ABSTRACT

Hua, Xia Ph.D., Purdue University, December 2014. Modeling the Dynamics and Stresses of Elongated Particles in Vertical Axis Mixers. Major Professor: Carl R. Wassgren, School of Mechanical Engineering.

Vertical axis mixers, such as high shear granulators and agitated filter dryers (AFDs), are commonly used in the processing of particulate materials. For example, AFDs are regularly used in the pharmaceutical industry to dry the wet active pharmaceutical ingredient (API) particles. During the drying process, an impeller blade agitates the bed to increase the drying rate and enhance drying uniformity. Unfortunately, the needle-shaped API particles tend to flow poorly, are frequently damaged, and can sometimes form undesirable agglomerates, causing manufacturing inefficiencies, flow stoppages, and unpredictable product quality. Therefore, it is important to gain an improved understanding of the system's particle behavior to aid in the design and optimization of unit operations. Previous work in vertical axis mixers, especially prior computational work, has assumed spherical particles. This thesis focuses on modeling and analysis of dynamics and stresses of elongated particles processed in vertical axis mixers. Elongated particles are of particular interest in the operation of pharmaceutical AFDs since the particles processed in such devices are often needle-shaped.

A discrete element method (DEM) model is used to examine the velocity, solid fraction, and particle orientation fields of non-cohesive, sphero-cylindrical particles agitated in a vertical axis mixer for a range of particle aspect ratios and bed depths. The model is validated against experimental measurements of the rotating shaft torque and bed surface velocity field. The particle trajectories within the bed are similar to those that have been reported previously for spheres, with a vortex circulating in the direction opposite of the blade rotation on horizontal planes of the bed. Increasing the particle aspect ratio generally decreases the particle velocities relative to the blade, implying reduced mixing. The solid fraction is largest just upstream of the blades and toward the base of the container. The former finding is different than what has been observed for spheres, but the latter is consistent with prior observations. The smallest solid fractions are located in the wake region and at the bed's free surface, which is similar to the patterns for spheres. In general, larger particle aspect ratios decrease the overall bed solid fraction as well as the solid fraction uniformity. Particles with an aspect ratio larger than one have major axes that are offset between 10 – 20 degrees from the flow streamlines. The degree of alignment between particles increases near boundary regions. In addition to the strong correlation between the particle principal orientation and velocity vectors, regions of larger velocity gradient magnitude result in smaller solid fractions and smaller degrees of three-dimensional alignment between particles.

In addition, the DEM model is used to predict the internal load and moment distribution within sphero-cylindrical 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 principal stress or Mises 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 occur at the particle's circumference. The largest average values of loads and moments increase with particle aspect ratio. The largest average maximum principal stress and Mises stress both increase with increasing particle aspect ratio. The trend of largest average maximum principal stress or Mises stress appears to have a positive curvature, which follows the trend of largest average bending moment most closely. The frequency distributions of maximum principal stress at high stress range can be fit to a Weibull distribution. Increasing blade speed, bed height and particle-particle friction coefficient generally leads to an increase in internal loads, moments and stresses, i.e. more particle breakage.