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Abstract

The topic of this work is the dynamic modeling and observation of polyhedral, growing crystals. This is motivated by the fact that besides size, shape is an important product property for particulate materials in various industries. Due to the underlying anisotropic molecular crystal structure, growth proceeds at different rates in different directions. Therefore, crystals assume a non-spherical, polyhedral, though, under ideal conditions also a symmetric shape. The work at hand is essentially divided into three major parts. At first, a system-theoretic framework is introduced and applied to describe the evolution of single crystals and of crystal populations. In the second part the extraction of shape information from suspension images is discussed. This data is finally used to determine growth kinetics enabling the description of the conducted experiments with the developed models.

It is shown that models decribing the development of a single crystal exhibit hybrid dynamics if the number of faces changes. In order to transfer this property to the population level, the class of systems that can be captured with population balances is widened to hybrid systems. Such systems are capable of performing switches in their velocity field or jumps in their state space. It is pointed out that different crystal morphologies exist in different parts of the state space, the so called morphology cones. On the bounding elements of the morphology cone hybrid dynamics is induced. It turns out that the morphology cones do not cover the whole state space and thus the computational time for the solution of evolution equations is reduced.

The shape evolution modeling studies are then augmented by the development of a crystal shape observation scheme. 3D shape descriptors of crystal populations cannot be measured directly with current devices. Therefore, an image processing routine is assembled that reduces 2D grayscale images of the crystal suspension so that individual particle projections are extracted. The estimation scheme to obtain the 3D shape is validated against synthetic (in-silico) image data. It is shown that the time-dependent shape distribution function of the synthetic images is reconstructed accurately. Also growth kinetics that control the shape evolution can be extracted from the image data. Since this is successfully tested on synthetic image data, the method is applied to observe the batch cooling crystallization of potassium dihydrogen phosphate. Two experiments are used to determine the supersaturation-dependent, face-specific growth rates. The obtained growth rates are cross-validated against the mass balance and independently conducted experiments.

Employing the developed techniques allows for a rigorous population balance modeling of crystals taking polyhedral shape into account. On the basis of the image-based crystal observation scheme, it is possible to determine face-specific growth rates. The so equipped population balance model can be included in a process model for crystallization and used to reproduce and predict the outcome of crystallization experiments.