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

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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 (Fig.1).

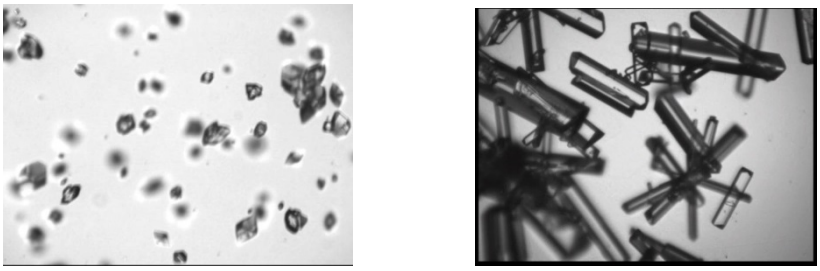

Figure 1: Citric acid crystals (left image) and ammonium oxalate crystals (right image) acquired by optical imaging.

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 [1]. 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 [2] that seems to be consistent with the data. This is defined as:

$$\Xi = \bigcup_{x_i \in \Phi} x_i + \Xi_i \tag{1}$$

where Φ is an homogeneous Poisson point process, and Ξ_i are independent identically distributed random convex sets. Here, and in the following, Ξ_0, called the primary grain or the typical grain of the Boolean model, denotes a further random convex set of the same distribution as the grains Ξ_i but independent of both the grains and the germ process Φ.

Several methods are used to connect the global characteristics of the Boolean model to the characteristics of the typical grain [3]. In the plane, the average value of the Minkowski functionals of the primary grain can be estimated by using the Miles formulas [4] or the minimum contrast method [2]. 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 have a shape that depends on several parameters (rectangle, ellipse ...), the estimation of the geometrical variations of the grain is not straightforward. The aim of the proposed work is to characterize and estimate the geometrical variations of the primary grain of the Boolean model without any assumption concerning its shape.

The proposed method consists in using the Steiner formula and the relationship between the mean geometric covariogram [5] of the typical grain 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:

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

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 $\mathbb{E}[A(\Xi_0)^2] < \infty$ it is possible to obtain an estimator for $\mathbb{E}[A(\Xi_0)^2]$ from an estimator of γ_{Ξ_0}. In the special case of the Boolean model, the mean geometrical covariogram can be obtained by the covariance C_Ξ, also called 2-points probability function by the following relationship:

$$\gamma_{\Xi_0}(u) = \frac{1}{\lambda} ln\left(1 + \frac{C_\Xi(u) - p_\Xi}{(1-p_\Xi)^2}\right) \tag{3}$$

where $p_\Xi = C_\Xi(0)$ is the fraction area of Ξ and λ the intensity of the Poisson point process. Let us notice that the Boolean is stable by convex dilations; 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 $(rK)_{r\geq 0}$ the second order moment of the area of the dilated grain $\mathbb{E}[A(\Xi_0 \oplus K)^2]$ is a polynomial function in r, it can be expressed by the Steiner's formula as follows:

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

where $W_{0,K}$ is the mixed area between Ξ_0 and K. The first order quantities $\mathbb{E}[A(\Xi_0)]$ and $\mathbb{E}[W_{0,K}]$ can be estimated by the 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 fitting on $\mathbb{E}[A(\Xi_0 \oplus K)^2]$. This method can be generalized to obtain n^{th} order moments of $(A(\Xi_0), W_{0,K})$, using n-points probability function [6].

The choice of the compact convex set K provides different characteristics of the primary grain. For example, if B denotes the unit disc then the mixed area is proportional to the perimeter of the primary grain: $W_{0,B} = \frac{U(\Xi_0)}{2}$.

Now let us define a compact set K as:

$$K = \bigoplus_{i=1}^{N} y_i S_{\theta_i} \tag{5}$$

where for all $i = 1, \cdots N,\ y_i \in \mathbb{R}_+$ and S_{θ_i} is a unit length segment oriented by $\theta_i \in [0, \pi]$. Then the mixed area can be express as:

$$W_{0,K} = \sum_{i=1}^{N} y_i H_{\Xi_0}(\theta_i) \tag{6}$$

where $H_{\Xi_0}(\theta)$ is the Feret's diameter of Ξ_0 in the direction θ. It also denotes the support function of the symmetrized grain $\frac{1}{2}(\Xi_0 \oplus \breve{\Xi}_0)$ in the direction θ, and it's well known that the support function of a set is enough to characterize it [2]. In this way, the characteristics of the random process $H_{\Xi_0}(.)$ can be estimated [6].

For example, for any $\theta_1 \in [0, \pi]$ with $N = 1, y_1 = 1$, we have $K = S_{\theta_1}$ and $W_{0,S_{\theta_1}} = H_{\Xi_0}(\theta_1)$. Then the first and second order moments of $H_{\Xi_0}(\theta_1)$ can be estimated for any θ_1, we have

$$\mathbb{E}[H_{\Xi_0}(\theta_1)] = \mathbb{E}[W_{0,S_{\theta_1}}] \tag{7}$$

$$\mathbb{E}[H_{\Xi_0}(\theta_1)^2] = \mathbb{E}[W^2_{0,S_{\theta_1}}] \tag{8}$$

Now, let $N = 2, y_1 = y_2 = 1$, for any $\theta_1, \theta_2 \in [0, \pi]$ we have $K = S_{\theta_1} \oplus S_{\theta_2}$ and $W_{0,S_{\theta_1} \oplus S_{\theta_2}} = H_{\Xi_0}(\theta_1) + H_{\Xi_0}(\theta_2)$, then the covariance of the process H_{Ξ_0} can be express as:

$$\mathbb{E}[H_{\Xi_0}(\theta_1) H_{\Xi_0}(\theta_2)] = \frac{1}{2}(\mathbb{E}[W^2_{0,S_{\theta_1} \oplus S_{\theta_2}}] - \mathbb{E}[W^2_{0,S_{\theta_1}}] - \mathbb{E}[W^2_{0,S_{\theta_2}}]) \tag{9}$$

Consequently, the first and second order characteristics of the random process H_{Ξ_0} can be estimated by this method.

The proposed method will be evaluated by simulating and characterizing several realizations of an isotropic Boolean model of rectangular grains.

References

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