Estimation of the Geometrical Variations of the Typical Grain within a Boolean Model

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Abstract:
The knowledge of the shape and size distributions of solid particle populations has been of increasing interest (both theoretical and practical) over the last decade. More particularly, crystals in liquid suspension are frequently used in industrial processes (e.g. for pharmaceutical technology) and is one of the LGF CNRS laboratory preoccupations. Their geometrical characterization is required for exploring the physico-chemical properties of crystallization processes. Using an in-situ camera, it is possible to get images of such crystal populations (as exposed in the following figure).
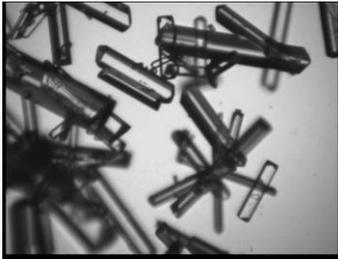
Ammonium oxalate crystals (Optical imaging)
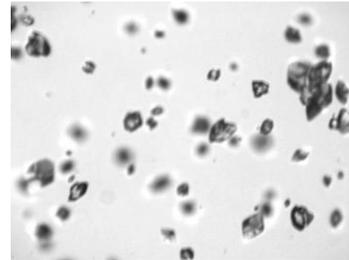
Citric acid crystals (optical imaging)

Image analysis is then needed for investigating their geometrical and morphological properties. Nevertheless, the individualization (and further geometrical characterization) of superimposed crystals remains a difficult task for high population densities. An alternative consists in using stochastic geometry that provides useful models for simulating a distribution of random geometrical patterns.

In this way, the objective of this work is to geometrically model these populations of crystals in order to get statistical geometrical characteristics of the individual crystals. We will use the homogeneous Boolean model that seems to be consistent with the data. Several methods are used to connect the global characteristics of the Boolean model to the characteristics of the typical grain. In the plane, Miles's formulae or the minimum contrast method can estimate the average value of the Minkowski functionals of the primary grain. Generally, the typical grain is assumed to have a known shape, such as discs. Thus, the first and second order moments of the radius of the primary grain are respectively proportional to its mean perimeter and its mean area. However, if we consider that the shape of the grain can vary, the Minkowski functionals of a random convex set are not enough to characterize its shape. For instance, for a Boolean model whose grains has a shape that depends on several parameters (rectangle, ellipse ...); the estimation of geometrical variations of the grain is not direct. The aim of our work is to characterize and estimate the variations of the primary grain of the Boolean model without any assumption concerning its shape, from a realization of the model in a bounded window.

The proposed method consists in using the Steiner formula and the relationship between the mean covariogram of the typical and the second order moment of its area. Indeed, it is well known that the second order moment of the area of the typical grain can be expressed as:

$$\mathbb{E}[A(\Xi_0)^2] = \int_{\mathbb{R}^2} \gamma_{\Xi_0}(u)du \tag{1}$$

where $\gamma_{\Xi_0}(u) = \mathbb{E}[A(\Xi_0 \cap \Xi_0 + u)]$ is the mean geometrical covariogram of the typical grain Ξ_0. Thus, under the hypothesis $\mathbb{E}[A(\Xi_0)] < \infty$ it is possible to obtain an estimator for $\mathbb{E}[A(\Xi_0)^2]$ from an estimator of $\gamma_{\Xi_0}(u)$. In the special case of the Boolean model, the mean geometrical covariogram can be obtained by the covariance $C_\Xi(u)$, also called 2-points probability function by the following relationship:

$$\gamma_{\Xi_0}(u) = \frac{1}{\lambda} \ln(1 + \frac{C_\Xi(u) - p_\Xi^2}{(1 - p_\Xi)^2})$$ (2)

where $p_\Xi = C_\Xi(0)$ is the fraction area of Ξ and λ the intensity of the point process. Let's notice that the Boolean is stable by convex dilation; that is to say, for each compact convex set K the random set $\Xi \oplus K$ is also a Boolean model of same intensity λ and of primary grain $\Xi_0 \oplus K$. Consequently for any compact convex set K the quantities $\lambda, \mathbb{E}[A(\Xi_0 \oplus K)]$ and $\mathbb{E}[A(\Xi_0 \oplus K)^2]$ can be estimated. Especially, considering a family of homothetic compact convex sets $(rK)_{r>0}$ the second order moment of the area of the dilated grain $\mathbb{E}[A(\Xi_0 \oplus rK)^2]$ is a polynomial function in r, it can be expressed by Steiner's formula as follows:

$$\mathbb{E}[A(\Xi_0 \oplus rK)^2] = \mathbb{E}[A(\Xi_0)^2] + 4r\mathbb{E}[A(\Xi_0)W_{0,K}] + r^2(4\mathbb{E}[W_{0,K}^2] + 2A(K)\mathbb{E}[A(\Xi_0)]) \\ + 4r^3 A(K)\mathbb{E}[W_{0,K}] + r^4 A(K)^2$$ (3)

where $W_{0,K}$ is the mixed area between Ξ_0 and K. The quantities $\mathbb{E}[A(\Xi_0)]$ and $\mathbb{E}[W_{0,K}]$ can be estimated by minimum contrast method or by Miles formulas.

Consequently, the quantities $\mathbb{E}[A(\Xi_0)^2]$, $\mathbb{E}[A(\Xi_0)W_{0,K}]$ and $\mathbb{E}[W_{0,K}^2]$ can be estimated by a polynomial approximation on $\mathbb{E}[A(\Xi_0 \oplus rK)^2]$. The choice of the compact convex set K provides different characteristics of the primary grain; for a disc, the mixed area $W_{0,K}$ is proportional to the perimeter $U(\Xi_0)$, and for a segment oriented by direction $\theta \in [0,2\pi]$ it is proportional to the Feret's diameter of Ξ_0 in the direction θ. This method can be generalized to obtain n^{th} order moments of $(A(\Xi_0), W_{0,K})$, using n-points probability function (article in preparation). The method has been evaluated by simulating several realizations of a test model: an isotropic Boolean model of rectangles bounded in a squared window of size 500×500, with intensity $\lambda = 100/500 \times 500$. The random sides of the rectangular typical grain are independent and follow the Gaussian laws $N(40,10)$ and $N(30,10)$. The results are presented in the following graph.
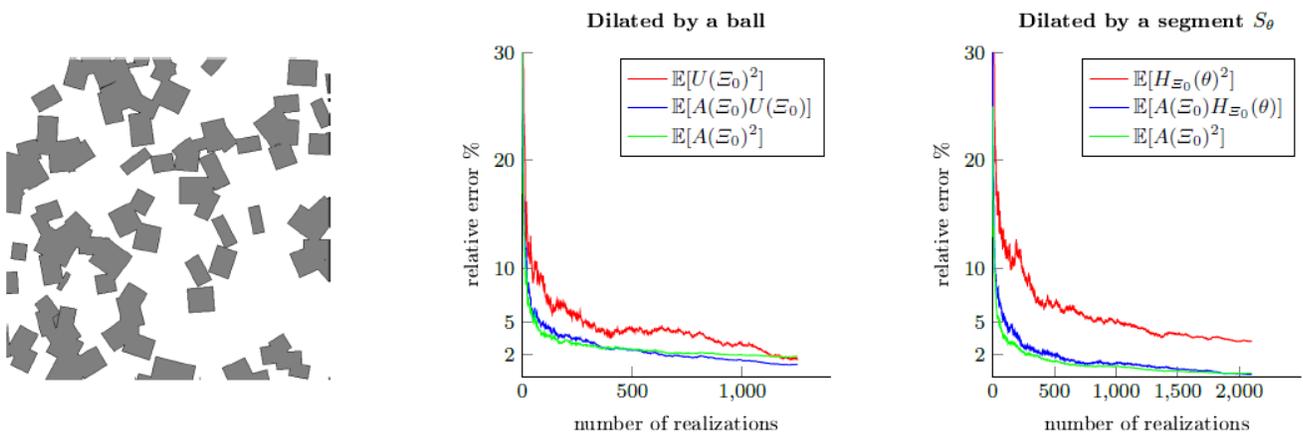
Currently, the authors try to investigate other compact convex sets K that could provide new geometrical information of the typical grain, such as its shape ratio.

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