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A GEOMETRIC PROBABILITY APPROACH TO ESTIMATING PARTICLE VOLUME DISTRIBUTION

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ABSTRACT

A fundamental problem in stereology is to estimate the particle volume distribution using planar profiles. A model has been developed to solve this problem. The model is based on three geometric probability equations and a small number of assumptions. These assumptions are that sectioning is isotropic and uniform, particle shape changes smoothly with particle volume and particles are convex. The model is based on dividing the particle volume distribution into bins with each bin representing a narrow range in particle volume. The planar profiles are allocated into the bins. The method of allocation is to ensure that for each bin the volume estimates obtained from applying the three geometric probability equations correspond closely to the bin particle volume. The model is verified by numerical simulation and experiment. The numerical simulation is based on sectioning ellipsoids. For the simulations the model for estimating particle volume distribution from planar profiles was found to be very accurate. The experimental verification has the advantage of testing the model on 'real' particles. The particle volume distribution model was applied to planar profiles from particles with a known size distribution. For this verification the estimated particle volume distribution was not as accurate as for the numerical simulations. The reason for this is most likely experimental error.

Key words: stereology, geometric probability, integral geometry, particle volume distribution, size distribution.

INTRODUCTION

A fundamental problem in stereology is to estimate the particle volume distribution using planar profiles. The basic problem is explained by considering Fig. 1. The figure consist of three bins and four segments. The bins represent narrow particle volume classes. Segment I illustrates 11 particles and the bins from which they came.

Segment II shows hypothetical isotropic uniform random (IUR) planar profiles of the particles. Notice that the size of the planar profiles can vary widely so that the size of a particular planar profile is not a good indicator of the size of the parent particle. In segment III the planar profiles are scrambled. The volume of their parent particles is unknown. This is the reality.

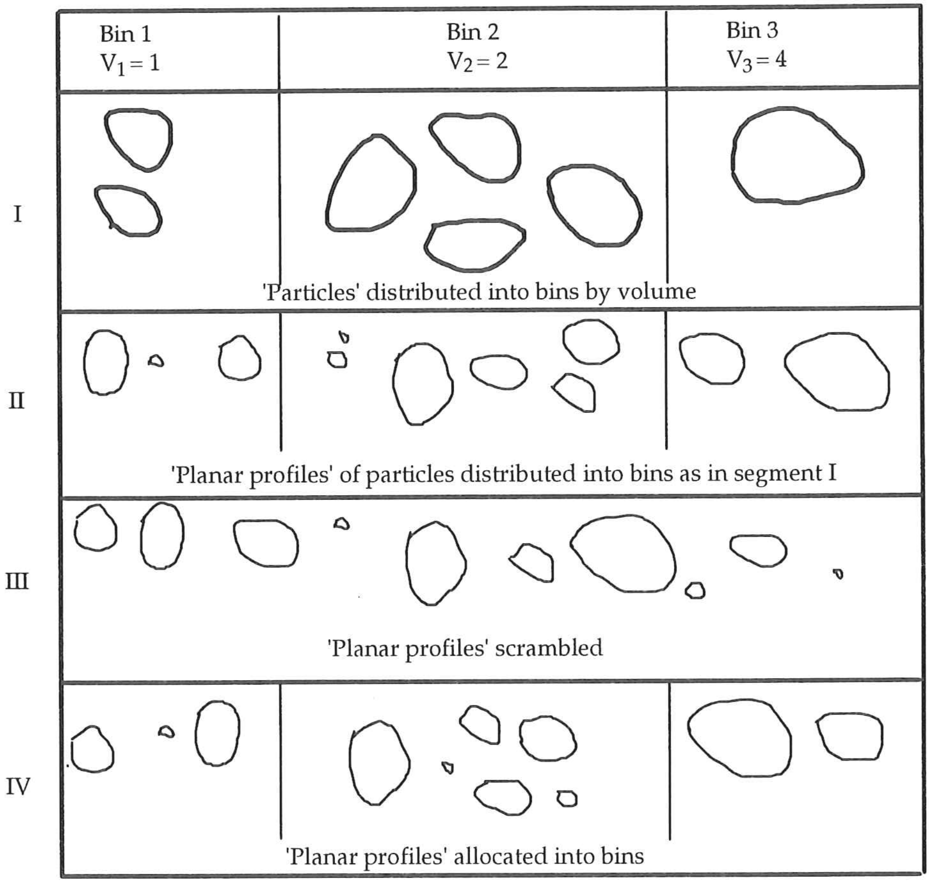

Fig. 1. Figure used to explain the allocation model for estimating the particle volume distribution from planar profiles.

THE PARTICLE VOLUME DISTRIBUTION MODEL

The basis of the particle volume distribution model is to allocate the planar profiles into bins so that the solution appears 'reasonable'. One would therefore expect that the estimated particle volume corresponds closely to the actual solution.

The question is: what useful information can be used to find a reasonable solution? Geometric probability, or integral geometry, gives stereological equations which, for convex particles (Miles, 1985), are independent of particle shape. The equations are based on the assumptions that sectioning is isotropic and uniform.

The geometric probability equations presented by Jensen (1991), Jensen & Gundersen (1985, 1987) and Gay (1995a&b) are the basis of the model. The equations are:

$$E_V(V^2)/E_V(V) = 2\, E_A(A^2\, d)/E_A(A) \quad (1)$$

$$E_V(V^3)/E_V(V^2) = 2\,\pi\; E_A(A^3\, \Delta)/E_A(A^2\, d) \quad (2)$$

$$E_V(S\, V)/E_V(S) = \pi/4\;\; E_A(A\, B\, s)/E_A(B) \quad (3)$$

Here V is volume and A is area. E() is the statistical expected value by number; with E_V implying with respect to volume and E_A with respect to planar profiles. d is average distance between all pairs of points within the same planar profile (see Fig.2). Δ is the average triangular area formed from all combination of three points within the same planar profile (see Fig. 3).

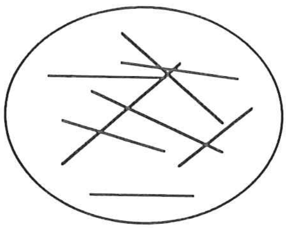

Fig. 2. Estimation of the average distance between pixels.

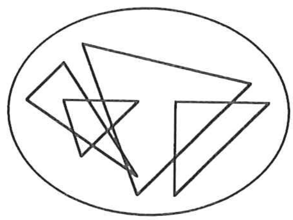

Fig. 3. Estimation of the average triangular area between pixels.

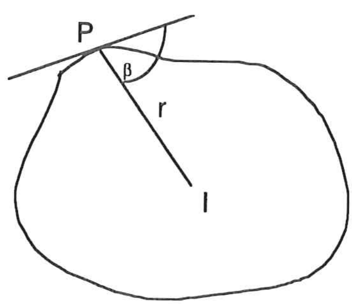

Fig. 4. Illustration for a planar profile indicating variables used to estimate the parameter 's'.

The parameter s in eqn. (3) is given by:

$$s = E\{\; r\, [\, \cos(\beta) + (\pi/2\text{-}\beta)\, \sin(\beta)]\; \} \quad (4)$$

In eqn. (4) the mean is with repect to both interior points within a planar profile and points on the perimeter. Fig. 4 illustrates. I is an interior point and P is a perimeter point. A ray intercept is constructed from the two points. r is the length of the ray intercept; β is the angle between the ray intercept and the tangent to the perimeter.

For particles of uniform volume, the left-hand side of Eqs. 1 to 3 is volume. Hence in segment II of Fig.1, one can see that when the equations are applied to the planar profiles within each bin the three geometric probability equations approximately equal the bin particle volume. This is the information needed to allocate the planar profiles given in segment III.

The planar profiles are sorted so that the three geometric probability equations within each bin provide reasonable estimates of the bin particle volume. The algorithm examines each planar profile and allocates it into a bin so that the sum of squares of the deviation of the geometric probability estimates from the bin particle volumes is minimised. The sorting algorithm is iterative so that once planar profiles are allocated they are continuously reallocated until convergence is reached. As well as the geometric probability equations the model also takes advantage of some realistic conditions. These conditions are that the particle shapes change smoothly from one bin to the next, the distribution is smooth and the density distribution has only one local maxima. These conditions are incorporated into the sorting algorithm by adding penalty functions. Full details of the model are given by Gay (1995a).

NUMERICAL VERIFICATION

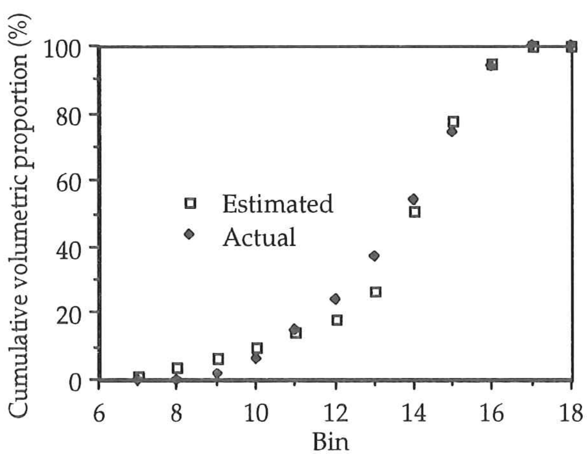

Fig. 5. Comparison of the actual and estimated particle volume distributions for the numerical simulation. A difference of four bins corresponds to a doubling in particle volume.

The particle volume model was verified both numerically and experimentally. For the numerical verification, sectioning was simulated through ellipsoids. The distribution of the ellipsoids varied using the following formulae:

ampx = 4 ... 6; ampy = ampx/4 ... ampx/3, and ampz = ampx/4 ... ampy.

Thus there is some variation in shape for both particles of the same volume and particles of different volume.

The computer program to section the ellipsoids also kept a record of the actual volume of the ellipsoid from which each planar profile was created. The particle volume distribution was divided into bins. The minimum particle volume for each bin is given by:

$$V_{min} = 4/3\ \pi\ 2^{Bin/4} \tag{5}$$

Hence the bins represent a fourth root 2 series in particle volume, or alternatively a difference in four bins corresponds to a doubling of particle volume.

Fig. 5 shows the estimated distribution compared with the actual distribution. There is reasonable agreement between the two distributions. The average discrepancy between the two distributions is 0.36 bins.

EXPERIMENTAL VERIFICATION

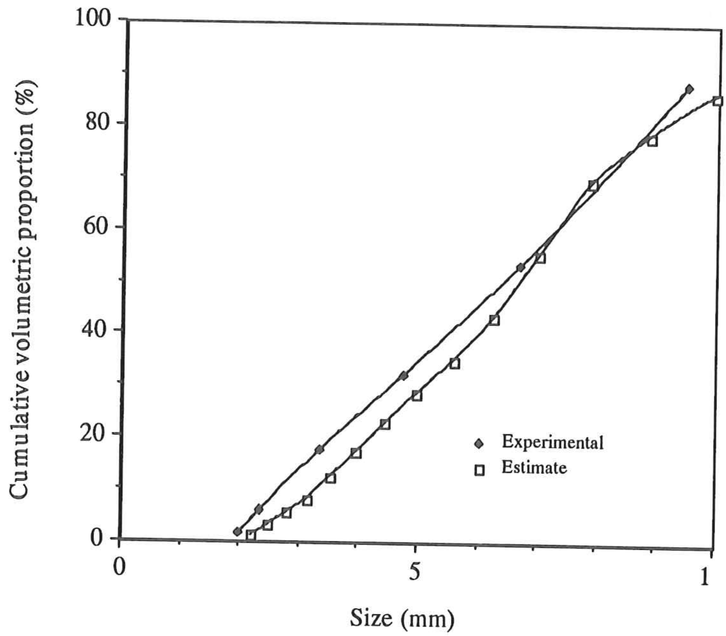

Fig. 6. Comparison of the stereologically-estimated size distribution with the experimental size distribution.

A set of particles were size-classed using sieving. Thus the 'size' distribution of the particles was estimated. These particles were sectioned and the particle volume distribution model was applied to the planar profiles. To estimate the relationship between mesh size and particle volume, particles from a narrow size class were also sectioned and a calibration constant was calculated. Using this calibration constant the relationship between particle volume distribution and size distribution was estimated.

Fig. 6 shows the stereologically-estimated and actual size distributions. It is clear that the stereologically-estimated size distribution is a reasonable approximation of the experimental size distribution. The largest discrepancy between the two distributions occurs at about 4 mm. In this case, it appears that about 25% of particles are less than 4 mm whereas the model estimates that 25% of particles are less than 4.6 mm. It is suggested that for most practical applications this discrepancy is negligible.

DISCUSSION AND CONCLUSIONS

The numerical simulation represents only one of three simulations contained in Gay's (1995) thesis. The results for the other two simulations were similar to that presented here in that the three geometric probability equations were verified and the particle volume distribution model was very accurate.

Both the numerical and experimental tests showed that for most practical purposes the particle volume distribution model was reasonably estimated by the particle volume distribution model. The particle volume distribution model is based on the density distribution having only one local maximum. The model should not be used in circumstances where this assumption is not true. With the inclusion of more geometric probability equations, such as those derived by Gay (1995a) the model will be even more accurate.

ACKNOWLEDGMENTS

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