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Methods for Estimating the Sizes of Large Inclusions in Clean Steels

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Abstract

The sizes of large inclusions within a cast of hard steel have a major influence on fatigue characteristics, but are not directly measurable by routine means. Recently, two methods have been proposed for estimation of the size distribution of large inclusions on the basis of measurements made on the sections of inclusions revealed in samples from a polished plane surface of the material. This paper reviews the two methods, showing that they are closely related and that properties found by each may be deduced from those found by the other. The paper also discusses the problem of inferring the distribution of the projected (3-dimensional) size of large inclusions from measurements made by either of the methods on sectional (2-dimensional) sizes. A simple new approximate solution to this stereological problem is proposed and is compared to existing approaches.

Keywords: STEELS; FATIGUE; IMAGE ANALYSIS; THEORY; STATISTICS OF EXTREMES

1 Introduction

The sizes of large inclusions within a cast of hard steel have a major influence on fatigue characteristics (Murakami [1]), and are therefore important indicators of the quality of the steel. However the sizes of inclusions vary from sample to sample and they cannot be measured directly by routinely-usable methods. It is therefore necessary to describe sizes by a statistical distribution and to use indirect methods of measurement to estimate this distribution. Knowledge of the distribution of large sizes enables the user to estimate such quantities as the typical size of the largest inclusion in a given volume of steel and to calculate the probability that the largest inclusion in a volume will exceed any specified size.

It was shown by Murakami & Usuki [2] and Murakami *et al* [3] that the effect of inclusion size on the fatigue limit can be quantified in terms of the square roots of the areas of large inclusions projected onto a plane perpendicular to the direction of stress. In this paper we therefore consider measurements of large inclusions revealed in polished sections of the steel. We review two ways of collecting such measurements and of processing the results to obtain estimates of the distribution of the largest inclusion in a volume. One of the methods, the Area Maximum (AM) method, first proposed in this field by Prof Y Murakami and co-workers, is based on the Gumbel distribution of statistical extreme value theory. The other method is based on the analysis of inclusions larger than a specified high threshold (Shi *et al* [4] and Davison & Smith [5]). There is a family of such *threshold methods*, differing in the distribution assumed for sizes exceeding the threshold. We consider here the particular threshold method, the Threshold Exponential or TE method, which assumes an exponential distribution for sizes larger then the threshold. Of all the threshold methods, this has the closest connection with the AM method. In both the AM and TE approaches the variable measured is the *sectional* size of inclusions, whereas the aspects of interest for fatigue properties are the sizes of the *projected* areas of inclusions. A stereological translation from *section sizes* to *projection sizes* will therefore be a necessary part of the estimation procedures.

This paper has two aims. The first is to show that although the AM and TE methods are based on measurements of different quantities and require different calculations they share a common basis in statistical extreme value theory. This knowledge is useful in clarifying the purposes for which each method can be used and for translating results between the two. The second aim of the paper is to exploit the connection between methods to derive a new approximate relationship between the distributions of *section size* of large inclusions revealed on a plane surface and the distribution of the true, but usually unobserved, 3-dimensional *projection size*. We suppose that, to a reasonable approximation, inclusions are spherical. The 3-dimensional size of an inclusion then coincides with its size as projected onto a plane surface. Prof Murakami's experimental work, summarized in [1], shows that it is the distribution of this projected size that is crucial for fatigue properties.

The plan of the paper is as follows. In §2 the AM and TE methods are reviewed and in §3 it is shown that both methods rest on a widely applicable model for the behaviour of the upper tail of the distribution of sizes of individual inclusions. The discussion reveals the relationship between characteristics of large inclusions estimated by the two approaches and it allows translation between the two. In §4 we discuss the extension from areal properties of inclusions revealed in measurements on planar sections to the volume properties crucial for fatigue. A new approximate practical solution to the stereological problem for large inclusions is presented and compared to existing approaches. The paper concludes in §5 with a summary and a discussion of the implications of the stereological approximations of §4.Appendices contain some technical material. For convenience in the stereological comparisons we discuss size in terms of the diameters of spheres or circles rather than in terms of square root areas, a difference merely of a constant of proportionality.

2 The Two Approaches

The basic procedures of the AM and TE methods are now described, including parameter estimation and graphical model checking. For clarity of exposition we restrict attention here to *section* sizes; the stereological translation to the largest *projection* inclusion size in a specified volume of steel is taken up in §4.

2.1 Area Maximum Approach

For the AM method (see for example Murakami [1], ESIS [6] and Beretta & Murakami [7]) a number, n say, of separate regions (*control areas*), each of the same area A_0 say, are chosen on the polished surface, and the diameter of the largest inclusion within each region is recorded. The result is a set of n observations of maximum diameters, $x_1, \ldots, x_n$ say. A Gumbel extreme value distribution is fitted to these data. The Gumbel distribution has distribution function

$$G(x : \lambda, \delta) = Pr(\text{Size} \leq x) = \exp\left\{-\left(\exp -\frac{x-\lambda}{\delta}\right)\right\}, \qquad (-\infty < x < \infty), \tag{2.1}$$

where $\delta > 0$ and λ are parameters, δ measuring variability and λ representing a typical size of the largest inclusion. In fact λ is the e^{-1} quantile of the distribution G and is referred to as the *characteristic largest* inclusion size in area A_0.

Several methods are available for estimating the parameters λ and δ. The simplest method is a graphical procedure based on the Gumbel plot. Suppose that the data are ordered from smallest to largest as $x_{(1)} \leq x_{(2)} \leq \ldots \leq x_{(n)}$. Then the Gumbel plot is a plot of $-\ln(-\ln(j/(n+1)))$ against $x_{(j)}$. Under the Gumbel distribution the points are expected to lie close to the line with slope $1/\delta$ and intercept $-\lambda/\delta$. Rough estimates of the parameters may be obtained from this. The linearity or otherwise of the plot also gives an informal check on adequacy of the Gumbel distribution and a simple way of comparing different data sets.

A more objective estimation procedure is based on maximum likelihood. The log-likelihood of the parameters based on data $x_1, x_2, \ldots, x_n$ is

$$l(\lambda, \delta) = \sum_j \ln G'(x_j : \lambda, \delta),$$

where G' is the probability density function of the Gumbel distribution function (2.1), that is, the derivative of G with respect to x. The function $l(\lambda, \delta)$ is maximized numerically with respect to λ and δ to obtain the maximum likelihood estimates of the parameters. (An EXCEL spreadsheet for the estimation is available at `http:/www.esisweb.org/activity/activity.htm`; see also ESIS [6]; and R-software to carry out these and related calculations is available at `http://www.maths.lancs.ac.uk/~stephena/ software`.) Besides the advantage of greater objectivity, the maximum likelihood method also gives standard errors: the negative of the inverse of the matrix of second derivatives of the log-likelihood with respect to λ and δ gives the variance-covariance matrix of the estimates. Beretta & Murakami [7] report extensive simulation experiments demonstrating the efficiency of the maximum likelihood estimates.

The fitted distribution may be used to estimate the size of the largest inclusion in a plane region larger than the control area A_0, or to compare largest inclusions from control areas of different sizes. For example the size of the largest inclusion in an area $A > A_0$ is a random quantity whose distribution is given by:

$$G^{A/A_0}(x : \lambda, \delta) = G(x : \lambda + \delta \ln(A/A_0), \delta). \tag{2.2}$$

The location parameter of this distribution, the characteristic value x_c,

$$x_c = \lambda + \delta \ln(A/A_0), \tag{2.3}$$

may be taken as a single summary value of the size of the largest inclusion in A.

An alternative single summary value is sometimes suggested, by analogy with the return level used to quantify hydrological and meteorological extremes. If A is an integer multiple of A_0 then a typical value for the largest inclusion in A can be defined as the size that would be expected to be exceeded by exactly one of the maxima from the A/A_0 sub-regions. The expected number of sub-region maxima larger than a size x is, from (2.1), $(A/A_0)(1 - G(x : \lambda, \delta))$, so the value of x that makes this expectation equal to 1 is

$$x = \lambda + \delta(-\ln(-\ln(1 - A_0/A))). \tag{2.4}$$

Expression (2.4) is referred to as the size of the maximum inclusion with return period $T = A/A_0$, and the same terminology is used even if A/A_0 is non-integer. Though the motivation for expressions (2.3) and (2.4) is different, in the important case when A_0 is small compared to A their numerical values are close. Indeed, when A_0/A is small, $-\ln(1-(A_0/A)) \approx A_0/A$ so that the logarithmic terms in (2.3) and (2.4) are almost the same.

2.2 Threshold Exponential Approach

For the TE method either a single area of the polished plane section of steel or multiple sub-areas are chosen for study. All inclusions on the total inspected area larger than a given size, u_0 say (called the threshold), are measured. Alternatively, for a pre-determined number N, the N largest inclusions on the total inspected area are measured, and the threshold value u_0 is then set equal to the size of the smallest of these. In either case, a set of measurements

$x_1, x_2, \ldots, x_N$ of the N diameters of all inclusions no smaller than u_0 in the inspected area is obtained. The statistical analysis is made on the excesses of these sizes over the threshold, that is on the values $y_i = x_i - u_0, i = 1, \ldots, N$. An exponential distribution with distribution function

$$H(y : \alpha) = 1 - e^{-y/\alpha}, \qquad (y > 0), \tag{2.5}$$

where α is a positive parameter, is fitted to these excess sizes by estimating the parameter α by the arithmetic mean $\bar{y}$ of $y_1, y_2, \ldots, y_N$:

$$\hat{\alpha} = \bar{y}. \tag{2.6}$$

Also, the rate of occurrence, $\mu(u_0)$ say, of inclusions of size greater than u_0 in the inspected area is estimated by

$$\hat{\mu}(u_0) = N/A_1, \tag{2.7}$$

where A_1 is the total area inspected.

These results may be used to estimate the size of the largest inclusion in other plane regions. For example, as will be shown in §3, under the assumptions of the TE Method the distribution of the largest inclusion in a region of area A has the Gumbel distribution function $G(x : \lambda, \delta)$ with parameters

$$\lambda = u_0 + \alpha \ln(A\mu(u_0)) \qquad \text{and} \qquad \delta = \alpha, \tag{2.8}$$

and these may be estimated by substituting $\hat{\alpha}$ and $\hat{\mu}(u_0)$ from (2.6) and (2.7).

For a single summary value for the size of the largest inclusion in region A, the location parameter λ in (2.8) may be employed, as in §2.1. In §2.1 an alternative motivation for this characteristic size of the largest inclusion in A was discussed, based on a return level argument. The natural analogue of this notion in the TE approach is the size that would be expected to be exceeded by exactly one inclusion within the region A. However, the results in §3 show that the resulting value is exactly the same as that given by expression (2.8).

To check the main assumption of the TE method (that of an exponential distribution for the excess sizes y), and to allow quick visual comparison of different sets of data, a Gumbel plot related to that in §2.1 may be used. Specifically, a plot of $-\ln(-\ln(j/(n+1)))$ against the reversed ordered values of $-\ln y_j$ should, if (2.5) is satisfied, produce an approximate straight line with unit slope and intercept $\ln \alpha$. In principle this could be used to estimate α, but is not necessary or advisable for that purpose because of the simplicity of (2.6) and the fact that (2.6) is already the maximum likelihood estimator, with corresponding optimality properties. On the other hand the plot may be used to check a proposed value for u_0. If this u_0 is used to calculate the y_j and a straight line plot is found, then u_0 and the assumption of an exponential distribution are vindicated. If there is definite non-linearity then a larger u_0 should be tried.

2.3 Relationship Between TE and AM Approaches

The relationship between the AM and TE approaches hinges on the relationship between the distribution of the size of the largest inclusion in an area (§2.1), and the distribution of excess size of inclusions larger than some high threshold (§2.2). A key factor in the relationship is the number of inclusions in a region, since the larger the number of inclusions, the greater the chance of observing a larger maximum. For a region of area A let $N(A)$ denote the random number of inclusions in A. In homogeneous material the distribution of $N(A)$ will depend only on the size of A and not on its shape or position, so that the expectation of $N(A)$ will be $E(N(A)) = \mu A$, where μ is the expected number of inclusions in unit area; that is, the rate of occurrence of inclusions. Moreover, if inclusions in separate regions are independent and occur sparsely enough never to coincide, then their locations will be described by a Poisson process (Stoyan *et al* [8]), so that the distribution of $N(A)$ will be Poisson with mean μA:

$$Pr(N(A) = k) = e^{-\mu A}(\mu A)^k/k!, \qquad k = 0, 1, \ldots$$

We can apply the same logic to large inclusions alone. For example, the distribution of the number, $N(A, u_0)$ say, of inclusions of size greater than a threshold size u_0 in area A is Poisson with mean $\mu(u_0)A$, where $\mu(u_0)$ is the expected number of inclusions of size greater than u_0 in unit area. Similarly for even larger sizes, say sizes greater than $u > u_0$, the number $N(A, u)$ of inclusions in A of size greater than u is Poisson distributed with mean $\mu(u)A$, where $\mu(u)$ is the appropriate expected number per unit area. Moreover, since inclusions in A of size greater than u form a proportion $Pr(X > u|X > u_0)$ of those larger than u_0, where X is inclusion size, $E(N(A,u)) = \mu(u)A$ is

$$\begin{aligned} E(N(A,u)) &= E(N(A,u_0)) \times Pr(X > u|X > u_0) \\ &= \mu(u_0)A Pr(X > u|X > u_0), \end{aligned}$$

and hence

$$\mu(u) = \mu(u_0)\, Pr(X > u|X > u_0)$$

so that *the distribution of* $N(A,u)$ *is Poisson with mean* $\mu(u_0)A\, Pr(X > u|X > u_0)$.

It is this fact that connects the threshold and area maximum approaches. The largest inclusion in area A, M say, will be no larger than u if and only if $N(A,u) = 0$. Hence, from the Poisson distribution,

$$\begin{aligned} Pr(M \leq u) &= Pr(N(A,u) = 0) \\ &= \exp(-\mu(u_0)\, A\, Pr(X > u|X > u_0)). \end{aligned} \tag{2.9}$$

If, as in §2.2, the conditional distribution of excess size $Y = X - u_0$, given that $X > u_0$, is exponential, then it follows that for any $u > u_0$,

$$\begin{aligned} Pr(X > u|X > u_0) &= Pr(Y > u - u_0|X > u_0) \\ &= e^{-(u-u_0)/\alpha} \end{aligned}$$

and so from (2.9)

$$\begin{aligned} Pr(M \leq u) &= \exp(-\mu(u_0)Ae^{-(u-u_0)/\alpha}) \\ &= \exp(-\exp(-(u-\lambda)/\delta)), \end{aligned}$$

for $u > u_0$, where

$$\lambda = u_0 + \alpha \ln(\mu(u_0)A) \qquad \text{and} \qquad \delta = \alpha. \tag{2.10}$$

Thus an exponential distribution for the excess size over threshold u_0 implies a Gumbel distribution for the largest inclusion M in an area, and the parameters are related by (2.10).

Conversely, if M has the Gumbel distribution $Pr(M \leq u) = \exp(-\exp(-(u-\lambda)/\delta))$, then by equating (2.1) and (2.9) we see that

$$\begin{aligned} Pr(X > u|X > u_0) &= \tfrac{1}{\mu(u_0)A} \exp(-(u-\lambda)/\delta), \quad \text{for } u > u_0 \\ &= \exp(-(u - \lambda + \delta \ln(\mu(u_0)A))/\delta), \end{aligned}$$

and since the left hand side takes the value 1 when $u = u_0$, it must be true that $u_0 = \lambda - \delta \ln(\mu(u_0)A)$ and hence that

$$Pr(X > u | X > u_0) = \exp(-(u - u_0)/\delta).$$

Thus a Gumbel distribution for M implies that excess size over u_0 must follow an exponential distribution, again with parameters related through (2.10).

In this sense therefore the AM and TE approaches are based on equivalent assumptions, with parameters related through (2.10).

2.4 Precision of Estimation

Anderson *et al* [9] compared the widths of confidence intervals for the characteristic size x_c obtained from the AM and TE methods. They found that for a clean air-melted steel in which the AM method utilized observations on $N = 40$ maximum inclusion sizes in control areas of size $A_0 = 200\text{mm}^2$, and the TE method was based on the sizes of all inclusions larger than $5\mu\text{m}$ in the total 8000mm^2 area inspected (395 inclusions altogether), the widths of 95% confidence intervals for x_c for a wide range of extrapolation areas A (10^3–10^8mm^2) were related by

$$\text{width(AM)} = -1.34 + 2.12\,\text{width(TE)},$$

to a good approximation. At $A = 10^3\text{mm}^2$ the width of the TE-based interval was 77% of the width of the AM-based interval, declining to 52% at $A = 10^8\text{mm}^2$. Though the details of these findings are specific to the steel analyzed, Anderson *et al* [9] give reasons to expect the TE method to give shorter confidence intervals generally.

3 Justifications

3.1 Justification for Area Maxima Method

The choice of the Gumbel distribution for observed maximum sizes is motivated in part by a limit result from extreme value theory, which shows that the distribution of the maximum of N independent and identically distributed observations, standardized for location and scale, converges to a Gumbel distribution as $N \to \infty$ for a very wide range of distributions of the individual observations, including Normal, log-Normal, exponential and Weibull distributions (in fact for any distribution of individual observations X for which $P(X > x)$ decays like an exponential of a polynomial in x); see, for example, Leadbetter *et al* [10]. A further, related, justification for use of the Gumbel distribution is its possession of the following stability property. Suppose that from a number $N = m \times k$ of independent and identically distributed observations we select the largest. Though the selection may be made directly, it could also be made in two stages: say by firstly selecting the largest of each successive set of m values, then taking the largest of the k resulting subset maxima. If individual observations have distribution function F then the fact that the two routes lead to the same result is expressed by the relation

$$F^N = (F^m)^k, \tag{3.1}$$

since, for any n, F^n is the distribution function of the maximum of n observations. If we wish to model maxima of different numbers of observations by a distribution function, G say, of some common general form, differing for different numbers only in location and scale, then if $G(x)$ is the distribution function of the maximum of m observations, the distribution function of the maximum of all N should be of form $G(Ax + B)$ for some constants $A > 0$ and B, and the relation (3.1) would require

$$G(Ax + B) = G^k(x),$$

which is called the max-stability condition for G. This condition limits the possible forms for G, but it is easily verified that the Gumbel distributions $G(x : \lambda, \delta)$ satisfy it with $A = 1/\delta$ and $B = -\ln k$.

Thus the Gumbel distributions constitute a family of models for data on maxima that can be expected to provide reasonable approximations whatever the distribution of individual measurements, and which embody in a simple way a fundamental structural feature of the data. Other distributions sometimes proposed – log-Normal distributions for example – do not share these properties.

3.2 Justification for Threshold Method

A justification for the key exponential assumption (2.5) of the ET method is that for a wide range of distributions of the size of individual measurements X the distribution of excess $X - u_0$ over a threshold u_0, for those sizes X that do exceed u_0, is approximated by an exponential distribution when u_0 is large enough. In fact it is found that whenever the distribution of individual sizes X has the property that maxima can be approximated by a Gumbel distribution then the distribution of excesses $Y = X - u_0$ over threshold u_0 may be approximated by an exponential distribution in the sense that

$$Pr(Y \leq y | X > u_0) \approx 1 - e^{-y/\alpha}, \quad (y > 0).$$

for large u_0 and some positive number α (Pickands [11]). Thus the exponential distribution is appropriate for excess sizes over a high threshold whenever the Gumbel distribution is appropriate for maxima. A second argument for use of the exponential distribution for excesses is that it is invariant to the value of the threshold, in the sense that if excesses $X - u_0$ of a threshold u_0 follow the exponential distribution (2.5) then (as is easily seen) for a higher threshold u_0' excesses over u_0', given that X indeed exceeds u_0', follow exactly the same exponential distribution (2.5) (the 'lack of memory' property: Feller [12].) Thus an exponential model for excesses has the property that the form of the model does not change as u_0 increases, an attractive property since the threshold value is in a sense incidental and should not be central to inference.

4 Stereology - the Largest Inclusion in a Volume

As shown in §3, the assumption of a Gumbel distribution for the sectional size of the largest inclusion observed in a control area is equivalent to the assumption of an exponential distribution for section sizes greater than a given threshold. Under these assumptions we now discuss the problem of estimating the distribution of the largest projection (3-dimensional) size of the inclusions in a volume; that is, of translating the information about planar sizes of large inclusions into information about spatial sizes. To do so we suppose that, to a reasonable approximation, inclusions are spherical and occur randomly within the material. We also assume that the density of inclusions is low enough to enable us to ignore the possibility of intersections.

To relate the exponential distribution of planar sectional sizes to the distribution of 3-dimensional projection sizes we use the inverse Wicksell transformation (Stoyan *et al* [8]). An alternative to assuming an exponential distribution for large section diameters would be to take section *areas* to be exponentially distributed, so that section diameters would follow a Rayleigh distribution. As Takahashi & Sibuya [13,14] point out, this would produce the mathematical simplification that under the Wicksell transformation projection diameters would follow an exact Rayleigh distribution too. However in many steels it is diameters rather than areas of large inclusions that are exponentially distributed and hence correspond to maxima that follow a Gumbel distribution, and so we concentrate here on this case. Figure 1 shows Gumbel plots of control area planar maximum inclusion diameters from a medium Carbon steel (Murakami [1]); the curvilinearity of the plot (a) for squared diameters contrasts with the approximate linearity of the plot (b) for diameters, confirming through the relationship in §2 that for this example an exponential model for section diameters rather than for areas is appropriate.

4.1 The Distribution of the Maximum Diameter of a Sphere

We derive the distribution of the diameter of the largest sphere in a volume on the assumption that the excesses over the threshold u_0 of the diameters D_a of sectional circles larger than u_0 are exponentially distributed with mean α. In general the distribution function F_{D_v} of the diameter D_v of a sphere is given by the inverse Wicksell transform of the distribution of the diameter of the sectional circle (Stoyan *et al* [8], p354). In the present case the inverse transform gives:

$$F_{D_v}(x) = 1 - \frac{2d_v}{\pi\alpha}\int_x^\infty \frac{e^{-(y-u_0)/\alpha}}{(y^2-x^2)^{1/2}}\,dy, \quad x \geq u_0,$$

where $(1/\alpha)e^{-(y-u_0)/\alpha}$, $y \geq u_0$, is the probability density of the diameter of the sectional circle in the range of sizes above the threshold. Here d_v is the mean sphere diameter. The conditional distribution of the sphere diameter given that it is larger than the threshold u_0 is:

$$F_{D_v|D_v>u_0}(x) = 1 - \frac{J(x/\alpha)}{J(u_0/\alpha)}, \quad x \geq u_0, \tag{4.1}$$

where

$$J(y) = \int_y^\infty \frac{e^{-z}}{(z^2 - y^2)^{1/2}}\, dz$$

This distribution is evidently independent of the parameter d_v. To find the distribution of the size of the largest sphere in a volume V we can argue as in §2.3, making use of the Poisson distribution. If μ_v is the mean number of spheres with diameters larger than u_0 in unit volume and if $x > u_0$, then the expected number of spheres with diameters greater than x in volume V is $\mu_v V(1 - F_{D_v|D_v > u_0}(x))$. The probability that the maximal inclusion diameter D_{vmax} in volume V is no greater than x is then the probability that there are no inclusions of size greater than x in V, which, from the Poisson distribution, is

$$F_{D_{vmax}}(x) = \exp\left\{-\mu_v V(1 - F_{Dv|Dv \geq u_0}(x))\right\}, \quad x \geq u_0.$$

The mean number of spheres μ_v is shown in Appendix A to be related to the mean number μ_a of circles with diameter larger than u_0 in a unit control area by:

$$\mu_v = \frac{2\mu_a}{\pi\alpha} e^{u_0/\alpha}\, J(u_0/\alpha). \tag{4.2}$$

In Appendix B it is also shown that if we write

$$J(x) = \sqrt{\frac{\pi}{2}} x^{-1/2} e^{-x} I(x) \tag{4.3}$$

then

$$\left(1 + \frac{1}{4x}\right)^{-1/2} \leq I(x) \leq 1. \tag{4.4}$$

When (4.1) – (4.3) are inserted into the expression for $F_{D_{vmax}}(x)$ we find that

$$F_{D_{vmax}}(x) = \exp\left\{-\frac{\mu_a V}{\alpha}\sqrt{\frac{2}{\pi}\frac{\alpha}{x}} \exp\left(-\frac{x - u_0}{\alpha}\right) I(x/\alpha)\right\} \tag{4.5}$$

In this expression the two quantities μ_a and α are unknown and must be estimated from the section measurements. How this is done differs between the AM and the TE methods, as follows.

4.2 Stereological Details for the TE-Method

With this method estimates of both α and μ_a are directly available from

$$\hat{\alpha} = \bar{x} - u_0, \qquad \hat{\mu}_a = \hat{\mu}(u_0) = N/A_1$$

where $\bar{x}$ is the mean of the observed inclusion diameters larger than u_0, N is the total number of inclusions with diameter greater than u_0, and A_1 is the total area over which measurements were made. Inserting these estimates in (4.5) gives the final estimate of the distribution of the maximum inclusion size in a body of volume V

$$\hat{F}_{D_{vmax}}(x) = \exp\left\{-\frac{V\hat{\mu}_a}{\hat{\alpha}}\sqrt{\frac{2}{\pi}\frac{\hat{\alpha}}{x}}\exp\left(-\frac{x-u_0}{\hat{\alpha}}\right)I\left(\frac{x}{\hat{\alpha}}\right)\right\} \tag{4.6}$$

$$\approx \exp\left\{-\frac{V\hat{\mu}_a}{\hat{\alpha}}\sqrt{\frac{2}{\pi}\frac{\hat{\alpha}}{x}}\exp\left(-\frac{x-u_0}{\hat{\alpha}}\right)\right\} \tag{4.7}$$

Here, $I(x/\hat{\alpha})$ is easily calculated numerically, or can be replaced by $(1+\hat{\alpha}/4x)^{-1/2}$ with an error less than 2% when $x/\hat{\alpha} > 1$, or by 1 with a slightly larger error. The latter leads to the approximation given in (4.7). The characteristic size x_c corresponding to volume V is obtained as the solution to the equation $F_{D_{vmax}}(x) = e^{-1}$. An exact analytic solution of this equation is not available, but numerical solution is straightforward. The following approximate solution (4.8) for large volumes V can be verified by inserting it into (4.7) and noting that the leading term in (4.8) is $\hat{\alpha}\ln(V\hat{\mu}_a/\hat{\alpha})$ when $V \to \infty$:

$$\hat{x}_c = u_0 + \hat{\alpha}\ln\left(\frac{V\hat{\mu}_a}{\hat{\alpha}}\sqrt{\frac{2}{\pi}}\right) - \frac{\hat{\alpha}}{2}\ln\left(\ln\left(\frac{V\hat{\mu}_a}{\hat{\alpha}}\sqrt{\frac{2}{\pi}}\right)\right) \tag{4.8}$$

The expressions (4.6) and (4.8) are estimates subject to uncertainty. The uncertainty may be expressed through confidence intervals for the true parameter values. This is particularly simple for the TE-method, since the estimates $\hat{\alpha} = \bar{x} - u_0$ and $\hat{\mu}(u_0) = N/A$ are independent and their standard deviations can be estimated by $\hat{\alpha}$ and $\sqrt{N/A}$ respectively. A Gaussian approximation based on a first order Taylor expansion of $\bar{x} - u_0$ and N/A around their expected values α and μ_a gives estimates of the standard deviations of $F_{D_{vmax}}(x)$ and x_c: see, for example, Coles [15]. Confidence intervals based on the approximate Normality of maximum likelihood estimators are then directly available. An alternative, likely to be more accurate in small samples, is to base confidence intervals on profile likelihood. See Coles [15].

4.3 Stereological Details for the AM-Method

In this case we solve (2.8) and replace unknown quantities with their estimates to get

$$\hat{\alpha} = \hat{\delta}, \qquad \hat{\mu}_a = \hat{\mu}(u_0) = A_0^{-1}\exp\left(\frac{\hat{\lambda} - u_0}{\hat{\delta}}\right),$$

where $\hat{\lambda}$ and $\hat{\delta}$ are the maximum likelihood estimates of the Gumbel parameters. By (4.5) the distribution of the maximum inclusion size in a body of volume V then is estimated by

$$\hat{F}_{D_{vmax}}(x) = \exp\left\{-\frac{V}{\hat{\delta}A_0}\sqrt{\frac{2}{\pi}\frac{\hat{\delta}}{x}}\exp\left(-\frac{x-\hat{\lambda}}{\hat{\delta}}\right) I(x/\hat{\delta})\right\} \tag{4.9}$$

$$\approx \exp\left\{-\frac{V}{\hat{\delta}A_0}\sqrt{\frac{2}{\pi}\frac{\hat{\delta}}{x}}\exp\left(-\frac{x-\hat{\lambda}}{\hat{\delta}}\right)\right\} \tag{4.10}$$

Here $I(x/\hat{\delta})$ as above can be calculated numerically or replaced by $\left(1+\hat{\delta}/4x\right)^{-1/2}$ or by 1, which leads to the approximation in (4.10). Again, to estimate the characteristic size x_c corresponding to the volume V requires numerical solution of $F_{D_{vmax}}(x) = e^{-1}$. Alternatively one can use the approximation

$$\hat{x}_c = \hat{\lambda} + \hat{\delta}\ln\left(\frac{V}{\hat{\delta}A_0}\sqrt{\frac{2}{\pi}}\right) - \frac{\hat{\delta}}{2}\ln\left(\frac{\hat{\lambda}}{\hat{\delta}} + \ln\left(\frac{V}{\hat{\delta}A_0}\sqrt{\frac{2}{\pi}}\right)\right) \tag{4.11}$$

which is verified in the same way as (4.8).

Confidence intervals corresponding to (4.9) and (4.11) are obtained as for the TE-method. The only difference is the estimation of the standard deviations and correlations of the parameter estimates $\hat{\lambda}$ and $\hat{\delta}$. For the maximum likelihood estimators, the correlation matrix of the estimators is obtained as the negative of the inverse of the second derivatives of the log-likelihood with respect to λ and δ, as described in §2.1.

4.4 Uemura & Murakami's Approximation

Uemura & Murakami [16] suggested an approximate solution to the stereological problem of inferring the distribution of the projection size of the largest inclusion in a volume from the distribution of the largest section diameter observed in plane sections. They suggested that the Gumbel distribution of the largest section diameter in a control area A_0 can be taken to be approximately the same as the distribution of the largest projection diameter in a volume $V_0 = A_0 \times h$, where h is the arithmetic mean of the square root areas of the largest sections of inclusions in n measured control areas A_0. The distribution of the projection diameter of the largest inclusion within a larger volume V may then be taken to be approximately

$$G^{V/V_0}(x : \lambda, \delta) = G(x : \lambda + \delta\ln(V/V_0), \delta),$$

so that the characteristic size for the largest inclusion in V is $x_c = \lambda + \delta\ln(V/V_0)$.

This approach can be compared to that in the present paper for the case when sample sizes are large enough for estimates to be close to their true values. Then $2h\sqrt{\pi}$ is approximately equal to the mean $0.577\ \delta + \lambda$ of the Gumbel distribution with parameters δ and λ, and Uemura & Murakami's approximating Gumbel distribution for the largest projection diameter in volume V takes the form

$$\exp\left\{-\exp\left(-\frac{x-\lambda-\delta\ln(V/V_0)}{\delta}\right)\right\} = \exp\left\{-\frac{2V}{A_0\sqrt{\pi}(0.577\ \delta+\lambda)}\exp\left(-\frac{x-\lambda}{\delta}\right)\right\} \quad (4.12)$$

This can be compared to the corresponding expression (4.10). Evidently the two expressions agree if $x = (0.577\ \delta+\lambda)^2/(2\delta)$, and are similar for x close to this value. Figure 2(a) shows the difference between the Uemura- Murakami estimate of the characteristic size of the largest inclusion in volume V obtained from (4.12) and the exact value obtained by equating (4.9) to e^{-1} and solving numerically. The result is plotted in relation to the scale parameter δ for typical values of λ/δ and the extrapolation factor $K = V/V_0 = 2V/(A_0\sqrt{\pi}(\lambda + 0.577\ \delta))$. There is relatively small variation with K, and the error is less than $\pm 1.5\delta$ for a wide range of Gumbel distributions. For comparison, Figure 2(b) shows the corresponding error in the estimate of the characteristic size obtained by equating (4.10) to e^{-1} and solving numerically. The error is much smaller and decreases with increasing extrapolation.

5 Summary & Conclusions

The paper has shown that the AM and TE methods are related both through the assumptions on which they are based and through the estimates that they yield. However, data requirements of the two methods are different: the AM method needs measurements only of control area maxima, whereas the TE method needs measurements of all inclusion exceeding a threshold size. In compensation the TE method yields more precise estimates of the characteristic size of the largest inclusion in larger amounts of material, and its calculations are very much simpler. It may be the more attractive alternative if automated measuring equipment is available.

Knowledge of the relationship between the methods facilitates derivation of a new solution to the stereological problem for large inclusions, and from that a new approximation. It is found that estimates of the characteristic size of the largest inclusion in a specified volume of material based on this new approximation differ in many cases from Uemura & Murakami's [16] estimates by no more than 1.5 times the scale parameter δ of the Gumbel distribution of section size maxima. Since values of δ might typically lie in the range 0.5–3.5μm, for many purposes Uemura and Murakami's approximation might be adequate. If greater accuracy is needed, then the results of §4, which are easy to evaluate numerically, may be used.

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References

[1] Murakami, Y. (2002) *Metal Fatigue: Effects of Small Defects and Inclusions*, Elsevier, Amsterdam.

[2] Murakami, Y. & Usuki, T. (1989) Prediction of Fatigue Strength of High-Strength Steels Based on Statistical Evaluation of Inclusion Size. *Trans. Jpn. Soc. Mech. Eng. A*, **55**, 213-221.

[3] Murakami, Y. Uemura, Y. & Kawakami, K. (1989) Some Problems in the Application of Statistics of Extreme Values to Estimation of the Maximum Size of Nonmetallic Inclusions in Metal. *Trans. Jpn. Soc. Mech. Eng. A*, **55**, 58-62.

[4] Shi, G., Atkinson, H. V., Sellars, C. M. & Anderson, C. W. (1999) Application of the Generalized Pareto Distribution to the Estimation of the Size of the Maximum Inclusion in Clean Steels. *Acta Mater.*, **47**,1455-1468.

[5] Davison, A. C. & Smith, R. L. (1990) Models for exceedances over high thresholds (with discussion). *J. R. Statist. Soc.* B, **52,** 393-442. **12**, 357–363.

[6] ESIS (2002) *Technical Recommendations for the Extreme Value Analysis of Data on Large Nonmetallic Inclusions in Steels.* Authors: Anderson, C. W., Beretta, S., de Maré, J. &

Svensson, T., *ESIS P11-02*, European Structural Integrity Society, Geesthacht, *pp 29*, ISSN 1616-2129.

[7] Beretta, S. & Murakami, Y. (1998) Statistical Analysis of Defects for Fatigue Strength Prediction and Quality Control of Materials, *Fatigue Fract. Eng. Mater. Struct.,* **21**, 1049-1065.

[8] Stoyan, D., Kendall, W. S. & Mecke, J. (1995) *Stochastic Geometry and its Applications,* 2nd edn., J. Wiley & Sons, Chichester & New York.

[9] Anderson, C. W., Shi, G., Atkinson, H. V., Sellars, C. M. & Yates, J. R. (2003) Interrelationship between statistical methods for estimating the size of the maximum inclusion in clean steels. *Acta Materialia*, **51**, 2331–2343.

[10] Leadbetter, M. R., Lindgren, G. & Rootzén, H. (1983) *Extremes and Related Properties of Random sequences and Processes*, Springer-Verlag, New York, Heidelburg, Berlin.

[11] Pickands, J. III (1975) Statistical inference using extreme order statistics. *Ann. Statist.* **3**,119-131.

[12] Feller, W. (1971) *An Introduction to Probability Theory and Its Applications* Wiley, New York.

[13] Takahashi, R. & Sibuya, M. (1996) The Maximum Size of Planar Section of Spheres and its Application to Metallurgy. *Ann. Inst. Stat. Math.*,**48**, 127-144.

[14] Takahashi, R. & Sibuya, M. (1998) Prediction of the Maximum Size in Wicksell's Corpuscle Problem. *Ann. Inst. Stat. Math.*,**50**, 361-377.

[15] Coles, S. G. (2001) *An Introduction to Statistical Modelling of Extreme Values*, Springer-Verlag, London.

[16] Uemura, Y. & Murakami, Y. (1990) A Numerical Simulation of Evaluating the Maximum Size of Inclusions to Examine the Validity of the Metallographic Determination of the Maximum Size of Inclusions. *Trans. Jpn. Soc. Mech. Eng.*, **56**, 162-167.

Appendix A: Justification of (4.2)

If a plane section is taken at random through a body, it intersects a sphere of diameter $D_v = x$ in a circle with diameter D_a larger than u_0 if the centre of the sphere lies within a slab of thickness $t = (x^2 - u_0^2)^{1/2}$ about the plane. The mean number per unit volume of such spheres with diameter between x and $x + \delta x$ is then $t\mu_v f_{Dv|Dv>u_0}(x)\delta x$, where the conditional density $f_{D_v|D_v>u_0}$ is

$$f_{D_v|D_v>u_0}(x) = \frac{d}{dx}F_{D_v|D_v>u_0}(x) = -\frac{1}{\alpha}\frac{J'(x/\alpha)}{J(u_0/\alpha)}$$

according to (4.1). Hence, summing up over all possible diameters, we get

$$\begin{aligned}
\mu_a &= \mu_v \int_{u_0}^{\infty} f_{D_v|D_v>u_0}(x)(x^2 - u_0^2)^{1/2}\, dx \\
&= -\frac{\mu_v}{\alpha}\int_{u_0}^{\infty} \frac{J'(x/\alpha)}{J(u_0/\alpha)}(x^2 - u_0^2)^{1/2}\, dx,
\end{aligned}$$

which gives

$$\mu_a = -\frac{\alpha\mu_v}{J(u_0/\alpha)}\int_{u_0/\alpha}^{\infty} J'(y)\,(y^2 - \frac{u_0^2}{\alpha^2})^{1/2}\, dy.$$

A result (supported by numerical computations and analytical approximations) for the Bessel function gives

$$-\int_{u_0/\alpha}^{\infty} J'(y)\,(y^2 - \frac{u_0^2}{\alpha^2})^{1/2}\, dy = \frac{\pi}{2}e^{-u_0/\alpha}.$$

From it and (4.2) we obtain:

$$\mu_v = \left(\frac{2\mu_a}{\pi\alpha}\right)\, e^{u_0/\alpha}\, J(u_0/\alpha).$$

Appendix B: Justification of (4.4)

We have

$$\begin{aligned}
J(y) &= \int_y^{\infty} e^{-z}/\sqrt{z^2 - y^2}\, dz \\
&= e^{-y}\int_0^{\infty} z^{-1/2}e^{-z}/\sqrt{z+2y}\, dz \\
&= 2^{-1/2}y^{-1/2}e^{-y}\int_0^{\infty} z^{-1/2}e^{-z}\left(1 + \frac{z}{2y}\right)^{-1/2} dz. \qquad \text{(B.1)}
\end{aligned}$$

Using the inequality $e^{-a/2} \leq (1+a)^{-1/2} \leq 1$ for $a \geq 0$ and the identity $\Gamma(1/2) = \int_0^{\infty} z^{-1/2}e^{-z}\, dz = \sqrt{\pi}$, we obtain

$$\left(1 + \frac{1}{4y}\right)^{-1/2}\sqrt{\pi} \leq \int_0^{\infty} z^{-1/2}e^{-z}\left(1 + \frac{z}{2y}\right)^{-1/2} dz \leq \sqrt{\pi}.$$

Now, comparing (4.3) and (B.1), we observe that

$$I(x) = \int_0^{\infty} z^{-1/2}e^{-z}\left(1 + \frac{z}{2y}\right)^{-1/2} dz/\sqrt{\pi},$$

and hence the approximation is established.

List of Figure Captions

Figure 1: Gumbel Plots for largest planar inclusions in a medium Carbon steel.

(a) Size = Squared Diameter; (b) Size = Diameter.

Dotted lines are informal linear approximations.

Figure 2: Errors in approximations for characteristic size of largest inclusion.

(a) (UM Approximation − Exact)/δ; (b) (New Approximation − Exact)/δ.

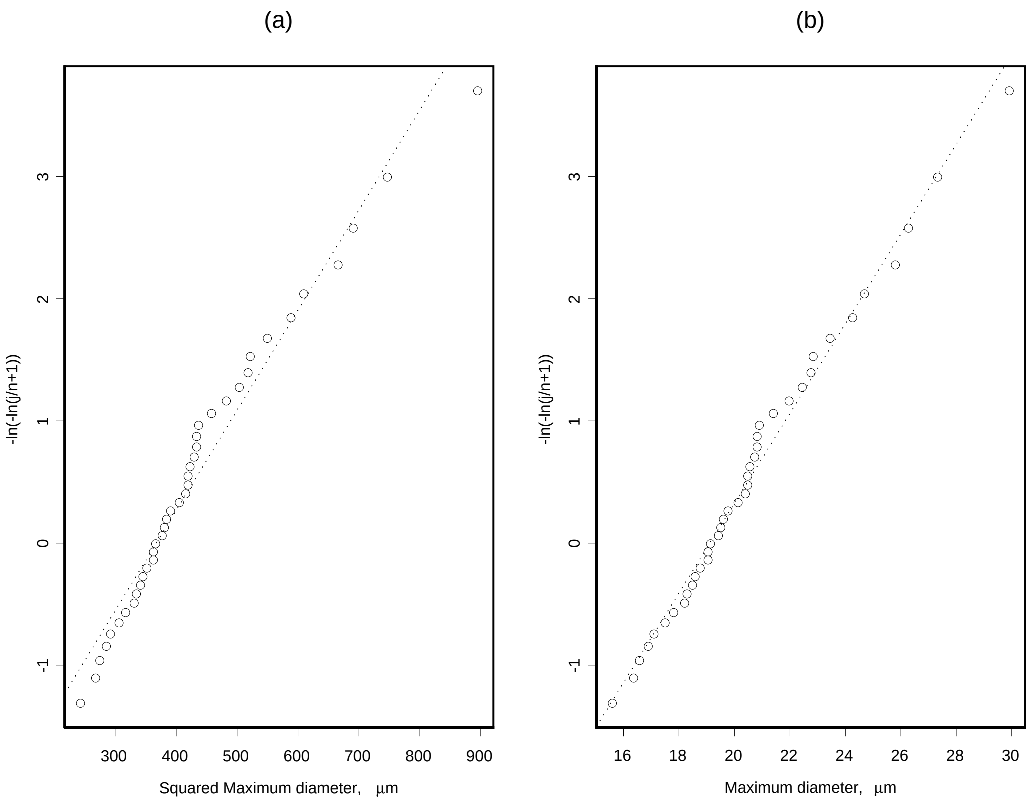

Figure 1: Gumbel Plots for Largest Planar Inclusions in a Medium Carbon Steel

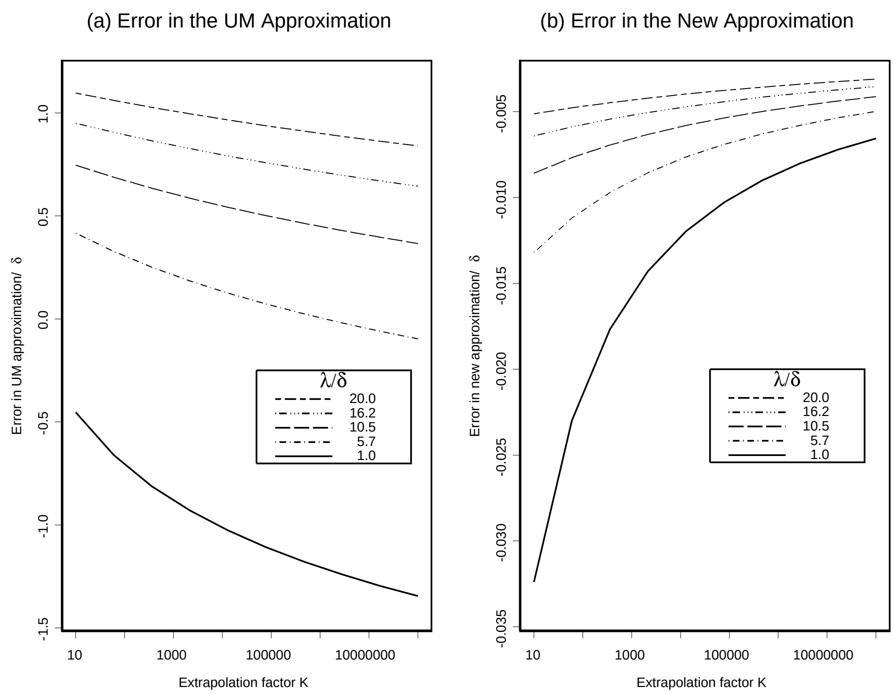

Figure 2: Errors in Approximations for Characteristic Size of Largest Inclusion