Comparison of Models for Coarse Particle Shape Evolution During Attrition in a Stirred Vessel

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Abstract

Particle breakage in stirred vessels is usually modeled using population balance equations (PBEs) to describe the evolution in particle size with time. Although shape has a strong effect on the particle properties and final product quality, changes in the particle shape distribution are often neglected. To account for changes in both size and shape simultaneously, a bivariate population balance must be used. This requires a bivariate breakage distribution function that accounts for the observed size and shape evolution in actual systems. Although bivariate breakage distribution functions have been developed that meet the constraints of mass conservation and exchangeability [1], they are not based on the fundamental physics of particle attrition. It is necessary to develop breakage distribution functions based on fracture mechanics that meet the constraints.

Two models have been developed – one by Gahn and Mersmann [2-3] and one by Ghadiri and Zhang [4-5] – that use fracture mechanics to predict the total particle volume lost due to attrition. The objective of this research is to test and compare the two theories to determine if they can explain the changes in particle size and shape due to attrition. This work focuses only on the larger particles, not the fines. This information is incorporated into the PBEs by including it in the breakage distribution function. Starting with the original coarse particle size and shape, the model accounts for the material removed from the parent particles due to attrition. The approach is to model the breakage distribution function as a bivariate function of the particle volume and the shape factor. A comparison of both models with experimental results for several systems is presented.

This work has wide applicability in that it directly affects any unit operation involving solids breakage in stirred vessels. This includes both stirred reactors with solid particles as well as crystallizers.

Previous Work

Gahn and Mersmann [2, 3] developed a physical attrition model based on a set of assumptions and on the material properties of hardness, fracture resistance, and the quasi-isotropic elastic constant. This work was based on the impact of a crystal with a hard surface such as an impeller. With this method, the number of fragments generated could be estimated as well as the minimum and maximum particle sizes. In addition, the volume of material abraded from a single particle, V_a, was predicted from the Vickers' hardness (H_v), the shear modulus (μ), the fracture resistance (Γ), the efficiency factor (K), and the plastic deformation work for a given particle (W_{pl}). In later work [6] this attrition model was applied to a crystallizer where both growth and breakage were occurring simultaneously. While these models quantitatively address the size distribution, they do not address particle shape.

A mechanistic model of impact attrition was developed [4, 5] based on fracture mechanics and physical properties such as hardness (H), fracture toughness (K_c), the characteristic particle length (l), and particle density (ρ) as well as the impact velocity (v). In this work the researchers developed an expression for the volume fraction of a particle lost due to impact, ξ. This expression used an experimentally obtained constant, α, and an attrition propensity parameter. The constant α was measured experimentally (Zhang and Ghadiri, 2002) for three materials: NaCl, KCl, and MgO. All of these studies were done with impact tests but not in a stirred vessel.

Theoretical Work

The two theories are compared to determine if they can explain the changes in particle size and shape due to attrition. This work focuses only on the larger particles, not the fines. Since the work of Ghadiri and Zhang [4, 5] only considers impact tests, it is necessary to adapt their work to breakage in a stirred vessel.

If the original volume of the parent particle is known, then the change in actual parent particle volume can be calculated by subtracting the volume lost due to attrition. This volume loss due to attrition changes the shape factor of the parent particle. Since both theories consider the contact of a crystal corner with a hard surface such as an impeller and since they consider materials that are more prone to attrition than to fragmentation, the experimental tests will focus on crystals with corners that are prone to attrition.

Experimental Method

Crystallization experiments were performed in a LabMax automated laboratory reactor system manufactured by Mettler-Toledo. This system includes a 1 liter jacketed glass vessel with an upflow impeller stirrer, a temperature control system, and a data acquisition system. A Julabo chiller provided cooling fluid for the LabMax. The computer included with this system controled the temperature of the vessel contents by controlling the temperature of heat transfer fluid circulated through the vessel jacket. The temperature of the vessel contents was measured by a PT-100 temperature probe and recorded.

Since many size analysis methods such as sieving only give a single particle dimension, image analysis was used to measure the aspect ratio of individual crystals. Image analysis was performed using a polarized light microscope with a data acquisition system. This system included a camera mounted on the microscope that connected to a computer with image analysis software.

In order to produce repeatable data, it was necessary to examine at least 900 particles from each experiment. Tests were performed more than once to check the repeatability of the data. Tests were performed with several systems including the sodium chloride/water system.

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