Donnerstag 19. Juli 2012

13:30 Uhr, Hörsaal H1

Zeit- und Raumänderung

Controlling the Morphology Evolution of Crystals: Modeling and First Experiments

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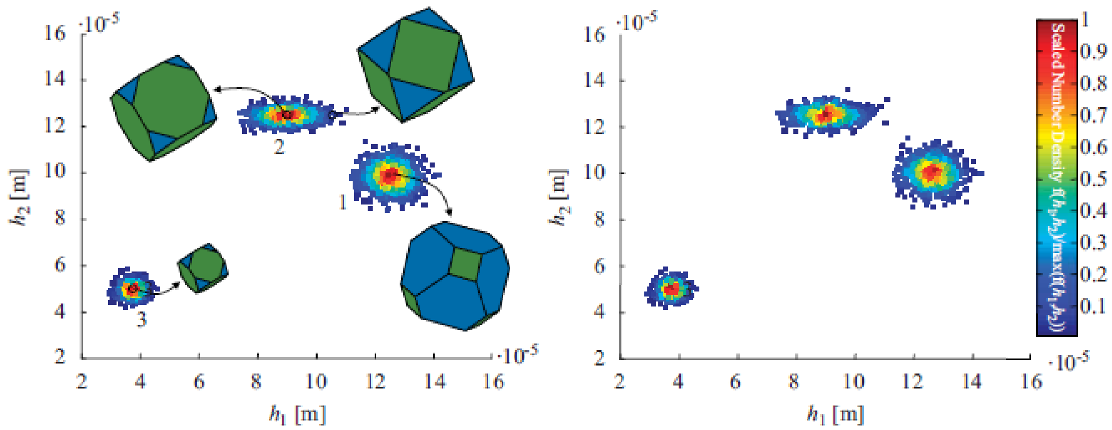

Fig. 1. Estimation of a trimodal crystal population consisting of 1000 crystals for each of the three populations. Left: scatter plot of samples from the original population including graphical representations of selected crystal morphologies. Right: scatter plot of the estimated population.

About 60% of all products produced by chemical companies are delivered as solids, among them many crystalline materials. Virtually all pharmaceutical production processes involve a crystallization step and most active pharmaceutical ingredients are administered in a crystalline form. Crystalline pharmaceuticals, agrochemicals, cosmetics and fine chemicals are high value added products for which crystal shape is an important quality factor. Examples where shape has been of interest range over the whole palette from bulk chemical products over nanoparticles to catalysts. Though it is well known that properties of dispersed phase products are strongly linked to their shape, process engineering research was so far focused on particle size and size distributions and only during the last years efforts have been started to include quantitative measures for shape and shape distributions, see e.g. Bajcinca et al. (2010), Borchert et al. (2009), Briesen (2006), Chakraborty et al. (2010), Kempkes et al. (2010) and Ma et al. (2002).

The understanding of a complex process requires a realistic and thus physically interpretable model. The dynamics of dispersed phase processes are at best captured with population balance equations. Modeling and numerical solution of population balance models accounting for crystal shape has been discussed in the literature as well, e.g. Borchert et al. (2009a,b), Briesen (2006) and Ma et al. (2002, 2008).

The observation of crystal shapes using video microscopy has been investigated by different groups, e.g. Eggers (2008). The improvement of the quality of the measurements can in principle be done via the enhancement of the image quality or further development of post- processing algorithms. That is, either the hardware of the sensor is improved or extended or processing algorithms for image analysis are equipped with advanced techniques in order to apply it to data acquired from the (commercially) available equipment. In principle, the evolution of crystal shape distributions can be observed in experiments and simulations ofprocess models can be performed. Though the coupling of observation and simulation opens a wide field of applications in crystallization, e.g. optimization of control strategies and estima- tion of kinetic parameters with regard to shape and size, only few work in this direction has been published, e.g. Patience and Rawlings (2001) and Wang et al. (2008).

Given the fact that microscopic images can be acquired, the questions the present contribution aims to answer are: How can crystal projections easily be related to the crystal's 3D body in order to measure the shape distribution of a population in terms as it is used in the model? How reliable is this information with regard to the identification of the growth kinetics of individual crystal facets, and with regard to the implementation of shape control algorithms?

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