THE PROBABILISTIC MODELLING OF FRACTURE TOUGHNESS

Stephen Slatcher*

A theoretical model predicts that, if the mode of fracture is cleavage, fracture toughness follows a 2-parameter Weibull distribution with a shape parameter equal to 2 (for J or CTOD measures of fracture toughness). The other parameter in the distribution comprises two factors, one being the crack front length and the other being a material constant. When a small number of fracture toughness data are to be used to predict the results of future tests or the effective fracture toughness of a cracked engineering body, the theoretical model provides information that increases the accuracy of the prediction.

INTRODUCTION

A fracture toughness test gives the fracture toughness representative of a rather small volume of material. This volume of material is located at the pre-crack tip of one particular test piece. What is actually required for practical applications is the fracture toughness of the material around the crack tip of a possible crack in an engineering structure or component. An important step in a fracture mechanics assessment is the inference from fracture toughness test results, of the effective fracture toughness in the engineering body. A conservative inference may be made deterministically, e.g. by using the minimum fracture toughness from 3 tests, but the problem is essentially statistical in nature. A statistical approach is outlined below.

From a set of fracture toughness test results one can infer the underlying probability distribution that happened to produce that set of observations. Then, knowing this underlying probability distribution, one can make probabilistic statements concerning the results of further fracture toughness tests, or concerning the effective fracture toughness of a cracked structure. It is convenient to approximate the

^{*}A.S Veritas Research, PO Box 300, N-1322 Høvik, Norway.

underlying distribution by parametric equations, so in practice the problem is basically one of fitting parametric distributions (e.g. lognormal or Weibull) to empirical fracture toughness data.

In doing this curve-fitting it is important to realize that the goal is to make good predictions (i.e. to make a fit close to the true population); it is not to provide a good fit to the particular set of data one may happen to possess. In order to make good predictions one should use not only the particular set of data, but also a knowledge of how similar sets of data are distributed and an understanding of the physical processes involved. One should also be aware of the possible danger of over-fitting. For equations of similar form, the larger the number of parameters that are fitted, the better the agreement with the data set to which the equation is fitted. However, this does not necessarily imply that the equation with a greater number of fitted parameters has better predictive capabilities. Small data sets often display features that are very untypical of the population, and the fitting of many parameters will in such cases merely reflect the peculiarities of the particular data set. The convenience aspects of keeping the number of adjustable parameters as low as possible should also be noted; in some cases it may be desirable to keep the approach simple and accept a less good approximation.

This paper will consider fracture toughness on the lower-shelf only, i.e. the micromechanism of fracture will be assumed to be cleavage with little or no ductile tearing prior to the cleavage event. It will concern itself with the prediction of the effective fracture toughness of cracked engineering bodies, by the fitting of a simple physically-based parametric distribution to fracture toughness data, and the consideration of the statistical crack front length effect.

A SIMPLE MODEL

Curry and Knott [1] first drew attention to the fact that cleavage fracture from a sharp crack tip is controlled by the interaction between the stress gradient due to the crack, and the distribution of microscopic flaw sizes ahead of the crack tip. Thus cleavage fracture could initiate from a small flaw close to the crack tip where the stresses are high, or from a larger flaw in a lower stress region further away from the crack tip. The crack initiation position and load would therefore depend on the number of flaws per unit volume, the size distribution of the flaws, and the form of the stress gradient. It was claimed [2] that this model could adequately predict fracture toughness from microstructural measurements. The statistical model was developed, and formulated with greater rigour, by Evans [3]. Wallin et al [4] stressed the fact that the model, when formulated in a physically reasonable way, actually predicted that fracture toughness was

statistically distributed. Wallin [5], agreeing with Pineau [6], came to the conclusion that fracture toughness, K_{Ic} , should be Weibull distributed with a shape parameter of 4. The minimum number of assumptions [7] required to reach this conclusion are stated and briefly discussed below:

- One can conceptually divide the body containing the crack into elements, such that the failure of one element implies failure of the whole body, and such that the strengths of the elements are stochastic variables, identically distributed and mutually independent. This implies that pop-ins must be interpreted as the critical event at which the fracture toughness is defined. Note, however, that some latitude is allowed for the definition of elemental failure. Thus, for a steel, a cracked ferrite grain need not necessarily constitute elemental failure. The conditions that the elemental strengths should be identically distributed and mutually independent are not very restrictive. If there are several microstructures along the crack front it is possible to apply equation (1) to each microstructural region, and treat the crack front in each region as a component in a series system. The result is an equation of the same form as equation (1) with an effective ψ that depends on the proportion of the crack front in each microstructure.
- All the stresses and strains at the first element to fail must dependent on J (the J-integral) and r (the perpendicular distance from the crack front), only through the ratio J/r. Thus it is assumed that the stresses and strains at the point of failure initiation are fully characterized by the J-integral. This is a common assumption in simple fracture mechanics analyses, but often breaks down, leading to so-called geometry (constraint) effects. It is conventional in the fracture mechanics literature to express the stresses and strains in the crack tip region as a function of J/r, but it is not clear to the author to what extent this reflects the actual physical situation, and to what extent it is mere convention.
- 3 The first element to fail must lie in a zone defined by r and θ (the angle, at the crack front, made with the plane ahead of the crack) such that, for any θ , r lies in the range $Jg(\theta) \leq r \leq Jh(\theta)$, where $g(\theta)$ and $h(\theta)$ are functions of θ . That is, for any angle θ , the lower and upper limits for the region where the fracture may initiate must be proportional to J. The lower limit may, for example, be zero, and the upper limit could be defined by a maximum flaw size if local flaws initiate failure.

Note that no assumptions about the details of the stress and strain fields around the crack have been made. Neither have any

assumptions been made about the detailed mechanics of elemental failure. These three assumptions lead to the following expression for the cumulative distribution function (CDF) for fracture toughness [7]:

$$F(J) = 1 - \exp(-B \psi J^2) \tag{1}$$

where ψ is given by

$$\psi = \int_{\theta = -\pi}^{\theta = +\pi} \int_{u = g(\theta)}^{u = h(\theta)} uf(u, \theta, \eta_1, \eta_2, \dots, \eta_k, \kappa_1, \kappa_2, \dots, \kappa_l) dud\theta$$
(2)

and

$$u = J/r \tag{3}$$

B is the length of the crack front; $\eta_1, \eta_2, ..., \eta_k$ are a set of parameters describing the flow properties of the material; and $\kappa_1, \kappa_2, ..., \kappa_l$ are a set of microstructural parameters that determine the distribution of elemental strength (e.g. κ_1 might be the average number of carbides per unit volume in a steel, while κ_2 and κ_3 might be the parameters that define the distribution of the carbide sizes). The function f () gives the probability per unit volume of elemental failure. In such an abstract form, the physical significance of the parameter ψ may be difficult to grasp, but it is in fact a material constant, which may be calculated [7] if sufficient information about the material and failure mechanisms is available (or assumed). Thus this model predicts that J_c follows a two-parameter Weibull distribution with a shape parameter of two, and the other parameter comprising two factors, namely the crack front length and a material constant. Since J is proportional to the crack-tip opening displacement (CTOD), and to the square of the stress intensity factor, critical values of CTOD are distributed as J_c , while K_{Ic} is Weibull distributed with a shape parameter equal to 4. The dimensions of ψ are dependent on the units of fracture toughness.

THE PARAMETRIC FORM

In this section the parametric form of equation (1) will be compared with actual fracture toughness data. Perhaps the most obvious way to proceed is to use a goodness-of-fit statistic to check for significant differences between the empirical fracture toughness data and equation (1) fitted to these data. However, this approach has its limitations. For data sets sizes of say 20 or less, significant deviations from equation (1) will probably not be detected. But neither will such data sets show significant deviations from, for example, a log-normal distribution, so little information is gained. One should also be careful in using the concept of statististical significance for large data sets,

because equation (1) will show significant deviations from sufficiently large data sets even if it is a sufficiently good representation of reality to make useful predictions.

For these reasons, the following method is used to evaluate how well equation (1) performs in making predictions. Three fitting techniques are used here:

- Equation (1) was fitted using the maximum likelihood method to estimate the single parameter represented by the product $B\psi$.
- 2 The two-parameter Weibull distribution was fitted estimating both parameters by the maximum likelihood method.
- 3 The log-normal distribution was fitted estimating the two parameters by the standard method.

These three fitting techniques, applied to a large (89 data) homogeneous set of cleavage fracture CTOD data, are illustrated in Figs. 1-3. The CTOD data were obtained in an ECSC collaborative project [8]. The material was 50 mm thick BS4360 grade 50D steel tested at -65°C, and the selection of the homogeneous set is explained in [7]. By eye, it can be seen that all three parametric distributions approximate reasonably well to the empirical data. The two-parameter Weibull distribution is better than the model distribution (equation (1)) because a greater number of parameters are fitted.

In order to compare the applicability of the three fitting techniques, sub-sets of the large data set were randomly selected, each fitting technique was applied to each sub-set, and the parametric distributions fitted to the sub-sets were compared with the empirical CDFs of the large distributions. Before presenting the results of this analysis, each of the steps in the above sentence will be expanded in the following paragraph.

Sub-sets containing 2, 3, 5, 10, 25 and 50 data were randomly selected from of the large 'parent' data set. 100 sub-sets of each size were selected from the parent data set. The so-called sub-sets were obtained by randomly selecting numbers in the range 0-1; the continuous form of the empirical CDF for the parent data set was then entered at the probability given by these random numbers, and the corresponding quantiles were selected to be members of the sub-set. The continuous form of the empirical CDF was defined as follows: the ith largest of N values in the data set is assigned the cumulative probability value (i-0.5)/N, cumulative probabilities in between these values are defined by linear interpolation, the cumulative probabilities for values lower than the lowest or higher than the highest in the data set are 0 or 1 respectively. The difference between the parametric distributions and the parent data set is quantified by the Kolmogorov-Smirnoff statistic, D, high values of D implying large

differences.

The median values of D for each set of 100 parametric distributions are plotted in Fig. 4.

The results show that for small data sets, the fitted model distribution is usually closest to the parent data set, whereas for larger data sets the distributions that involve the fitting of two parameters are superior. We can conclude that, for many practical applications where fitting to rather small data sets is involved, equation (1) is a useful approximation to reality. For small data sets the fitting of two parameters gives poorer predictive capabilities. In [7], tentative guidelines are given for how one might decide whether or not to use the model distribution rather than a two-parameter Weibull or a log-normal distribution.

THE CRACK FRONT LENGTH EFFECT

An important feature of equation (1) is the crack front length term. This crack front length term is due to a statistical size effect (simply speaking, the longer the crack front length, the greater the possibility of sampling a brittle region). It is a convenient feature of the Weibull distribution that statistical size effects enter the form of the distribution in such a simple way, but it is by no means necessary that a quantity should be Weibull distributed in order to exhibit a statistical size effect. If a crack front length may be divided into small equally loaded (in terms of a fracture mechanics parameter) elements, if the crack is brittle with respect to these elements (i.e. if one element fails, total failure occurs), and if the strengths of the elements are identically distributed and mutually independent stochastic variables, then the CDF of fracture toughness measured on test pieces of crack front length p, $F_p(J)$, is related to the fracture toughness for crack front length q, $F_q(J)$, by the relationship

$$F_p(J) = 1 - (1 - F_q(J))^{p/q}$$

$$(4)$$

irrespective of the forms of the CDFs. This is explained in greater detail in [9].

The predictive capabilities of equation (4) are illustrated by Fig. 5 [9]. Here distributions A and B are empirical cumulative distributions for test pieces of different breadth (i.e. crack front length), but otherwise nominally identical, and tested under nominally identical conditions. The data were again taken from [8], and actually the data comprising distribution A are the large data set from the previous section, plus some higher CTOD values for material close to the edges of the plates. The prediction of the CDF for B was made from distribution A, applying equation (4). The prediction is very good for

the lower CTOD values of practical interest, and this encouraging result strengthens confidence in equation (1) since the form of equation (4) is essential if equation (1) is to be correct.

The practical consequence of the statistical crack front length effect is that if the crack in the engineering body possesses a different crack front length to that used in the fracture mechanics testing, then this fact should be allowed for in any fracture mechanics calculations involving brittle fracture. It is proposed that if only few fracture toughness data are available, the material constant ψ should be determined by the maximum likelihood technique. Considering a set of fracture toughness data, $J_{c,i}$, i=1,2,...N, and assuming that J_c is distributed as in equation (1), the maximum likelihood estimator for ψ is given by

$$\hat{\psi} = N / B \sum_{i=1}^{N} J_{c,i}^2 \tag{5}$$

Then, having estimated ψ , equation (1) can be taken to give the distribution of fracture toughness for any particular crack front length. If one knows how the fracture mechanics parameter varies over the crack front, it is not too difficult to incorporate this variation into the calculation [10]. In [9], it is suggested that the variation is included in the form of an effective crack front length. It is also simple to include a crack front length effect in deterministic fracture mechanics calculations if one wishes to use a particular fractile of the toughness distribution, irrespective of crack length, as input to the calculation [9].

CONCLUSIONS

- A theoretical model predicts that, if the mode of fracture is cleavage, fracture toughness follows a 2-parameter Weibull distribution with a shape parameter equal to 2 (for J or CTOD measures of fracture toughness) or 4 (for K based measures). The other parameter in the distribution comprises two factors, one being the crack front length and the other being a material constant.
- 2 Though approximate, the theoretical model provides information that, when applied in the fitting of a parametric distribution to a small number of fracture toughness data, gives better fits than Weibull or log-normal distributions that require the fitting of two parameters.
- 3 The statistical crack front length size effect, which is a feature of the theoretical model, has been demonstrated experimentally, and may readily be incorporated in fracture mechanics analyses that consider brittle fracture.

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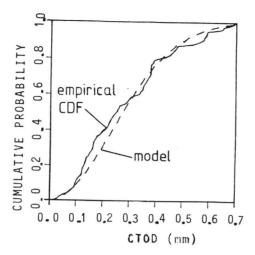


Fig. 1 The model distribution (equation 1) fitted to 89 CTOD data.

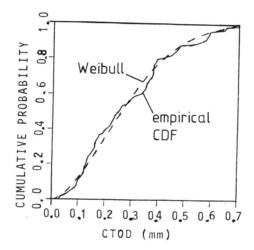


Fig. 2 The two-parameter Weibull distribution fitted to 89 CTOD data.

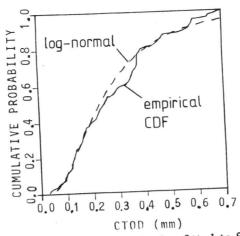


Fig. 3 The log-normal distribution fitted to 89 CTOD data.

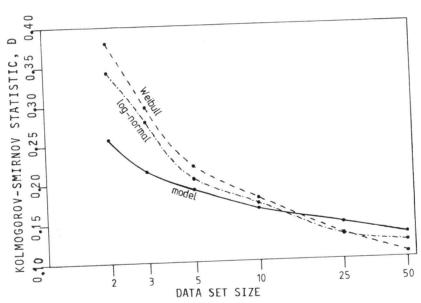


Fig. 4 The deviation between parametric distributions fitted to sub-sets of a parent data set, and the parent data set itself. The median deviation (quantified by the Kolmogorov-Smirnov statistic) of 100 Monte-Carlo simulations is plotted for each set size.

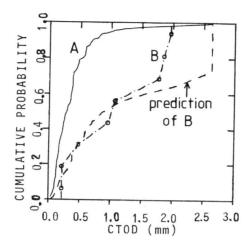


Fig. 5 A comparison between: the empirical cumulative frequencies of the critical CTOD values for the test pieces of breadth 50 mm (distribution A); the empirical cumulative frequencies of the critical CTOD values for a set of test pieces of breadth 12.5 mm (distribution B); and a prediction of distribution B based on distribution A and equation 4.