ABSTRACT

Kumar, Rohit Ph.D., Purdue University, August 2018. Predicting Breakage of Needle-shaped Large Aspect Ratio Particles Using Discrete Element Method (DEM). Major Professor: Carl Wassgren, School of Mechanical Engineering.

Particle attrition is inevitable during processing of granular material and has been reported to cause manufacturing inefficiencies, unpredictable product quality, dust hazards, flow problems, etc. Of particular interest to this study is attrition of large aspect ratio needle-shaped active pharmaceutical ingredients (APIs) in an agitated filter dryer (AFD). Prior experimental works on particle attrition in AFDs have been successful at predicting the overall bulk behavior. However, for an in-depth understanding of the attrition phenomenon, particle level kinematics and dynamics information is required. The particle level details can be obtained through computational discrete element method (DEM) models, but most of the previous DEM studies have either assumed spherical particles or have not incorporated actual particle breakage. This thesis proposes a state-of-the-art particle breakage model to predict breakage of needle-shaped particles, utilizing spherocylinder geometry, in agitated systems. Needle-shaped particles are of particular interest since the API particles obtained from crystallization process often have large aspect ratio.

Particle breakage occurs due to stresses developed in the particle from particle-particle and particle-boundary contacts. Therefore, it is important to examine different normal force model and use an accurate contact force model to be able to predict particle breakage correctly. In this study, the effect of three different contact force models on various aspects of static and dynamic assemblies of spherocylinders is investigated. Three force models investigated were: (i) a Hertzian force model (HFM) which assumes a circular contact area; (ii) a linear overlap force model (LFM) with a constant stiffness; and (iii) a modified HFM (MFM) that accounts for various contact

areas and contact transitions. Comparison of the contact force, contact overlap, contact duration, normal specific impact energy, and orientation distributions are made, as well as the particle packing fractions and blade torques. These investigations revealed that for non-cohesive powders the contact force models have no significant impact on the contact force distributions and bulk properties, such as blade torque, particle orientation, and solid fraction, and a simple model can be used for force calculations. However, if more detailed contact information, such as contact area, contact overlap, contact duration, impact energy, or collision frequency, are needed, then a more accurate contact area specific force models should be used. Previous studies have shown that particle attrition only becomes significant when the moisture content in the powder is very small, indicating that attrition becomes significant for non-cohesive powders. Therefore, in this study, a simplified Hertzian force model is used.

Additionally, a state-of-the-art DEM particle breakage model has been developed to simulate the breakage of needle-shaped particles. Forces and moments are calculated at multiple imaginary breakage planes on the particle, which are then used to calculate the maximum normal and shear stress. If the maximum normal or the maximum shear stress exceeds the particle yield strength then the particle breaks at the given breakage plane. The breakage model is validated by comparing the simulation results with experiments of cylindrical chalk sticks under uni-axial compression. This model is used to examine different aspects of particle breakage in a small scale AFD. It is observed that smaller particles after breakage get deposited around the blade and at the bottom of the container. Most of the particle breakage occurs at the blade tip near the circumference of the cylindrical container of the AFD. Investigations also revealed that the initial particle aspect ratio characteristics don't affect the resulting particle aspect ratio characteristics, provided that enough work is done on the particle bed. The extent of particle breakage increased with increment in particle elastic modulus and load of the overlying material, and decrement in particle yield strength. It is found that the extent of particle breakage increased with the number

of blade revolutions but remained the same per blade revolution. Impact of initial particle aspect ratio characteristics, material properties, and operating conditions are also examined on particle specific breakage rate and daughter particle distribution. Particle specific breakage rate increased with increment in elastic modulus and load of the overlying material, and decrement in particle yield strength. Initial particle aspect ratio characteristics didn't have any influence on the specific breakage rate. Investigations on the daughter particle distribution showed a self-similar behavior, with breakage frequently occurring at the particle center, and are independent of initial particle aspect ratio characteristics, material properties, and operating conditions. The specific breakage rate and the daughter particle distribution information from DEM simulation is utilized in a population balance model (PBM) to predict the resulting particle size distribution (PSD) for extended time periods. The PSDs obtained from PBM fit well with log-normal distribution, which is frequently used to define the PSD of real powders. The PBM predictions are verified by comparing the PSDs obtained from the PBM to that obtained from the DEM.