TOWARDS CONTROL OF CRYSTAL SHAPE. CRYSTALLIZATION AND DISSOLUTION.

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Crystalline materials are of considerable interest to diverse applications such as in pharmaceutical products, catalysts, solar cells, nanotechnology and so on. The properties that serve the application are closely linked to crystal morphology which has spurred noticeable activity in recent times in the literature [1-3] to explore the extent to which shapes can be subject to rational manipulation using mathematical models. It will be the purpose of this presentation to provide a panoramic view of issues in the modeling of crystal shape distributions towards the design and control of products with consequently enhanced properties relevant to the application.

Modeling the dynamics of crystal shape in a crystallization process involves tracking the shape evolution of single crystals as well as how the population acquires a distribution of shapes in a supersaturation environment that is influenced by the collective growth of all crystals in the population. As shape control implies preference for asymmetry, population balance models must contend with high dimensionality of the number density by finding ways to exploit any residual aspects of symmetry.[4] The formulation complete with transitions between different morphologies will be presented with examples including model fitted parameters through analysis of images from hot stage microscopy. For example, the dissolution images of succinic acid can be used to obtain the polar plots of dissolution rates at different undersaturations.

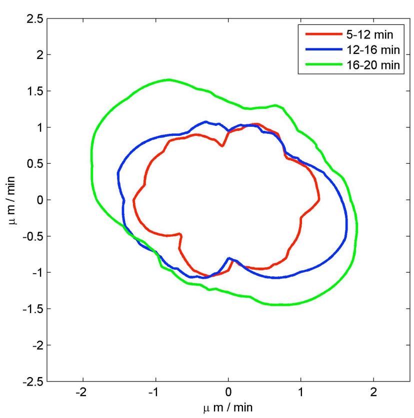

Figure 1. The polar plot of dissolution rates calculated from the timeline images of the dissolution of succinic acid taken from Snyder et al. [5]

The shape of polar plots depends on the atomic structure of the crystalline materials and the environmental conditions. It is shown that the surface evolution equations subjected to the polar plots of growth/dissolution rates can be used to determine the shape evolution of single crystals.

The success of such a modeling effort clearly depends upon concomitant developments in measurement techniques for not only the morphology of single crystals but also that of distributions of the same in a population.[6] A description of morphology is presented which together with confocal microscopy is shown to possess the speed to obtain morphology distributions. The strategy to measure crystal morphology is briefly described in Figure 2 which involves acquiring tomographic images of crystals using confocal microscopy followed by image processing and analysis.

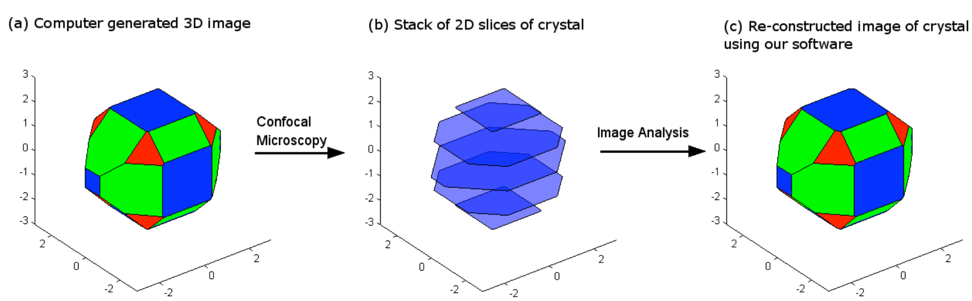

Figure 2. The methodology to measure morphology of 3-D crystal

As an example application of the methodology under development, we focus on producing crystals with shapes that would reduce dissolution times of the product, an issue with pharmaceuticals. An illustrative example of dissolution of square crystal, presented in Figure 3, shows that the dissolution flux increases with time as crystal shape is changing incorporating more fast dissolving faces. As such a demonstration will also call for modeling the dissolution process, we address population balance modeling of dissolving crystals which has some features in remarkable contrast to those of crystallization. While industrial practice has numerous other strategies for manipulation of crystal products, we believe that the methods presented herein could contribute to their implementation in a quantitative way.

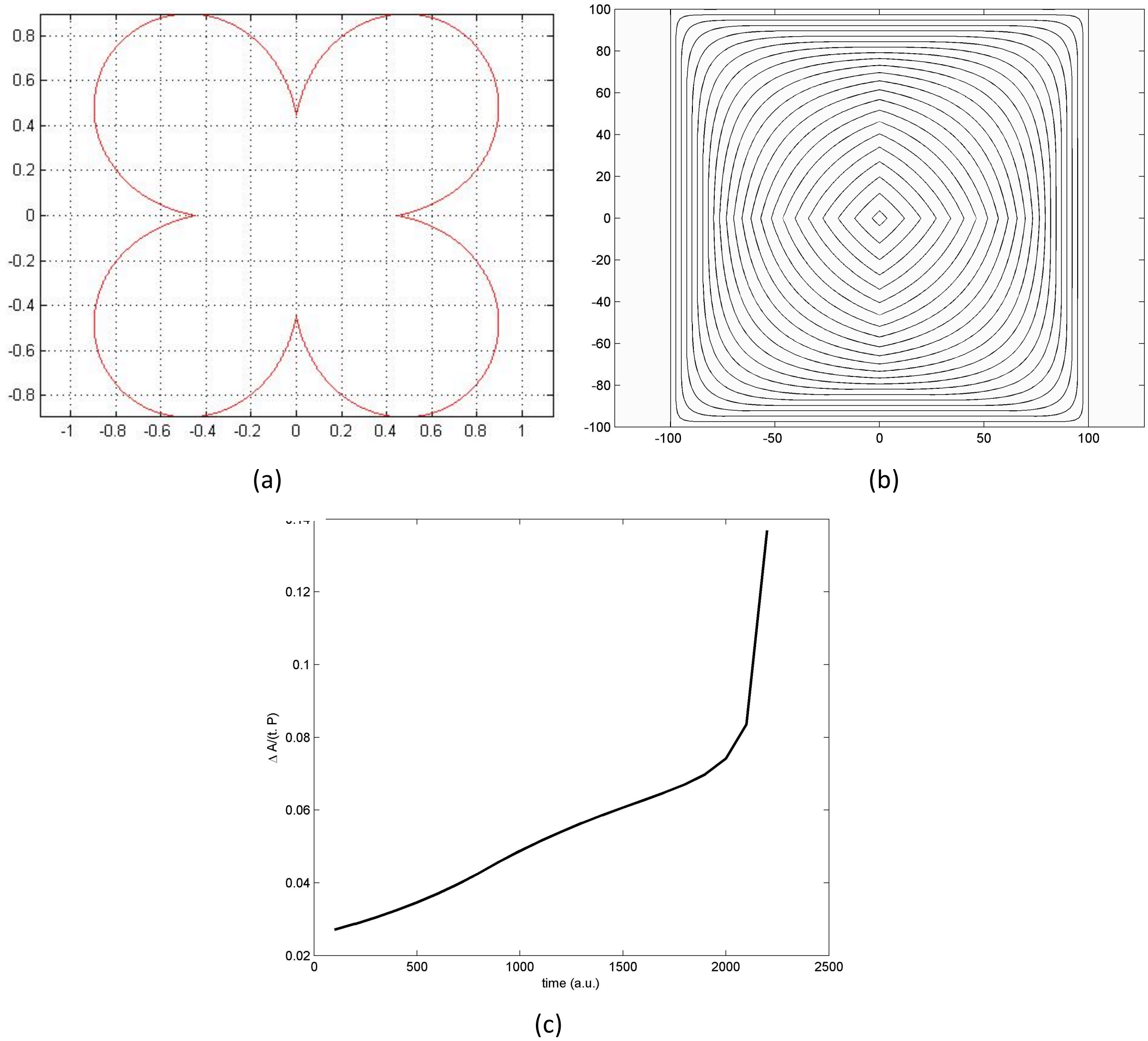

Figure 3. An illustrative example showing the effect of crystal shape on dissolution flux. a) the polar plot of dissolution rates, b) evolution of crystal shape subjected to dissolution rate in a, c) dissolution flux increasing with time as crystal shape is evolving.

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