Size and shape estimation of 3-D convex objects from their 2-D projections: application to crystallization processes

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Summary

The aim of this paper is to present a new projective stereological method that enables to estimate the size and the shape of a three-dimensional convex object from measurements only made on its two-dimensional projections. To do so, some geometrical and morphometrical measurements on the projected shadows of the three-dimensional convex object are done and the value of the three-dimensional convex object size and shape parameters are retrieved using the maximum likelihood estimation method. The proposed method is then applied to estimate three-dimensional particle size distributions during crystallization processes.

Introduction

Finding the real size and shape of a three-dimensional (3-D) object from its two-dimensional (2-D) projections is a quite difficult task. Indeed, first of all, except for a sphere, a 3-D object has several different 2-D projections and secondly a 2-D object resulting from a projection can come from various 3-D objects. For example, a disc of radius \( r \) can either come from a sphere of radius \( r \) or a prolate spheroid of equatorial radii \( r \). The set of methods used to estimate higher dimensional information from lower dimensional samples is called stereology (Underwood, 1970; Russ & Dehoff, 2000). From either 2-D planar cross-section images through a 3-D object (Gundersen & Jensen, 1987; Cruz-Orive, 1997; Sahagian & Proussevitch, 1998; Higgins, 2000; Howard & Reed, 2005) or its 2-D projection images (Underwood, 1972; King, 1982; Outal et al., 2008; Eggers et al., 2008), stereology attempts to extract quantitative 3-D information such as the volume or the surface area of the 3-D object. The main drawback of classical projective stereology is that without any assumptions about the shape of the 3-D object, that is, the 3-D object type (ellipsoid, elliptical cylinder, etc.) and its anisotropy, it is not possible to determine its real size from its 2-D projections.

For this reason, it has been decided to develop a new projective stereological method, called ‘Projective Stereological Size and Shape Estimator’ (P3SE), that allows to estimate not only the size but also the shape of a 3-D convex object from measurements only made on its 2-D projections. The paper is organized as follows. In the second section, some concepts and tools useful for the understanding of this paper are reminded. In the third section, the proposed P3SE method is explained. In the fourth section, it is evaluated on simulated data. In the fifth section the P3SE method is compared to the classical projective stereological method and in the sixth section it is used to estimate 3-D size distributions of particles during crystallization processes. At last, some conclusions and several prospects are given.

Concepts and tools used in this paper

Shape diagrams

Two-dimensional compact sets can be described by using various geometrical functionals (Minkowski, 1903; Michielsen & De Raedt, 2001; Sevink, 2007): the most common used in convex and integral geometry are the minimum and maximum Feret diameters, denoted by, respectively, \( \omega \) and \( d \), the radii of the inscribed and circumscribed circles, denoted by, respectively, \( r \) and \( R \), and the perimeter and the area, denoted by, respectively, \( P \) and \( A \) (Fig. 1). These geometrical functionals satisfy geometric inequalities, allowing to define morphometrical functionals that are normalized ratios between two geometrical

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functionals. The resulting morphometrical functionals are all valued within the real interval \([0, 1]\) and are invariant under similitude transformations, that is, through translations, rotations and scalings. From these geometrical functionals, 2-D shape diagrams can be defined. A shape diagram (Santaló, 1961; Hernández Cifre & Segura Gomis, 2000; Hernández Cifre et al., 2001; Rivollier et al., 2010a,b,c) enables to represent the morphology of a 2-D compact set in the Euclidean 2-D plane from two morphometrical functionals, that is to say from three geometrical functionals because the two denominators of the morphometrical functionals use the same geometrical functional. Let any triplet of the considered six geometrical functionals \((A, P, r, R, \omega, d)\) and \((M^1, M^2)\) be the associated morphometrical functionals. The corresponding shape diagram \(D\) is the mapping from \(K(E^2)\) (the family of compact sets of the Euclidean 2-D plane) to \([0, 1]^2\), that maps a 2-D compact set \(S\) to its corresponding morphometrical functionals’ value \((M^1, M^2)\). Formally, a shape diagram \(D\) is defined as

\[
D: \begin{align*}
K(E^2) & \rightarrow [0, 1]^2 \\
S & \mapsto (M^1, M^2).
\end{align*}
\]

Thirty-one shape diagrams can be defined, denoted by \((D_k)_{k \in \{1, 11\}}\), respectively. Rivollier et al. (2010a, 2010b, 2010c) have studied in details all these shape diagrams and have concluded that the shape diagram \(D_{12}\) \((M^1 = \omega / d, M^2 = 4A / \pi d^2)\), is the one that best discriminates arbitrary 2-D compact convex sets. Consequently, the shape diagram \(D_{12}\) is used in this study. Fig. 2 shows a plot of the \(D_{12}\) shape diagram: in black is represented the convex domain boundary (the domain in which all 2-D compact convex sets are mapped) and in colour the locations of several 2-D compact convex sets.

The computer simulator

To set up, validate and quantify the performance of the proposed \(P3SE\) method, a computer simulator has been created. The computer simulator is a software tool able to generate \(n (n \in \mathbb{N}^*)\) orthographic projections of a 3-D object. Figure 3 shows \(n = 5\) random (uniform law) orthographic projections of a cube. Figure 4 shows the five types of 3-D objects modelled within the computer simulator: ellipsoid, elliptical cylinder, rectangular cuboid, rectangular pyramid and rectangular bipyramid. All these 3-D object types have three varying size parameters, denoted by \(a (a > 0), b (b > 0), \) and \(c (c > 0),\) and therefore two shape parameters also known as aspect ratios, denoted by \(\alpha_1 = \frac{a}{d}\) and \(\alpha_2 = \frac{a}{c}\).

Although the proposed \(P3SE\) method could be developed for any 3-D convex objects, only results based on the following assumptions are presented in this paper: it is assumed that a 3-D object is convex with a known type (ellipsoid, elliptical cylinder, rectangular cuboid, etc.), \(\alpha_1 = 1\) (\(\alpha_1\) represents the flatness of the 3-D object), and \(\alpha_2 \geq 1\) (\(\alpha_2\) represents the elongation of the 3-D object). From now on, a 3-D convex object modelled within the computer simulator is denoted by \((CO, a, \alpha_2)\), where \(CO\) denotes its type (ellipsoid, elliptical cylinder, rectangular cuboid, rectangular pyramid, rectangular bipyramid), \(a\) its size parameter (length) and \(\alpha_2\) its shape parameter (elongation).
Fig. 3. Random (uniform law) orthographic projections of a cube.

The P3SE method

The proposed geometrical descriptor and Stereological Shape Diagram-based Descriptor (SSDD)

The proposed geometrical descriptor $f_{CO, a, \alpha_2}$. Let $(CO, a, \alpha_2)$ be a 3-D convex object modelled within the computer simulator of type $CO$, size parameter $a$ and shape parameter $\alpha_2$. Let $A$ be the continuous positive real valued random variable called ‘projected area’ associated to a 2-D projection of $(CO, a, \alpha_2)$. The proposed geometrical descriptor, denoted by $f_{CO, a, \alpha_2}$, is defined as the probability density function of $A$. Formally, $f_{CO, a, \alpha_2}$ is defined as follows:

$$f_{CO, a, \alpha_2}: \{ [A_{\min, CO, a, \alpha_2}, A_{\max, CO, a, \alpha_2}] \} \rightarrow \mathbb{R}^+$$

where $A_{\min, CO, a, \alpha_2}$ ($A_{\max, CO, a, \alpha_2}$, respectively) represents the minimum (maximum, respectively) projected area of the 3-D convex object $(CO, a, \alpha_2)$.

For some simple 3-D objects, like prolate spheroid or oblate spheroid, it is possible to get an analytical expression of $f_{CO, a, \alpha_2}$ (Vickers & Brown, 2001). However, numerical methods should be applied when the 3-D convex objects get more complex.

Towards that end, for a 3-D convex object $(CO, a, \alpha_2)$, $N$ ($N = 1\,000\,000$) uniformly distributed 3-D random rotations are first performed. For each 3-D spatial orientation, the orthographic projection onto the plane $z = 0$ is then carried out, and at last, for each projection $p_i$ belonging to $\{p_i\}_{i \in [1, N]}$, the area is calculated. The proposed geometrical descriptor $f_{CO, a, \alpha_2}$ is thus constructed from the $N$ projected area values, using Knuth’s bin optimization algorithm (Knuth, 2006). Figure 5 shows the computed $f_{CO, a, \alpha_2}$ for the cube of size parameter $a = 10 (\alpha_1 = \alpha_2 = 1)$.

Reproducibility of the geometrical descriptor $f_{CO, a, \alpha_2}$. To validate the construction of the proposed geometrical descriptor $f_{CO, a, \alpha_2}$, and in particular the number $N$ of projections used to compute it, the reproducibility of $f_{CO, a, \alpha_2}$ has been studied:

(1) for a 3-D convex object $(CO, a, \alpha_2)$, $f_{CO, a, \alpha_2}$ is generated $m$ ($m = 100$) times and the mean number of bins of the family $\{f_{CO, a, \alpha_2}^{i}\}_{i \in [1, m]}$ is calculated: $B_{\text{mean}} = \frac{1}{m} \sum_{i=1}^{m} B_i$, where $B_i$ stands for the number of bins of $f_{CO, a, \alpha_2}^{i}$.
(2) for the same 3-D object, \(N (N = 1\ 000\ 000)\) random (uniform law) orthographic projections are generated and for each projection \(p_i\) of \(\{p_i\}_{i\in[1,N]}\), the area is calculated. From these \(N\) projected area values, a normalized histogram \(h\) is constructed using \(B_{\text{mean}}\) bin number;

(3) the step 2 is repeated \(m (m = 100)\) times, generating thus a family of probability density functions, denoted by \(\{h_{CO,a,\alpha_2}^i\}_{i\in[1,m]}\).

It should be noticed that, contrary to the elements of the family \(\{f_{CO,a,\alpha_2}^i\}_{i\in[1,m]}\), the elements of \(\{h_{CO,a,\alpha_2}^i\}_{i\in[1,m]}\) are all calculated with the same number of bins \(B_{\text{mean}}\). Therefore, the elements of this family can be mutually compared. Thus, to quantify the reproducibility of \(f_{CO,a,\alpha_2}\), the mean validation error, denoted by \(MVE\), is calculated between \(h_{\text{mean}} = \frac{1}{m} \sum_{i=1}^{m} h_{CO,a,\alpha_2}^i\) and \(\{h_{CO,a,\alpha_2}^i\}_{i\in[1,m]}\) (Eq. 1):

\[
MVE = \frac{1}{m} \sum_{i=1}^{m} \frac{\|h_{\text{mean}} - h_{CO,a,\alpha_2}^i\|_1}{\|h_{\text{mean}}\|_1},
\]

where \(\|\cdot\|_1\) denotes the \(L_1\) norm.

Table 1 shows the mean validation error (MVE) for both isotropic and anisotropic 3-D convex objects, that is, for the 3-D convex objects of type ellipsoid, elliptical cylinder, rectangular pyramid, rectangular cuboid, rectangular bipyramid, size parameters \(a \in [1, 100]\) and shape parameters \(\alpha_2 \in [1, 50]\). As one can notice, in the worst case \(MVE = 2.5\%\). For a lot of application issues, where the desired \(MVE\) is generally of at least 10% or 5%, \(f_{CO,a,\alpha_2}\) is reproducible. Therefore the number \(N\) of projections used to compute \(f_{CO,a,\alpha_2}\) is sufficient.

The proposed Stereological Shape Diagram-based Descriptor (SSDD) \(g_{CO,a}\). Let \((CO, a, \alpha_2)\) be a 3-D convex object and \(\mathcal{P}_{CO,a,\alpha_2} \subset \mathbb{R}^2\) be the set of its orthographic projections (note that for all \(p \in \mathcal{P}_{CO,a,\alpha_2}, p\) is a compact convex set).

The proposed Stereological Shape Diagram-Based Descriptor (SSDD) is based on the shape diagram \(D_{12}\). Since shape diagrams are invariant under similitude transformations, this descriptor is also invariant under these transformations. Therefore it is independent of the size parameter \(a\) of a given 3-D convex object \((CO, a, \alpha_2)\).

Let \(M = (M^1, M^2) = (\omega/\bar{d}, 4A/\pi d^2)\) be the continuous random vector called ‘projected morphometrical functionals’ associated to a 2-D projection of \((CO, a, \alpha_2)\). The SSDD, denoted by \(g_{CO,a}\), is defined as the joint probability density function of \(M^1\) and \(M^2\). Formally, \(g_{CO,a}\) is defined as follows:

\[
g_{CO,a} : D_{12}(\mathcal{P}_{CO,a,\alpha_2}) \rightarrow \mathbb{R}^*_+ \quad M \mapsto g_{CO,a}(M).
\]

For some simple 3-D objects, like spheres, it is possible to get an analytical expression of \(g_{CO,a}\). However, numerical methods should be applied when the 3-D convex objects get more complex.

Towards that end, for a 3-D convex object \((CO, a, \alpha_2)\), \(N (N = 10\ 000\ 000)\) 3-D uniformly distributed random rotations are first performed. For each 3-D spatial orientation, the orthographic projection onto the plane \(z = 0\) is then carried out, and at last, for each projection \(p_i\) belonging to \(\{p_i\}_{i\in[1,N]}\), the value of the morphometrical functionals \(M^1\) and \(M^2\) are calculated. The SSDD \(g_{CO,a}\) is thus constructed from the 10 million projected morphometrical functional values discretizing \([0, 1]\) with a step size of about 0.003 \(\times\) 0.003. Figure 6 shows the computed \(g_{CO,a}\) for the cube \((CO = \text{Rectangular cuboid}, a \in \mathbb{R}^*_+, \alpha_2 = 1)\).

Reproducibility of the SSDD \(g_{CO,a}\). To validate the construction of the proposed SSDD \(g_{CO,a}\), and in particular the number \(N\) of projections used to compute it, the reproducibility of \(g_{CO,a}\) has been studied: for a 3-D convex object \((CO, a, \alpha_2)\), \(g_{CO,a}\) is generated \(m (m = 100)\) times \(\{g_{CO,a}^i\}_{i\in[1,m]}\) and the MVE is calculated between \(g_{\text{mean}} = \frac{1}{m} \sum_{i=1}^{m} g_{CO,a}^i\) and \(\{g_{CO,a}^i\}_{i\in[1,m]}\) (Eq. 2):

\[
MVE = \frac{1}{m} \sum_{i=1}^{m} \frac{\|g_{\text{mean}} - g_{CO,a}^i\|_1}{\|g_{\text{mean}}\|_1},
\]

where \(\|\cdot\|_1\) denotes the \(L_1\) norm.

Table 2 shows the \(MVE\) for both isotropic (\(\alpha_2 = 1\)) and anisotropic (\(\alpha_2 = 50\)) 3-D convex objects of type ellipsoid, elliptical cylinder, rectangular bipyramid, rectangular cuboid, rectangular pyramid (\(a \in \mathbb{R}^*_+\)). As one can notice, in the worst case \(MVE = 1.28\%\). For a lot of application issues, where the desired \(MVE\) is generally of at least 10% or 5%, \(g_{CO,a}\) is reproducible. Therefore the number \(N\) of projections used to compute \(g_{CO,a}\) is sufficient.
Table 1. Reproducibility of the geometrical descriptor $f_{\text{CO},a,\alpha_2}$. The mean validation error, $MVE$, expressed in percent, has been calculated for both isotropic and anisotropic 3-D convex objects of type ellipsoid, elliptical cylinder, bipyramid, rectangular cuboid, pyramid, size parameters $a \in [1, 100]$ and shape parameters $\alpha_2 \in [1, 50]$.

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<tr>
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<td></td>
<td>$a = 1, \alpha_2 = 1$</td>
<td>$a = 1, \alpha_2 = 50$</td>
<td>$a = 100, \alpha_2 = 1$</td>
<td>$a = 100, \alpha_2 = 50$</td>
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<tr>
<td>$MVE$</td>
<td>1.71</td>
<td>1.91</td>
<td>1.67</td>
<td>1.92</td>
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<td>$a = 100, \alpha_2 = 50$</td>
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<tr>
<td>$MVE$</td>
<td>1.99</td>
<td>2.48</td>
<td>1.96</td>
<td>2.50</td>
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<td></td>
<td>Bipyramid</td>
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<td>$a = 1, \alpha_2 = 1$</td>
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<td>$a = 100, \alpha_2 = 1$</td>
<td>$a = 100, \alpha_2 = 50$</td>
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<tr>
<td>$MVE$</td>
<td>0.84</td>
<td>0.54</td>
<td>0.83</td>
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<td></td>
<td>Rectangular cuboid</td>
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<td>$a = 1, \alpha_2 = 1$</td>
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<tr>
<td>$MVE$</td>
<td>0.56</td>
<td>0.58</td>
<td>0.57</td>
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<td></td>
<td>Pyramid</td>
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<td>$a = 1, \alpha_2 = 1$</td>
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<tr>
<td>$MVE$</td>
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<td>0.57</td>
<td>0.88</td>
<td>0.57</td>
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Estimation of the parameters value of a 3-D convex object from its 2-D projections

Estimation of the size parameter $a$ value. In this section, it is assumed that the value of the shape parameter $\alpha_2$ is known. Therefore, under the assumptions made in the section ‘The computer simulator’, to retrieve the parameters value of a 3-D convex object $(CO, a, \alpha_2)$ it is only necessary to estimate the value of its size parameter $a$. To do so, the maximum likelihood of $a$ of the geometrical descriptors is used.

Let $a$ be the continuous positive real valued random variable ‘projected area’ associated to a 2-D projection of an unknown 3-D convex object $(CO, a, \alpha_2)$ and let $(A_1, A_2, \ldots, A_n)$ be $n$ realizations ($n \in \mathbb{N}^+$) of $A$. As the $n$ realizations are independent, identically distributed, the likelihood of the size parameter $a$ in relation to the $n$ realizations $(A_1, A_2, \ldots, A_n)$ is defined as Eq. (3):

$$L_{\text{CO},a,\alpha_2}(a) = \prod_{i=1}^{n} f_{\text{CO},a,\alpha_2}(A_i), \quad (3)$$

where

$$f_{\text{CO},a,\alpha_2}: \begin{cases} \mathbb{R} \to \mathbb{R}_+ \quad & \text{if } A_i \in [A_{\text{min,CO},a,\alpha_2}, A_{\text{max,CO},a,\alpha_2}] \\ 0 & \text{if } A_i \not\in [A_{\text{min,CO},a,\alpha_2}, A_{\text{max,CO},a,\alpha_2}] \end{cases}$$

and $f_{\text{CO},a,\alpha_2}$ is the geometrical descriptor defined in the section ‘The proposed geometrical descriptor $f_{\text{CO},a,\alpha_2}$’.

Consequently, the maximum likelihood of the size parameter $a$ can be written as Eq. (4):

$$\hat{a} = \arg \max_{a \in \mathbb{R}_+} L_{\text{CO},a,\alpha_2}(a). \quad (4)$$

Estimation of the shape parameter $\alpha_2$ value. In this section, it is proposed to estimate the value of the shape parameter $\alpha_2$. To do so, the maximum likelihood of $\alpha_2$ of the SSDDs is used.

Let $M = (M^1, M^2) = (\alpha_2/d, 4A/\pi d^2)$ be the continuous random vector ‘projected morphometrical functionals’ associated to a 2-D projection of an unknown 3-D convex

Table 2. Reproducibility of the stereological shape diagram-based descriptor (SSDD) $f_{\text{CO},a,\alpha_2}$. The mean validation error, $MVE$, expressed in percent, has been calculated for both isotropic and anisotropic 3-D convex objects of type ellipsoid, elliptical cylinder, bipyramid, rectangular cuboid, pyramid and shape parameters $\alpha_2 \in [1, 50]$.

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<td>$\alpha_2 = 1$</td>
<td>$\alpha_2 = 50$</td>
<td>$\alpha_2 = 1$</td>
</tr>
<tr>
<td>$MVE$</td>
<td>$\simeq 0$</td>
<td>0.13</td>
<td>0.40</td>
<td>0.21</td>
<td>1.28</td>
<td>0.18</td>
<td>0.64</td>
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</table>
object \((CO, a, \alpha_2)\) and let \((M_1, M_2, \ldots, M_n)\) be \(n\) realizations \((n \in \mathbb{N}^+)\) of \(M\). As the \(n\) realizations are independent, identically distributed, the likelihood of the shape parameter \(\alpha_2\) in relation to the \(n\) realizations \((M_1, M_2, \ldots, M_n)\) is defined as Eq. (5):

\[
L_{\text{CO}}^2(\alpha_2) = \prod_{i=1}^{n} g_{\text{CO},\alpha_2}(M_i), \tag{5}
\]

where

\[
g_{\text{CO},\alpha_2} : \begin{cases} [0, 1]^2 \rightarrow \mathbb{R}^+ \\ M_i \mapsto \begin{cases} f_{\text{CO},\alpha_2}(M_i) & \text{if } M_i \in D_{12}(P_{\text{CO},\alpha_2}) \\ 0 & \text{if } M_i \notin D_{12}(P_{\text{CO},\alpha_2}) \end{cases} \end{cases}
\]

and \(g_{\text{CO},\alpha_2}\) is the proposed SSDD defined in the section ‘The proposed Stereological Shape Diagram-based Descriptor (SSDD) \(g_{\text{CO},\alpha_2}\)’.

Consequently, the maximum likelihood of the shape parameter \(\alpha_2\) can be written as Eq. (6):

\[
\hat{\alpha}_2 = \arg\max_{\alpha_2 \in [1;+\infty]} L_{\text{CO}}^2(\alpha_2). \tag{6}
\]

Joint estimation of the size parameter \(a\) and the shape parameter \(\alpha_2\) value. To estimate both the value of the size parameter \(a\) and the value of the shape parameter \(\alpha_2\), the maximum likelihood estimation method is still used.

Let \(A\) be the continuous random variable ‘projected area’ and \(M = (M_1, M_2) = (\omega/\pi, 4A/\pi d^2)\) be the continuous random vector ‘projected morphometric functionals’ associated to a 2-D projection of an unknown 3-D convex object \((CO, a, \alpha_2)\). Let \(n\) \((n \in \mathbb{N}^+)\) orthogonal projections of \((CO, a, \alpha_2)\) and \((A_1, M_1), (A_2, M_2), \ldots, (A_n, M_n)\) be the corresponding observations. The likelihood of the size parameter \(a\) and the shape parameter \(\alpha_2\) in relation to these \(n\) observations is defined as Eq. (7):

\[
L_{\text{CO}}(a, \alpha_2) = L_{\text{CO}}^2(\alpha_2) \int_{\mathbb{R}^+} L_{\text{CO},\alpha_2}(v)dv, \tag{7}
\]

where \(L_{\text{CO}}^2(\alpha_2)\) is the likelihood of \(\alpha_2\) in relation to the \(n\) observations \((M_1, M_2, \ldots, M_n)\) and \(L_{\text{CO},\alpha_2}(a) = \int_{\mathbb{R}^+} L_{\text{CO},\alpha_2}(v)dv\) is the likelihood of \(a\) knowing \(\alpha_2\) in relation to the \(n\) observations \((A_1, A_2, \ldots, A_n)\).

Thus, the maximum likelihood of the size parameter \(a\) and the shape parameter \(\alpha_2\) can be written as Eq. (8):

\[
(\hat{a}, \hat{\alpha}_2) = \arg\max_{(a, \alpha_2) \in [1;+\infty] \times [1;+\infty]} L_{\text{CO}}(a, \alpha_2). \tag{8}
\]

Evaluation of the performance of the proposed P3SE method on simulated data

Estimation results of the size parameter \(a\) value

To evaluate the performance of the proposed method to estimate the value of the size parameter \(a\), tests have been run as follows: for a 3-D convex object \((CO, a, \alpha_2)\) (the value of \(\alpha_2\) is known), \(n\) \((n \in \mathbb{N}^+)\) random (uniform law) orthographic projections are generated by the computer simulator and the value of \(a\) is estimated from these \(n\) projections using the method exposed in the section ‘Estimation of the size parameter \(a\) value’. To get reliable statistical data, this process is repeated \(m\) \((m = 10000)\) times for each \(n\) and the performance of the proposed method is quantified by calculating the relative mean error between the real value of \(a\) and the estimated values of \(a\) \(\left(\{\hat{a}_i\}_{i \in [1,m]}\right)\) as a function of \(n\) (Eq. (9)).

\[
\text{RME}_n(a, \{\hat{a}_i\}_{i \in [1,m]}) = \frac{1}{m} \sum_{i=1}^{m} \frac{|a - \hat{a}_i|}{a}. \tag{9}
\]

where \(|.|\) denotes the absolute value function and \(\hat{a}_i\) the \(i\)th estimated value of \(a\).

Figure 7 shows the relative mean error \(\text{RME}_n(a, \{\hat{a}_i\}_{i \in [1,m]})\) as a function of \(n\) \((n = 1, 2, \ldots, 20, 50, 100, 200, 500)\) for the 3-D convex objects (Ellipsoid, 10, \(\alpha_2 \in [1, 2, 5, 10, 20, 50]\), Elliptical cylinder, 10, \(\alpha_2 \in [1, 2, 5, 10, 20, 50]\), Rectangular bipyramid, 10, \(\alpha_2 \in [1, 2, 5, 10, 20, 50]\), Rectangular cuboid, 10, \(\alpha_2 \in [1, 2, 5, 10, 20, 50]\)). As one can notice, the more projections \(n\) are realized, the better the estimation of the size parameter \(a\) value is. Moreover, the larger \(\alpha_2\) is, the more difficult the estimation of \(a\) becomes (Presles et al., 2010). Nevertheless, the relative mean error, \(\text{RME}_n(a, \{\hat{a}_i\}_{i \in [1,m]})\), does not vary linearly according to \(\alpha_2\). Only two projections are necessary to estimate \(a\) with a mean error lower than 10%, whatever the studied 3-D convex object is.

Estimation results of the shape parameter \(\alpha_2\) value

To evaluate the performance of the proposed method to estimate the value of the shape parameter \(\alpha_2\), tests have been run as follows: for a 3-D convex object \((CO, a, \alpha_2)\), \(n\) \((n \in \mathbb{N}^+)\) random (uniform law) orthographic projections are generated by the computer simulator and the value of \(\alpha_2\) is estimated from these \(n\) projections using the method exposed in the section ‘Estimation of the shape parameter \(\alpha_2\) value’. To get reliable statistical data, this process is repeated \(m\) \((m = 10000)\) times for each \(n\) and the performance of the proposed method is quantified by calculating the relative mean error between the real value of \(\alpha_2\) and the estimated values of \(\alpha_2\) \(\left(\{\hat{\alpha}_i\}_{i \in [1,m]}\right)\).
Fig. 7. Relative mean error $RME_n(a, \{\hat{a}_i\}_{i \in [1, m]})(m = 10,000)$ between the real value of $a$ and the estimated values versus the number of projections $n$ for several 3-D convex objects of size parameter $a = 10$ and shape parameters $\alpha_2 \in \{1, 2, 5, 10, 20, 50\}$. (a) Ellipsoid, (b) Elliptical cylinder, (c) Rectangular bipyramid, (d) Rectangular cuboid and (e) Rectangular pyramid.
as a function of \( n \) (Eq. 10).

\[
RME_n(\alpha_2, \{\hat{\alpha}_2^i\}_{i \in \llbracket 1, m \rrbracket}) = \frac{1}{m} \sum_{i=1}^{m} \frac{\lvert \alpha_2 - \hat{\alpha}_2^i \rvert}{\alpha_2},
\]

(10)

where \( \lvert . \rvert \) denotes the absolute value function and \( \hat{\alpha}_2^i \) the \( i \)th estimated value of \( \alpha_2 \).

Figure 8 shows the relative mean error \( RME_n(\alpha_2, \{\hat{\alpha}_2^i\}_{i \in \llbracket 1, m \rrbracket}) \) as a function of \( n \in \{1, 2, \ldots, 20, 50, 100, 200, 500\} \) for the 3-D convex objects (Ellipsoid, \( a \in \mathbb{R}^+ \), \( \alpha_2 \in \{1, 2, 5, 10, 20\} \)), (Elliptical cylinder, \( a \in \mathbb{R}^+ \), \( \alpha_2 \in \{1, 2, 5, 10, 20\} \)), (Rectangular bipyramid, \( a \in \mathbb{R}^+ \), \( \alpha_2 \in \{1, 2, 5, 10, 20\} \)), (Rectangular cuboid, \( a \in \mathbb{R}^+ \), \( \alpha_2 \in \{1, 2, 5, 10, 20\} \)). As one can notice, the more projections \( n \) are realized, the better the estimation of the shape parameter \( \alpha_2 \) value. Moreover, the larger \( \alpha_2 \) is (more anisotropic the 3-D convex object is), the more difficult the estimation of the value of \( \alpha_2 \) becomes. However, only four projections are necessary to estimate \( \alpha_2 \) with a mean error lower than 10%, whatever the studied 3-D convex object is.

Estimation results of the size parameter \( a \) and the shape parameter \( \alpha_2 \) value

To evaluate the performance of the proposed method to estimate both the value of the size parameter \( a \) and the shape parameter \( \alpha_2 \), tests have been run as follows: for a 3-D convex object \( (CO, a, \alpha_2) \), \( n \in \mathbb{N}^+ \) random (uniform law) orthographic projections are generated by the computer simulator and the value of the ordered pair \((a, \alpha_2)\) is estimated from these \( n \) projections using the method exposed in the section ‘Joint estimation of the size parameter \( a \) and the shape parameter \( \alpha_2 \) value’. To get reliable statistical data, this process is repeated \( m \) (\( m = 10000 \)) times for each \( n \) and by calculating the following relative mean error as a function of \( n \) (Eq. 11).

\[
RME_n((a, \alpha_2), \{\hat{\alpha}_2^i, \hat{\alpha}_2^i\}_{i \in \llbracket 1, m \rrbracket}) = \frac{1}{m} \sum_{i=1}^{m} \left( \frac{\lvert a - \hat{a}_i \rvert}{a} + \frac{\lvert \alpha_2 - \hat{\alpha}_2^i \rvert}{\alpha_2} \right),
\]

(11)

where \( \lvert . \rvert \) denotes the absolute value function, \( \hat{a}_i \) denotes the \( i \)th estimated value of \( a \) and \( \hat{\alpha}_2^i \) the \( i \)th estimated value of \( \alpha_2 \).

The error has been quantified by adding the relative errors between \( a \) and \( \hat{a}_i \) and \( \alpha_2 \) and \( \hat{\alpha}_2^i \), because \( a \) and \( \alpha_2 \) are not homogeneous with respect to their dimensions.

Figure 9 shows the relative mean error \( RME_n((a, \alpha_2), \{\hat{\alpha}_2^i, \hat{\alpha}_2^i\}_{i \in \llbracket 1, m \rrbracket}) \) as a function of \( n \in \{1, 2, \ldots, 20, 50, 100, 200, 500\} \) for the 3-D convex objects (Ellipsoid, \( 10, \alpha_2 \in \{1, 2, 5, 10, 20\} \)), (Elliptical cylinder, \( 10, \alpha_2 \in \{1, 2, 5, 10, 20\} \)), (Rectangular bipyramid, \( 10, \alpha_2 \in \{1, 2, 5, 10, 20\} \)), (Rectangular cuboid, \( 10, \alpha_2 \in \{1, 2, 5, 10, 20\} \)). (Rectangular pyramid, \( 10, \alpha_2 \in \{1, 2, 5, 10, 20\} \)).

First of all, it can be noticed that whatever the studied 3-D convex object is, the more projections \( n \) are realized, the better the estimation of the value of \((a, \alpha_2)\) is. Moreover, the larger \( \alpha_2 \) is (more anisotropic the 3-D convex object is), the more difficult the estimation of the value of \((a, \alpha_2)\) becomes. Nevertheless, the relative mean error \( RME_n((a, \alpha_2), \{\hat{\alpha}_2^i, \hat{\alpha}_2^i\}_{i \in \llbracket 1, m \rrbracket}) \) does not vary linearly according to \( \alpha_2 \). Only seven projections are necessary to estimate \((a, \alpha_2)\) with a mean error lower than 10%, whatever the studied 3-D convex object is. Note that this number of projections should be minimized because the relative mean error \( RME_n((a, \alpha_2), \{\hat{\alpha}_2^i, \hat{\alpha}_2^i\}_{i \in \llbracket 1, m \rrbracket}) \) is calculated by adding the relative errors of \( a \) and \( \alpha_2 \) and not by calculating the relative error of the ordered pair \((a, \alpha_2)\).

The classical projective stereological method versus the proposed P3SE method

The classical projective stereological method

In classical projective stereology, the volume of a 3-D convex object can be estimated by (Underwood, 1972):

\[
\hat{V} = \overline{L_1} \times \overline{A},
\]

(12)

where \( \overline{L_1} \) denotes the mean intercept length from \( n \) penetrations of the 3-D convex object by random straight lines in 3-D and \( \overline{A} \) the mean projected area. Without any assumptions about the shape of the 3-D convex object, it is not possible in classical projective stereology to estimate its volume from measurements only made on its 2-D projections. However, if the type and the anisotropy factors of the 3-D convex object are known, \( \overline{L_1} \) can be expressed as a function of the mean projected height \( \overline{H} \) (the average mean projected Feret diameter) (Underwood, 1970).

For example, for a sphere of radius \( r \), \( \overline{L_1} = \frac{2}{3} \overline{H} \) and therefore:

\[
\hat{V} = \frac{2}{3} \overline{H} \times \overline{A}.
\]

(13)

Contrary to Eq. (12), Eq. (13) is expressed only by means of projected parameters and note that the radius \( r \) of the sphere can also be expressed as a function of \( \overline{H} \) and \( \overline{A} \): \( r = \left( \frac{1}{\pi} \overline{H} \times \overline{A} \right)^{\frac{1}{3}} \).

The classical projective stereological method can therefore be used to estimate the size of a 3-D convex object from its 2-D projections and be compared to the P3SE method.

Comparison results

To compare the two methods, tests have been run using the computer simulator. For a 3-D convex object \((CO, a, \alpha_2)\) of type \( CO \), size parameter \( a \) and shape parameter \( \alpha_2 \) (as explained in the section ‘The classical projective stereological method’, the value of \( \alpha_2 \) has to be assumed known), \( n \in \mathbb{N}^+ \) random (uniform law) orthographic projections are generated by the
Fig. 8. Relative mean error $RME_n(\alpha_2, \{\hat{\alpha}_2^i\}_{i\in[1,m]}) (m = 10,000)$ between the real value of $\alpha_2$ and the estimated values versus the number of projections $n$ for several 3-D convex objects of shape parameters $\alpha_2 \in \{1, 2, 5, 10, 20\}, (a) Ellipsoid, (b) Elliptical cylinder, (c) Rectangular bipyramid, (d) Rectangular cuboid and (e) Rectangular pyramid.
Fig. 9. Relative mean error $RME_n((a, \alpha_2), ([\hat{a}_i, \hat{\alpha}_2^j])_{i \in [1,m]})$ ($m = 10000$) between the real value of $(a, \alpha_2)$ and the estimated values versus the number of projections $n$ for several 3-D convex objects of size parameter $a = 10$ and shape parameters $\alpha_2 \in \{1, 2, 5, 10, 20\}$. (a) Ellipsoid, (c) Elliptical cylinder, (c) Rectangular bipyramid, (d) Rectangular cuboid and (e) Rectangular pyramid.
Fig. 10. Relative mean errors $RME_n(a, [\hat{a}^1, \hat{a}^m])$ and $RME_n(a, [\hat{a}_s^1, \hat{a}_s^m])$ ($m = 10,000$) between the real value of $a$ and the estimated values versus the number of projections $n$ for several 3-D convex objects of size parameter $a = 10$ and shape parameters $\alpha_2 \in \{1, 2, 5, 10, 20, 50\}$. The full line represents the relative mean error $RME_n(a, [\hat{a}^1, \hat{a}^m])$ of the proposed P3SE method. In dotted line is the relative mean error $RME_n(a, [\hat{a}_s^1, \hat{a}_s^m])$ of the classical projective stereological method. (a) Elliptical cylinder and (b) Rectangular cuboid.

The computer simulator and the value of the size parameter $a$ is estimated from these $n$ projections by each of the two methods: the P3SE method exposed in the section ‘Estimation of the size parameter $a$ value’ and the projective stereological method exposed in the section ‘The classical projective stereological method’. To get reliable statistical data, this process is repeated $m$ ($m = 10,000$) times for each $n$ and for each method, the relative mean error between the real value of $a$ and the estimated values of $a$ is calculated as a function of $n$ (Eq. 14):

$$RME_n(a, [\hat{a}^1, \hat{a}^m]) = \frac{1}{m} \sum_{i=1}^{m} \frac{|a - \hat{a}^i|}{a},$$

$$RME_n(a, [\hat{a}_s^1, \hat{a}_s^m]) = \frac{1}{m} \sum_{i=1}^{m} \frac{|a - \hat{a}_s^i|}{a}. \quad (14)$$

Fig. 11. The experimental system: (a) the EZProbe® sensor and (b) the scheme of the system.
where $\hat{a}_i$ ($\hat{a}_s$, respectively) denotes the $i$th estimated value of $a$ by the $P3SE$ method (by the classical stereological method, respectively) and $\{\hat{a}_i\}_{i \in \{1, m\}}$ ($\{\hat{a}_s\}_{i \in \{1, m\}}$), respectively) denotes the family of estimated $a$ values by the $P3SE$ method (by the classical stereological method, respectively).

Figure 10 shows the relative mean errors $RME_n(a, \{\hat{a}_i\}_{i \in \{1, m\}})$ and $RME_n(a, \{\hat{a}_s\}_{i \in \{1, m\}})$ as a function of $n \in \{1, 2, \ldots, 20, 50, 100, 200, 500\}$ for the 3-D convex objects (Rectangular cuboid, $10, \alpha_2 \in \{1, 2, 5, 10, 20, 50\}$) and (Elliptical cylinder, $10, \alpha_2 \in \{1, 2, 5, 10, 20, 50\}$) (no reference in the literature has been found for the other 3-D convex object types modelled within the computer simulator).

As one can notice, whatever the value of $\alpha_2$ is, the $P3SE$ method better estimates the value of the size parameter $a$ than the classical projective stereological method. Moreover, contrary to the classical projective stereological method, the proposed $P3SE$ method enables to estimate not only the size (parameter $a$) but also the shape (parameter $\alpha_2$) of a 3-D convex object, which is an overwhelming advantage.

Application to the estimation of 3-D particle size distributions during crystallization processes

In this section, it is proposed to use the $P3SE$ method to estimate 3-D size distributions of particles during crystallization experiments.

Materials and experimental setup

Crystallization experiments have been performed with particles crystallizing in water in a 3 L lab-scale batch jacketed crystallizer, equipped with a profiled pale propeller (Mixel TT) and four baffles. The stirring rate was set to 250 revolutions per minute (rpm). The temperature of the crystallizing suspension was controlled by means of hydro-alcoholic fluid circulating in the jacket. The imaging system used to monitor the experiments was an in situ imaging probe: the ‘EZProbe sensor’® (Fig. 11(a)) developed at the University of Lyon 1. The probe was immersed into the reactor as shown in Figure 11(b) and filmed a restricted volume region within the suspension. The imaging system is able to acquire video sequences of 2-D projections of 3-D particles with the following specifications: 25 frames per second, 256 grey level images of size $640 \times 480$ pixels with a spatial resolution up to $4 \mu m^2$ per square pixel.

It is important to notice that:

(1) as the suspension is homogenized by mechanical agitation, it can be assumed that the viewed particles are representative of the crystals in suspension;

(2) having regard to the frame rate (25 images per second), it is possible to visualize the same particle on several consecutive images (Fig. 12) and moreover it takes a random orientation in space between two consecutive images.

Thereafter, it is assumed that the size distributions calculated by image analysis are representative of the particles present in the reactor and the particles take an uniformly distributed random orientation in space between two consecutive images.
3-D size distributions of ammonium oxalate particles

As shown in Fig. 13, an ammonium oxalate particle can be modelled, in first approximation, by a rectangular cuboid of length $a$, width $b = a$ ($a_1 = 1$) and height $c = a_2 a$ with $a_2 \geq 1$ (Mielniczek-Brzózka & Sangwal, 1995; Sangwal et al., 1996). An ammonium oxalate particle can therefore be modelled by a 3-D convex object (Rectangular cuboid, $a \in \mathbb{R}^+$, $a_2 \geq 1$). The assumptions made previously are thus satisfied and therefore the $P$3$\Sigma E$ method can be used to estimate the size and the shape of these particles.

Before being able to apply the proposed method to estimate 3-D size distributions of ammonium oxalate particles from a video sequence, it is first necessary to identify each projected shadow (segmentation step) and then make a video tracking to locate the several (if any) projected views of the same particle. Although these steps could have been completed automatically (Calderon De Anda et al., 2005; Larsen et al., 2006; Yilmaz et al., 2006; Sarkar et al., 2009; Ahmad Suleiman et al., 2011), they were accurately performed manually by an expert to not affect the results (segmentation and tracking errors).

Once these two steps achieved, the $P$3$\Sigma E$ method estimates the value of the ordered pair ($a$, $a_2$) of each particle and particle size distributions, denoted by 3DPSDs, are deduced.

The $P$3$\Sigma E$ method versus a 2-D method. To compare the $P$3$\Sigma E$ method with a 2-D method (Gherras & Fèvotte, 2012) that uses the same input data as the $P$3$\Sigma E$ method, the following process has been performed. For each segmented shadow, the 2-D rectangle of width $l$ and length $L$ presenting the same area and perimeter as the projection is calculated. Assuming that each ammonium oxalate particle can be modelled by a rectangular cuboid of length $l$, width $l$, height $l$, particle size distributions, denoted by 2DPSDs, are deduced.

Figure 14 shows six size distributions in volume (number of particles vs. the volume) calculated by the two methods at three different times of a crystallization experiment. If $t_0$ represents the time when the ammonium oxalate particles start to build up, that is, the nucleation, the two first distributions have been calculated on the interval $t_0 + 1 \pm \frac{2}{3} \Delta t$ min, the two seconds on the interval $t_0 + 10 \pm \frac{2}{3} \Delta t$ min and the two thirds on the interval $t_0 + 15 \pm \frac{2}{3} \Delta t$ min ($\Delta t = 2/60$ min). As one can notice, the time evolution of the 2DPSD and the 3DPSD is well consistent with the crystallization process. More precisely, due to the development of both crystal nucleation and growth, both PSDs spread and the growth of the initial seed particles leads to the emergence of new particle size distribution classes.

To quantify more precisely the error in volume of each method, the following simulation has been performed: for a 3-D convex object (Rectangular cuboid, $a \in \mathbb{R}^+$, $a_2 \geq 1$) of volume $V_{\text{real}} = a \times a \times a_2 a$, $n = 1$ random (uniform law) orthographic projection is generated by the computer simulator and the volume of the 3-D convex object is estimated from this projection by each of the two methods. To get reliable statistical data, this process is repeated $m$ ($m = 10000$) times and the performance of each method is quantified by calculating the relative mean error between the real volume of the 3-D convex object and the family of estimated volumes (Eqs 15 and 16).

$$RME(V_{\text{real}}, \{V_{2D}^i\}_{i\in[1,m]}) = \frac{1}{m} \sum_{i=1}^{m} \frac{|V_{\text{real}} - V_{2D}^i|}{V_{\text{real}}}, \quad (15)$$

where $V_{2D}^i$ and $\{V_{2D}^i\}_{i\in[1,m]}$ denote respectively the $i$th estimated volume and the family of estimated volumes by the 2-D method.

$$RME(V_{\text{real}}, \{V_{P3\Sigma E}^i\}_{i\in[1,m]}) = \frac{1}{m} \sum_{i=1}^{m} \frac{|V_{\text{real}} - V_{P3\Sigma E}^i|}{V_{\text{real}}}, \quad (16)$$

where $V_{P3\Sigma E}^i$ and $\{V_{P3\Sigma E}^i\}_{i\in[1,m]}$ denote respectively the $i$th estimated volume and the family of estimated volumes by the proposed $P$3$\Sigma E$ method.

Figure 15 shows the result of this simulation for the 3-D convex objects of type rectangular cuboid, size parameter $a = 10$ and shape parameters $a_2 \in \{1, 2, 5, 10, 20\}$. As one can notice, whatever the value of $a_2$ is, the proposed $P$3$\Sigma E$ method estimates more precisely the volume of (Rectangular cuboid, $a$, $a_2$). Moreover, since the 2-D method does not take into account the fact that the same particle can be viewed on several consecutive images, the volumes estimated by the $P$3$\Sigma E$ method have been estimated from only one projection. Therefore, the values of the relative mean error $RME(V_{\text{real}}, \{V_{P3\Sigma E}^i\}_{i\in[1,m]})$ should be minimized.

The $P$3$\Sigma E$ method versus the Coulter counter. To compare the $P$3$\Sigma E$ method with a ‘3-D method’, the Coulter counter has been used (Beckman Coulter, https://www.beckmancoulter.com). The Coulter counter is a rather reliable offline measurement device that is currently used for particle sizing and counting, for example, in the field of biology (blood cells, microscopic algae, etc.). It detects the change in electrical conductance of a small aperture as a fluid containing particles/cells is drawn through. The particle size measured by the Coulter counter is the diameter of the sphere whose volume is equal (approximately) to that of the particle.

The particle size estimated by the $P$3$\Sigma E$ method is the value of the ordered pair ($a$, $a_2$) of each particle. By calculating for each particle, the corresponding volume and by converting this volume to the equivalent volume sphere diameter, it is possible to compare the distributions measured by the Coulter counter to the distributions calculated by the $P$3$\Sigma E$ method. Figure 16 shows the size distributions estimated by both methods at the ‘beginning’ of a crystallization process. The Coulter counter distribution has been measured by using an aperture tube of size 1.000 $\mu$m and therefore only particles with an equivalent volume sphere diameter between [30 $\mu$m: 600 $\mu$m] has been recorded. For comparison purposes, the 3DPSD has been calculated on the same interval.
Fig. 14. Size distributions of ammonium oxalate particles calculated at three different times of a crystallization experiment ($t_0$ denotes the beginning of the nucleation, $\Delta t = 2/60$ min). (a) 2DPSD at $t_0 + 1 \pm \frac{\Delta t}{2}$ min; (b) 3DPSD at $t_0 + 1 \pm \frac{\Delta t}{2}$ min; (c) 2DPSD at $t_0 + 10 \pm \frac{\Delta t}{2}$ min; (d) 3DPSD at $t_0 + 10 \pm \frac{\Delta t}{2}$ min; (e) 2DPSD at $t_0 + 15 \pm \frac{\Delta t}{2}$ min; (f) 3DPSD at $t_0 + 15 \pm \frac{\Delta t}{2}$ min.
As one can notice, the two distributions are similar. This result is important because it validates experimentally the proposed P3SE method.

Conclusion and prospects

In this paper, a new projective stereological method, called Projective Stereological Size and Shape Estimator (P3SE) has been presented. This method allows to estimate the size and the shape of a 3-D convex object from its 2-D projections. Under the assumptions that the type of the 3-D convex object is known and the 3-D convex object has three size parameters $a$, $b$ and $c$ such as $a > 0$, $\alpha_1 = \frac{b}{a} = 1$ ($\alpha_1$ represents the flatness of the 3-D object) and $\alpha_2 = \frac{c}{a} \geq 1$ ($\alpha_2$ represents the elongation of the 3-D object), it has been shown in particular that it is possible to estimate the value of the ordered pair $(a, \alpha_2)$ from measurements only made on the projected shadows of the 3-D convex object. The more projections of the 3-D convex object there are, the better the estimation of the $(a, \alpha_2)$ value is [about seven projections are necessary to estimate $(a, \alpha_2)$ with a mean error lower than 10%, whatever the studied 3-D convex object is], and the larger $\alpha_2$ is (more anisotropic...
the 3-D convex object is), the more difficult the estimation of the \((\alpha_1, \alpha_2)\) value becomes. However, the relative mean error between the real value of \((\alpha_1, \alpha_2)\) and the estimated values does not increase linearly with \(\alpha_2\). Moreover, it has been shown that the proposed method better estimates the value of the size parameter \(\alpha_1\) than the classical projective stereological method and contrary to the latter, the P3SE method does not necessarily require assumption about the anisotropy (shape parameter \(\alpha_2\)) of the 3-D convex object, which is an overwhelming advantage.

The proposed P3SE method has finally been applied to estimate 3-D size distributions of ammonium oxalate particles crystallizing in water. Results have been compared with a 2-D method that uses the same input data as the P3SE method and have been validated experimentally by comparing them to the Coulter counter.

Although only results on some 3-D convex objects have been proposed in this paper, this work could be extended to any 3-D convex objects. The authors are currently working on both increasing the number of 3-D convex object types modelled within the computer simulator and removing the hypothesis \(\alpha_1 = 1\).

References


