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Mathematical Modelling of the Evolution of the Particle Size Distribution during Ultrasound-Induced Breakage of Aspirin Crystals

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Highlights

- A mathematical model is derived for the crystal breakage that results from ultrasound
- Population balance models are developed for three models of binary breakage events
- Dependencies of cavitation rate on applied power and solvent viscosity are provided
- Agreement with experiments is good for aspirin crystals undergoing sonofragmentation
- Analysis supports the model in which crystals break into two equal-sized particles

Abstract

While the effects of ultrasound on crystals have been heavily investigated experimentally, population balance models that describe the effects of all physical parameters such as solution viscosity and applied power on the crystal size distribution have been lacking. This article presents one of the first population balance models for describing the crystal breakage that results from ultrasound. Aspirin crystals dispersed in various solvents, dodecane and silicon oils of known viscosity, were subjected to ultrasound to study this sonofragmentation that occurs due to cavitation when bubbles violently collapse, creating extreme conditions in the immediate vicinity of the bubbles. Population balance models are developed with three models for binary breakage events and cavitation rate proportional to the applied power and exponentially related to solvent viscosity. The resulting population balance models provide reasonable agreement with the experimental data over the ranges of applied power and solvent viscosity investigated, with nearly overlapping crystal size distributions for applied power between 10 and 40 W. The statistical analysis supports the breakage model in which cavitation bubbles cause the aspirin crystals to break into two equal-sized particles.

Keywords: ultrasound; population balance modeling, crystallization; particle technology; kinetics estimation

1 Introduction