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The internal loads, moments, and stresses in rod-like particles in a low-speed, vertical axis mixer

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HIGHLIGHTS

- New model for predicting internal loads, moments and stresses in rod-like particles.
- Predictions made for varying particle properties and process conditions in a mixer.
- Maximum absolute principal stresses fit well with a Weibull distribution.
- Largest stresses occur at particle center-plane and circumference on average.
- Stresses increase with aspect ratio and fill; friction and speed not as important.

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ABSTRACT

A discrete element method (DEM) model is used to predict the internal load and moment distribution within rod-like particles in a low-speed, vertical axis mixer. The internal loads and moments are combined with small deformation beam bending theory to determine the internal stress distributions. Parametric studies using the model examined the influence of particle aspect ratio, blade rotational speed, and material properties. The spatial distributions of loads and moments, averaged over all particles and time steps, are symmetric about the particle center-plane with a maximum at the particle center-plane. In addition, the largest average maximum absolute principal stress is observed to occur along the particle circumference at the center-plane of the particle. These results indicate that particle failure is not only most likely to occur at the center-plane of the particle, but the failure will begin at the particle's circumference. The largest average loads, moments, and maximum absolute principal stress increase with particle aspect ratio. The frequency distributions of maximum absolute principal stress at the high stress range are fit well with a Weibull distribution. Increasing blade speed, bed height and particle–particle friction coefficient generally lead to an increase in internal loads, moments, and stresses. The largest maximum absolute principal stresses occur at the base of the mixer and in front of the blades near the mixer circumference where the bed depth is the greatest.

1. Introduction

Vertical-axis mixers, such as high shear granulators and agitated filter dryers (AFDs), are commonly used in the processing of particulate materials. In an AFD, active pharmaceutical ingredient (API) particles produced by crystallization are filtered, washed, and dried. During the drying process, an impeller blade agitates the bed to increase the drying rate and enhance drying uniformity. Unfortunately, the rotating blade can also frequently lead to unwanted particle breakage or attrition, which can impact the properties of the bulk powder, such as particle size distribution, flowability, bulk density, segregation behavior, and dissolution rate, which, in turn, can lead to deleterious manufacturing and product performance.

Numerous experimental and computational studies have been performed to investigate the influence of impeller speed, fill level, mixer size, blade angle, particle size distribution, and inter-particle friction and cohesion on particles in a mixer. These studies have provided excellent insight into how particles move in such systems; however, the work on particle attrition, especially quantitatively predictive work, is limited. Previous experimental work

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has generally involved the reporting of trends or empirical correlations. Computational work has typically assumed spherical particles, although many particles, such as the API materials typically processed in AFDs, are rod-like in shape. In addition, only a handful of studies have investigated the loading state within individual particles. Having such information would be particularly useful when investigating particle breakage.

In this paper, a novel approach is proposed for predicting the internal load, moment, and stress distributions within individual rod-like particles. This model is used to examine how these distributions change as particle aspect ratio, material properties, and operating conditions vary for particles in a vertical-axis mixer. These distributions are particularly useful when combined with standard material failure theories to predict particle breakage rates and resulting size distributions.

2. Background

There have been numerous studies, both experimental and computational, concerning particle movement and mixing in vertical-axis mixers. A detailed review can be found in the background section of Hua et al. (2013). Here, the focus is on particle attrition in vertical-axis mixers, with additional discussion concerning the modeling of rod-like particles.

2.1. Particle attrition in vertical axis mixers

Particle attrition in vertical axis mixers has been studied using both experimental and computational methods. The experimental studies are presented first followed by the computational studies.

Lekhal et al. (2003, 2004) examined the change in mean particle size within an AFD for two types of material: cubic crystals of KCl and needle-shaped crystals of L-threonine. They found that for both materials, attrition only became significant when the moisture content in the materials was below a threshold value, i.e., when the material was nearly dry. They also observed that for KCl, the size decrease was not sensitive to agitator speed, but the size decrease for the L-threonine was. For both materials, size decreased with the number of agitator revolutions and approached a constant value after a large time, most likely because the crystals either became sufficiently rounded in the case of cubical KCl, or the L-threonine needles broke to a small enough aspect ratio that the loads were no longer sufficient to continue breakage.

Lamberto et al. (2011) developed an attrition cell for assessing API sensitivity to mechanical stress in an AFD. The attrition cells were similar in design to a scaled-down AFD. A small amount of material was characterized, placed in a narrow cylinder, and a movable lid was placed on the material's surface. A load was applied to the lid to mimic the weight of overlying material. The material in the cylinder was then agitated by a rotating blade, similar to what would occur in an AFD. After a specified amount of time, the material was characterized again and an attrition measure was calculated. Lamberto et al. utilized the change in mean particle size to characterize the attrition of materials and ranked the materials with a breakage classification (hard, medium, or easy to break), which was used as a guide for how to process at larger scale.

Am Ende et al. (2013) performed similar experimental work. They assessed materials utilizing an FT4 powder rheometer with a rotating agitator located at the end of a vertical shaft, which also applied a specified normal load. This device was similar in design to the attrition cell discussed in the previous paragraph. Compared with Lamberto et al. (2011), this group not only ranked materials according to attrition potential, but also investigated the influence of different operating parameters on material attrition, including blade speed, agitation time, sample volume, and applied normal force. They reported that increasing blade speed, agitation time, or normal force led to more attrition, with normal force being the most significant factor. The attrition cell data showed reasonable agreement with data from a pilot plant AFD.

Hare et al. (2011) described a combined discrete element method (DEM)-experimental approach to predict the extent of paracetamol particle breakage due to impeller agitation. Spherical particle DEM simulations of a small-scale, agitated dryer were performed to determine the normal stresses and shear strains in various parts of the particle bed. The data were combined with the attrition correlation of Neil and Bridgwater (1994) to predict total attrition within the dryer, with the correlation parameters fit from annular shear cell experiments. The predictions showed reasonable agreement with a corresponding agitated dryer experiment. In addition, Hare et al. reported that in both the simulations and experiments, the total bed attrition was independent of impeller speed for a given number of impeller revolutions, i.e., the attrition was a function of total strain and not of strain rate. This result was consistent with the findings of Am Ende et al. (2013) and Lekhal et al. (2003, 2004). Moreover, the simulation demonstrated that more than 50% of the attrition occurred in the bottom third of the bed, toward larger radial distances, and in the vicinity of the mixer blade.

More fundamental studies on multi-particle attrition frequently relied on the use of shear cells rather than vertical axis mixers. In most instances, these studies utilized spherical or angular particles as opposed to rod-like particles. In general, these studies measured bulk attrition rates and particle size distributions and attempted to relate these quantities to material or operating parameters (e.g., Gwyn, 1969; Neil and Bridgwater, 1994; Potapov and Campbell, 1997; Paramanathan and Bridgwater, 1983; Bridgwater et al., 2003; Ning and Ghadiri, 2006).

In addition to these bulk level studies, there have been investigations focused on particle attrition and breakage at the particle level using computational methods. Of particular interest in these studies is that the simulated particles can be damaged directly in the simulations. For example, Potapov and Campbell (1997) performed 2D DEM shear cell simulations using initially square particles that were comprised of a collection of bonded Delaunay triangles. When the load on a bond exceeded a critical value, the bond was broken and thus the particle could attrit over time. Thornton (1999) and others (Mishra, 2001; Kafui, 2000) examined particle, or more aptly, agglomerate, breakage due to crushing and impact using a similar technique. These DEM agglomerates were roughly spherical in shape, with the bonded elements consisting of smaller spheres. As with Potapov and Campbell, when the bond load exceeded a critical value, the bond would break. The approach of using "glued spheres" with breakable bonds is now a common method in DEM for studying attrition and breakage problems (see, for example, Liu, 2010; Antonyuk, 2011; Nguyen, 2014).

2.2. DEM simulations of rod-like particles

Few previous DEM studies have incorporated rod-like particles. Due to the additional computational time required for contact detection, most researchers perform DEM simulations using spheres rather than more realistic particle shapes. Those simulations that do incorporate more complex shapes generally rely on the use of glued sphere approximations, which provide the simplicity of sphere–sphere contact detection and the flexibility of generating a wide variety of particle shapes, but at the cost of artificially rough particle surfaces (Kodam et al., 2009; Gallas and Sokolowski, 1993; Nolan and Kavanagh, 1995; Price et al., 2007), smaller coefficients of restitution (Kodam et al., 2009), and the