction coefficients. The large friction coefficients enable the input energy to break the particles more efficiently.