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A COMPARISON OF QUANTITATIVE METHODS OF SHAPE CHARACTERIZATION

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ABSTRACT

The three quantitative methods of shape description investigated in this work are:- Form Factors, Fourier Analysis and Fractal Dimensions. It is concluded that it is unrealistic to expect that any one type of shape coefficient will adequately quantify all the aspects of particle morphology that contribute to the physical properties of powders in bulk. Useful information may be obtained if care is taken in choosing the method of analysis to match the purpose of the investigation or by combining data from each of the methods.

INTRODUCTION

The bulk properties of particulate solids depend on the size and shape distributions of their constituent particles. Shape analysis has lagged far behind that of size because of the inherent difficulties in quantifying morphic properties.

Shape may be arbitrarily subdivided under the following headings which relate to the scale of scrutiny with which the particles are examined. (Kaye, 1981)

External Morphology: the low resolution shape description such as might affect packing behaviour.

Topography: by analogy to physical geography this describes the medium resolution irregularities (peninsulars and bays) on the particle boundary.

Texture: describes the microscopic surface features.

METHODS OF MEASUREMENT

- 1) Form Factors. These are dimensionless groups of metric quantities chosen so as to be a measure of some shape attribute. (Gibbard et al, 1972)
- 2) Fourier Series Expansion. This method transforms the particle perimeter into a periodic function which is then expanded as a Fourier series. The method used for this work converts the boundary points into polar co-ordinates with respect to the centre of gravity as origin. Thus:-

R(
$$\theta$$
) = A_o + $\sum_{n=1}^{\infty}$ A_nCOS(n θ - φ _n)

Where R(θ) is the radius as a function of the polar angle θ , A_n is the amplitude and φ_n the phase angle of the nth harmonic. (Erlich and Weinberg, 1970)

3) Fractal Dimensions. A measure of the space filling capacity of an irregular boundary. (Mandelbrot, 1982)

Measurements and analyses were performed on a Quantimet 720 using the methods described by Flook (1982) for the Fourier method and Flook (1978) for the fractal method.

MAIN FINDINGS AND CONCLUSIONS

It was found that form factors are easy to measure but give a crude indication of shape which may lead to ambiguous interpretation. Eg. the circularity factor $(4\pi \text{ x area/perimeter}^2)$ measures the deviation from a true circle, a low value for this factor may be caused by an elongated particle or a rounded one with a roughly textured surface. The joint use of two or more different form factors can resolve this ambiguity.

The Fourier method can encode particle shapes to any required accuracy, but the series must be expanded to a relatively large number of terms to obtain satisfactory shape information. Figure la shows a profile which was encoded as an harmonic series. Expanding this series to 5 terms regenerated the shape shown in fig. 1b. Although the expansion to 75 terms shown in fig. 1c indicates a more faithful reproduction of the original profile the number of coefficients imposed difficulty in using this technique as a general method of analysis. Figure 1d is the regenerate using the constant term plus the all the harmonic terms from 5 to 75 and demonstrates that the high frequency shape

information missing from fig. 1b arises from both the texture and sharp deflections in the profile boundary.

There are further difficulties with the Fourier method if we wish to render the harmonic terms invariant to rotation and reflection of the profile. A scheme has been devised to achieve this but at the expense of generating more terms. An alternative method is to use only the amplitude terms, which are invariant, and to ignore the phase terms which cause the problem. The effect of this omission is shown in figs. le,f; where the profiles have been regenerated using the first 75 harmonic amplitudes with their phase angles randomised and set to zero respectively.

Despite these restrictions the method has been found useful in several applications where low numbers of harmonic terms were sufficient to monitor subtle changes in shape which were difficult to resolve using alternative methods.

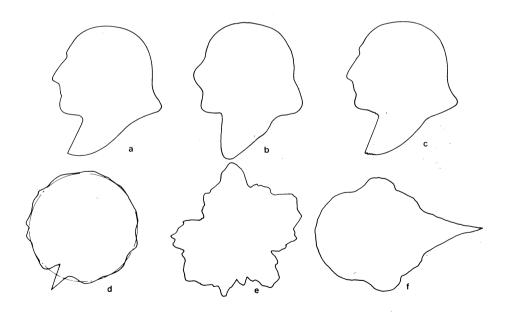


Figure 1. Profiles regenerated by Fourier series expansion using different conditions.

Fractal dimensions have been found unsuitable for general shape analysis (Schwarz, 1979) but they are extremely useful for characterizing highly textured or contorted shapes (Flook, 1978 and 1979). For example, the fractal plots of agglomerates often show three distinct regions. To investigate the influence of the various parts of the structure on the fractal plot a profile of a typical agglomerate was modified as shown in fig. 2 and the corresponding fractal plots are shown in fig. 3.

Analysis of the results show the expected textural and structural regions with the transition point corresponding to the area per unit length of perimeter (Flook, 1978). The structural regions of flocs A' and A" give a fractal dimension of 1.32 and 1.34 compared with 1.54 for floc A. This arises from the decrease in the complexity of the profile by the removal of the inner boundary. It can also be seen that the tailing-off at higher stride lengths is associated with the overlapping of the structuring elements from opposite boundaries at the higher dilation values. The structural fractal region of floc A" extends to the limit of dilation and well beyond the limits reached by the closed boundary plots.

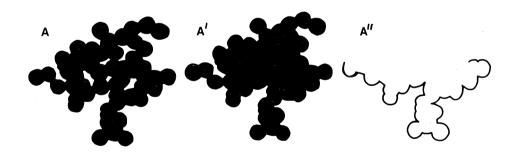


Figure 2. Modified floc profiles.

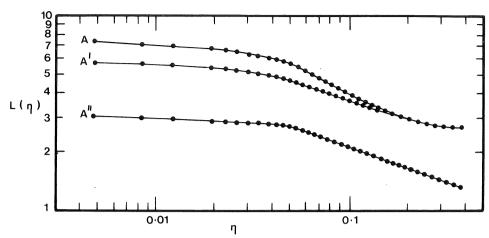


Figure 3. Fractal plots of modified profiles. η = stride length $L(\eta)$ = perimeter estimate at stride length η

N.B. Units normalised with respect to the maximum Feret's diameter.

CONCLUSIONS

The use fo form factors is well established and should be the preferred method where possible because of the simplicity of their interpretation.

The Fourier method can be contemplated as a method for shape analysis if only a small number of coefficients is required or if their number can be reduced to a manageable level by mathematical combination.

Further practical experience on a wider range of materials is required before the fractal method can be used with any degree of confidence. The main problem is likely to be related to the definition of the range over which the dimension is determined since most natural materials are unlikely to exhibit statistical self-simularity over the useful range of measurement. The method is most promising in the application of shape characterization of highly convoluted or textured profiles where other methods become problematical.

The main conclusions are summarised in table 1. Further work needs to be done to resolve some of the remaining difficulties with each of these techniques and to include other methods (e.g. mathematical morphology).

Table 1. Summary of main finding	Table	1.	Summary	of	main	finding
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MEASUREMENT METHOD SHAPE PROPERTY	FORM FACTOR	HARMONIC ANALYSIS	FRACTAL DIMENSIONS
EXTERNAL MORPHOLOGY	Good	Good: can discriminate subtleties of shape.	Poor
TOPOGRAPHY	Good but a combination may be needed to avoid ambiguities	Moderately good: the number of harmonics may become a problem for extreme topographical features.	Moderate: experience is required to interpret the plots.
TEXTURE	Poor unless range of shapes is restricted and/or multiple factors used.	Poor	Good for many highly textured profiles

REFERENCES

Erlich R, Weinberg B. An exact method for the characterization of grain shape. J. Sed. Petrology 1970; 40: 205-212. Flook AG. The use of dilation logic on the Quantimet to achieve fractal dimension characterization of textured and structured profiles. Powder Technology 1978; 21: 295-298. Flook AG. The characterization of textured and structured profiles by the automated measurement of their fractal dimensions. Proceedings of PARTECH Symposium, Nuremberg 1979; 591-599.

Flook AG. Fourier analysis of particle shape. In: Stanley-Wood NG and Allen T, eds. Particle size analysis 1981. Wiley Heyden Ltd, 1982: 255.

Giddard DW, Smith DJ, Wells A. Area sizing and pattern recognition on the Quantimet 720. Microscope 1972; 20: 37-4.

Kaye BH. Direct characterization of fineparticles. New York: John Wiley, 1981; 302-302.

Mandelbrot BP. The fractal geometry of nature. San Francisco: WH Freeman, 1982; 25-33.

Schwarz H. Two-dimensional feature-shape indices. Proceedings of 5th International Congress for Stereology. 1979; 64-67.

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