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**ESTIMATION OF LOWER-BOUND  $K_{Jc}$  ON PRESSURE  
VESSEL STEELS FROM INVALID DATA\***

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## ESTIMATION OF LOWER-BOUND $K_{Jc}$ ON PRESSURE VESSEL STEELS FROM INVALID DATA

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**REFERENCE:** McCabe, D. E., and Merkle, J. G., "Estimation of Lower-bound  $K_{Jc}$  on Pressure Vessel Steels from Invalid Data," *Fatigue and Fracture Mechanics: 28th Volume, ASTM STP 1321*, J. H. Underwood, B. D. MacDonald, and M. R. Mitchell, Eds., American Society for Testing and Materials, 1997.

**ABSTRACT:** Statistical methods are currently being introduced into the transition temperature characterization of ferritic steels. The objective is to replace imprecise correlations between empirical impact test methods and universal  $K_{Ic}$  or  $K_{Jc}$  lower-bound curves with direct use of material-specific fracture mechanics data. This paper will introduce a computational procedure that couples order statistics, weakest-link statistical theory, and a constraint model to arrive at estimates of lower-bound  $K_{Jc}$  values. All of the above concepts have been used before to meet various objectives. In the present case, the scheme is to make a best estimate of lower-bound fracture toughness when resource  $K_{Jc}$  data are too few to use conventional statistical analyses. The utility of the procedure is of greatest value in the middle-to-high toughness part of the transition range where specimen constraint loss and elevated lower-bound toughness interfere with the conventional statistical analysis methods.

**KEYWORDS:** fracture toughness,  $K_{Ic}$ ,  $K_{Jc}$ , lower bound, constraint, order statistics, weakest link

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### INTRODUCTION

Good progress is being made relevant to the problem of defining the transition temperature of ferritic steels. The problem has been in learning how to deal with excessive scatter in fracture mechanics data based on  $K_{Ic}$  and/or  $K_{Jc}$  values. Statistical methods are now being used to model the data scatter patterns and to pinpoint the

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characteristics that can be used to more accurately compare one material or material condition with another.

Values of  $K_{Ic}$  are now being used that imply elastic-plastic stress intensity factors determined at the point of onset of cleavage fracture. Such instabilities are triggered by minute microstructural impurities that are almost always present in commercially produced steels. These can be carbides and/or nonmetallic inclusions of varied sizes that are scattered randomly throughout the microstructure [1]. To trigger cleavage, a particle must be of a critical size and by chance be located within the highly stressed volume of material local to the crack tip [2]. The resulting scatter of  $K_{Ic}$  data due to this probabilistic phenomenon usually produces ratios of from 2 to 3 times between the lowest to the highest values; assuming, of course, that data replication is sufficient to demonstrate this. It follows that crack tip volume sampling effects that produce data scatter can also lead to a statistical thickness effect in which large specimens tend to exhibit lower toughness than small specimens. This can be explained by using a statistical weakest-link theory.

In general, statistical methods have been able to explain much of what has been observed experimentally. However, there are other influential conditions that need to be taken into account as well. As already mentioned, cleavage fracture is triggered by particles of a critical size exposed to a critical tritensile combination of stress and plastic strain that develops along the crack front. The stress ratios and plastic strain magnitudes are controlled by the degree of crack tip constraint. Therefore, constraint must be well managed to successfully use statistical models on the data. Constraint is a function of material strength, specimen thickness, and specimen or component geometry. This aspect of transition range behavior has generated a second and somewhat independent focal point for research work [3]. Care can be taken to control constraint in laboratory tests, but the application of laboratory-generated data to engineering problems requires added attention to possible constraint differences.

This paper uses both statistical and constraint modeling to deal with the special problems sometimes encountered in engineering applications. We will consider the case where the background data are too few to use conventional statistics, and show a method of imposing extrapolation limits on the weakest-link size effect model to generate an estimate of the lower bound of fracture toughness.

Background information will be covered first that applies to the more precise determination of median  $K_{Ic}$  and standard deviation that is possible when a sufficient data sampling plan is used. This approach will provide benchmark information for comparison to the backup method of lower certainty proposed here.

## **BACKGROUND ON STATISTICAL MODELS**

The three-parameter Weibull statistical model has been chosen as the best one to fit  $K_{Ic}$  data distributions [4]. It has the versatility to fit a wide variety of data distributions, one of which is the typical fracture mechanics-based fracture toughness data distribution.

Cumulative probability for failure,  $P_f$ , at or before stress intensity driving level,  $K_{Jc}$ , is calculated by the following modification of the three-parameter Weibull equation:

$$P_f = 1 - \exp \left\{ - \left[ \frac{(K_{Jc} - K_{min})}{(K_o - K_{min})} \right]^b N \right\} . \quad (1)$$

Parameters  $K_o$ ,  $K_{min}$ , and  $b$  are three Weibull data population fitting constants obtained from data sampling. The model of Eq. (1) also shows a fourth parameter,  $N$ , that describes the phenomenon of weakest-link behavior that develops only in the low-to-middle part of the transition range of fracture toughness. Term  $N$  is a size ratio and, for test specimens of different sizes where all dimensions are scaled proportionally, specimen thickness is used; i.e.,  $N = B_2/B_1$ . In theory, the dimension  $B_1$  is arbitrary and once  $B_1$  is selected,  $K_o$  is determined by the order statistics of sample data. For example, when replicate tests are made on specimens of thickness  $B_1$  and median  $K_{Jc(1)}$  has been determined, median  $K_{Jc(2)}$  for specimens of thickness  $B_2$  can be calculated using the following relationship:

$$K_{Jc(2)} = (K_{Jc(1)} - K_{min}) (1/N)^{1/b} + K_{min} . \quad (2)$$

Equation (2) is derived from Eq. (1) and it models the weakest-link size effect described earlier. The trend set by Eq. (2) has been extended outside the range covered by typical test specimen sizes for predicting large flaw effects in engineering applications [5]. Crack size ratio instead of thickness is then used in term  $N$ . The end point of extrapolation on Eq. (2) is 20 MPa $\sqrt{m}$  and the present work will propose an existence of a truncation point at higher  $K_{Jc}$  values based on a constraint limit rationale. To obtain the three Weibull parameters of Eq. (1) that represent the total data population, it is important to know how large the data sampling must be. Early Weibull parameter fitting work was done without such consideration [4]. Subsequently, Wallin [6] conducted a much-needed sensitivity study and it was determined that parameters  $K_{min}$  and Weibull slope,  $b$ , require huge numbers of replicate tests; of the order of 50 to 100. However, in this same study, it was determined that when  $K_{min}$  is set to 20 MPa $\sqrt{m}$ , Weibull slope for ferritic steels tended to centralize to a constant value of 4. Data were taken from several experiments to demonstrate the centralizing tendency with increased sample size described above. This discovery has been used to convert what had been an interesting technical observation into a practical engineering tool that is amenable to standardization practices. Hence, Eqs. (1) and (2) become more consistent and universally reproducible. To determine the Weibull scale parameter,  $K_o$ , requires only 6 replicate tests. With Weibull slope known and essentially constant, the standard deviation,  $\sigma$ , on data scatter is precisely characterized from the following [7]:

$$\sigma = 0.28 K_{Jc(\text{med})} \left( 1 - \frac{20}{K_{Jc(\text{med})}} \right) \text{ MPa}\sqrt{\text{m}}, \quad (3)$$

where  $K_{Jc(\text{med})}$  is the calculated median toughness value.

Equations (1) through (3), used with the two fixed Weibull parameters, have been tested repeatedly with experimental results and, although small data samplings cannot always accurately match and confirm the two fixed parameters, the evidence of the centralizing tendency to these values is quite convincing.

Finally, Wallin [6] has determined that the median of  $K_{Jc}$  fracture toughness for ferritic steels will fit a common transition curve; namely, 1T compact and bend bar specimens (25 mm thick) will fit the following curve:

$$K_{Jc(\text{med})} = 30 + 70 \exp [0.019(T - T_0)] \text{ MPa}\sqrt{\text{m}}. \quad (4)$$

This curve is known as the "master curve," and it can be noted that Eq. (4) is of the same mathematical form as the American Society of Mechanical Engineers (ASME) *Boiler and Pressure Vessel Code* equations for static lower-bound  $K_{Jc}$  and crack arrest  $K_{Ia}$ . In those cases, the curves are positioned using reference temperature,  $RT_{NDT}$  [8]. For the master curve, reference temperature is  $T_0$  and, when test temperature,  $T$ , is set at the reference temperature,  $K_{Jc(\text{med})}$  is 100  $\text{MPa}\sqrt{\text{m}}$ .

Again, the concepts presented to this point will be used to set the more exact characterization of fracture toughness. The following sections deal with an application that is specialized toward seeking a lower bound of  $K_{Jc}$  fracture toughness for the data distribution of the material. It will be assumed that sample size is insufficient. A constraint-based model is then applied to a lower-bound  $K_{Jc}$  estimate to find a safe  $K_{Jc}$  value for use in engineering applications.

## ORDER STATISTICS

Steinstra et al. [9] have described how lower-bound tolerance estimates on  $K_{Jc}$  can be made from small data samplings. The method is aided by having prior knowledge of the Weibull slope of the data population. When  $K_{Jc}$  values are arranged in order of increasing magnitude, the cumulative probability value can be estimated independently from each datum using the so-called "Beta distribution estimator." These estimates are determined for a discretionally selected value of cumulative probability. For example,  $P_f = 0.10$  will be used predominantly here. At the same time, one must choose a confidence level on the determination. The concept involves the development of a set of coefficients,  $\eta$ , that, when multiplied by ranked data, will provide estimates of  $K_{Jc(0.1)}$

values that are expected to reside in the 10% lower tail of the population distribution. The process of developing the multiplier coefficients is explained in detail elsewhere [8]. Table 1 is an example of such coefficients, set up to cover from one to six data sample sizes.

TABLE 1--Coefficient, "η," for  $P_f = 0.10$  and 90% confidence on the estimate.

K <sub>Jc</sub> rank	Number of tests					
	1	2	3	4	5	6
1	0.4625	0.550	0.6087	0.6541	0.6916	0.7239
2		0.434	0.5042	0.5516	0.5888	0.6198
3			0.4206	0.4822	0.5238	0.5564
4				0.4122	0.4686	0.5062
5					0.4062	0.4587
6						0.4016

A hypothetical example will be used here to illustrate the use of order statistics (see Fig. 1). Assume three 1T compact specimens had been tested at 100°C, giving K<sub>Jc</sub> values of 165, 190, and 235 MPa√m. These are ranked as shown in Table 2 and the appropriate coefficients from Table 1 are assigned (column 3).

TABLE 2--Estimates of K<sub>Jc</sub> at or below the  $P_f = 0.10$  level.

Rank	K <sub>Jc</sub> (MPa√m)	Coefficient (η)	K <sub>Jc(0.1)</sub> (MPa√m)
1	165	0.6087	108
2	190	0.5042	106
3	235	0.4026	110

The Beta distribution estimation assumes two-parameter Weibull with a slope of 4; so for a three-parameter model, the following equation was used:

$$K_{Jc(0.1)} = (K_{Jc} - 20) \eta + 20 \text{ MPa}\sqrt{\text{m}} . \quad (5)$$

The solid and dashed curves in Fig. 1 represent the assumed master curve characteristic of the material population. The true K<sub>Jc</sub> at the 10% tolerance bound of the data population is about 140 MPa√m and the filled square datum approximates the order statistic placement of all three order statistic estimates. Such values, when based on few data, carry the potential of being overly conservative. The following order statistic example will be based on actual experimental data.

Figure 2 shows a master curve and tolerance bound developed from the testing of about 150 1T compact specimens. The data came from a round-robin activity sponsored by the Materials Properties Council and the Japanese Society for the Promotion of Science [10]. Eighteen laboratories were involved. A 508 class 2 steel was tested at three test temperatures:  $-50$ ,  $-75$ , and  $-100^{\circ}\text{C}$ . Duplication for each variable (test temperature and laboratory) was five specimens. In this case, the order statistic exercise was to determine how well each data set could predict the lower tolerance bound of the master curve. The 10% tolerance bound on the master curve was margin adjusted  $16^{\circ}\text{C}$  to cover the uncertainty in reference temperature,  $T_{\sigma}$ , from the five-specimen sample size. A 95% confidence level is imposed.<sup>2</sup> The same tolerance bound and confidence level was imposed on the order statistic estimates. Clearly, the order statistics estimates related well to the more rigorous determinations of the three-parameter Weibull method.

### ADJUSTMENT TO LOWER-BOUND TOUGHNESS

Equation (2) can follow the size effect trend of median  $K_{Jc}$  values suitably for data obtained from test specimens. However, some questions arise when the test temperature is high in the transition range and when the equation is used on in-service flaws that could perhaps be an order of magnitude or more larger than that of the test specimens. Observe that predicted  $K_{Jc(2)}$  in Eq. (2) will tend toward  $20\text{ MPa}\sqrt{\text{m}}$  as size ratio tends to infinity. It is argued here that such a trend will cease to be maintained as upper-shelf temperature is approached and the model should break down. It seems only reasonable to expect that real  $K_{\min}$  must rise to J-R curve levels at the upper-shelf part of the transition range. In addition, it is important to recognize that  $K_{\min} = 20\text{ MPa}\sqrt{\text{m}}$  is used as a deterministic parameter of the Weibull model and there must be some departure between the model and real material behavior at temperatures high in the transition range [11,12]. Figure 3 depicts how this departure is envisioned. Here, 1T compact specimens are tested at a test temperature where the median  $K_{Jc}$  is  $300\text{ MPa}\sqrt{\text{m}}$ . The distribution for 10T compact specimens is calculated using weakest-theory. A constraint-based data truncation point is calculated to be at  $144\text{ MPa}\sqrt{\text{m}}$  using a procedure that is to be covered presently.  $K_{Jc}$  data to the left of the vertical line cannot be developed experimentally, irrespective of the specimen size used. To experimentally demonstrate the phenomenon at such temperatures as depicted here is difficult for more than one reason. In Fig. 3, it appears that the smaller 1T specimens have an advantage against data truncation because only 3% of the possible test data are influenced. However, small specimens will develop severe top-end  $K_{Jc}$  data loss due to excessive loss of constraint; a subject not addressed in this paper. On the other hand, an experiment with adequate numbers of 10T specimens would never be considered practical.

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<sup>2</sup>Test Method for the Determination of Reference Temperature,  $T_{\sigma}$ , for Ferritic Steels in the Transition Range, Appendix C, Draft 12, American Society for Testing and Materials, January 31, 1996.



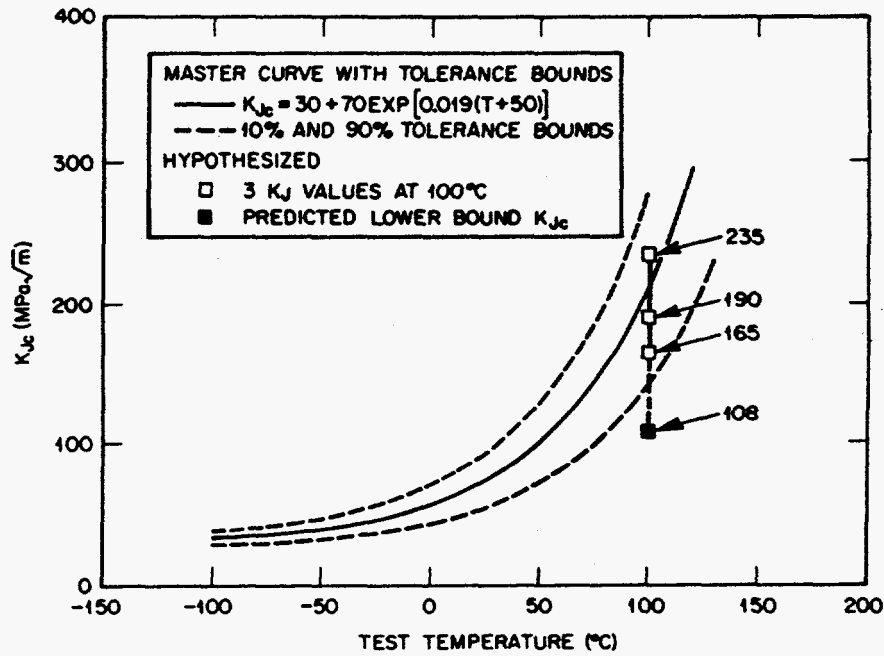


FIG. 1--Schematic representation of a three-specimen sample from material defined by the master curve with 10% and 90% tolerance bounds.

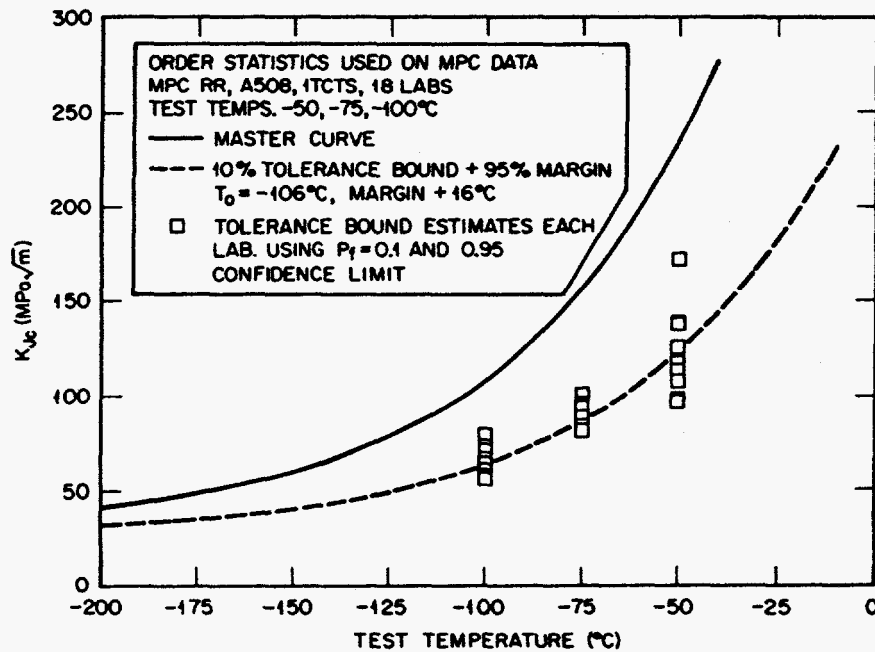


FIG. 2--Data for A 508 class 2 steel from 18 participating laboratories from a round robin sponsored by the Materials Properties Council and the Japanese Society for the Promotion of Science. Each data point represents an estimate of the 10% tolerance bound from five replicate tests.

## DETERMINATION OF LOWER-BOUND $K_{Jc}$ TOUGHNESS

The constraint model to be applied here emanates from the most senior model used in the technology of fracture mechanics [13]. We assume that the critical maximum constraint is achieved when thickness,  $B_2$ , satisfies the following inequality:

$$B_2 > \alpha_o (K_{Jc}/\sigma_{ys})^2 . \quad (6)$$

The right side of Eq. (6) can be input into ratio  $N$  of Eq. (2) to project the trend of  $K_{Jc}$  decrease with increased thickness. Then an equation of the following cubic form results:

$$\left( \frac{K_{Jc(2)}}{K_{min}} \right)^{3/2} - \left( \frac{K_{Jc(2)}}{K_{min}} \right)^{1/2} - 2G = 0 , \quad (7)$$

$$\text{where } 2G = \left( \frac{K_{Jc(0.1)}}{K_{min}} - 1 \right) \left( \frac{\sqrt{B_1/\alpha_o}}{K_{min}/\sigma_{ys}} \right)^{1/2} . \quad (8)$$

The following simple steps will produce a  $K_{Jc}$  of maximum constraint if  $G > \sqrt{1/(3)^3}$ :

$$M_1 = G + \sqrt{G^2 (-1/3)^3} .$$

$$M_2 = G - \sqrt{G^2 (-1/3)^3} .$$

$$\text{Let } y = M_1^{1/3} + M_2^{1/3} .$$

$$\text{Then } K_{Jc(2)} = y^2 (K_{min}) . \quad (9)$$

Alternatively, the following empirical power law can be used:

$$K_{Jc(2)} = 44.78(G)^{0.538} \text{ MPa}\sqrt{\text{m}} . \quad (10)$$

Substitution of  $K_{Jc(2)}$  into Eq. (6) will define the limiting thickness of full constraint where increased specimen thickness will not further reduce  $K_{Jc}$ . The choice of  $\alpha_0$  to be used in Eqs. (6) and (8) can be based on experimental evidence. If  $\alpha_0 = 2.5$  were used,  $K_{Jc(2)}$  and  $B_2$  would satisfy the validity limits for  $K_{Jc}$  [13] in the American Society for Testing and Materials (ASTM) Standard Test Method for Plane-Strain Fracture Toughness of Metallic Materials (E 399). However, experimental work on ferritic steels has indicated that  $\alpha_0 = 1$  is the more accurate coefficient [14]; this is the value selected to be used in the examples that follow.

Figure 4 is again a schematic example of specimen size effects. It shows the three-parameter Weibull trend of median fracture toughness (solid line), with open squares for 1/2T, 1T, 2T, 4T, and 6T compact specimens, the  $P_f = 0.10$  (dotted line) curve is calculated using Eqs. (1) and (2). The open-diamond points represent exact  $P_f = 0.1$  predictions for lower-bound  $K_{Jc}$  at each specimen thickness. When these lower-bound values,  $K_{Jc(0.1)}$ , are adjusted using Eqs. (8) and (9), the  $K_{Jc(2)}$  values shown as filled squares result. The lower bound of  $K_{Jc}$  toughness is defined and the separation between the dashed line and the dotted line indicates the extent of  $K_{Jc}$  lower-bound adjustment applied to data distributions.

The Heavy-Section Steel Irradiation Program Fifth Irradiation Series can be used as a challenging example application of the proposed procedure [15]. Test data replications varied from two to nine specimens and specimen sizes varied from 1T to 8T. There were nominally eight test temperatures selected along the transition range. Two materials were submerged-arc welds in A 533 grade B plate (72W and 73W) that differed only in copper content. The ASME reference temperatures ( $RT_{NDT}$ ) were known precisely ( $\pm 5^\circ\text{C}$ ) for both unirradiated and irradiated conditions.

Figures 5 and 6 show unirradiated  $K_{Jc}$  data for 73W (0.31% Cu) material as tabulated (Fig. 5) and then after order statistics and constraint adjustments for lower-bound  $K_{Jc}$  have been applied (Fig. 6). Again, the fracture toughness truncation used corresponds to  $\alpha_0 = 1.0$  in Eq. (6). The ASME lower-bound  $K_{Jc}$  curve shown in Fig. 6 is reputed to correspond to a 2% confidence limit (short dash). The 2% cumulative probability tolerance bound line (long dash) based on the master curve is also shown.

Figures 7 and 8 are the same as Figs. 5 and 6, except that the material is weld 72W (0.23% Cu). In this case, lower-bound predictions tend to be a little nonconservative at the low test temperatures.

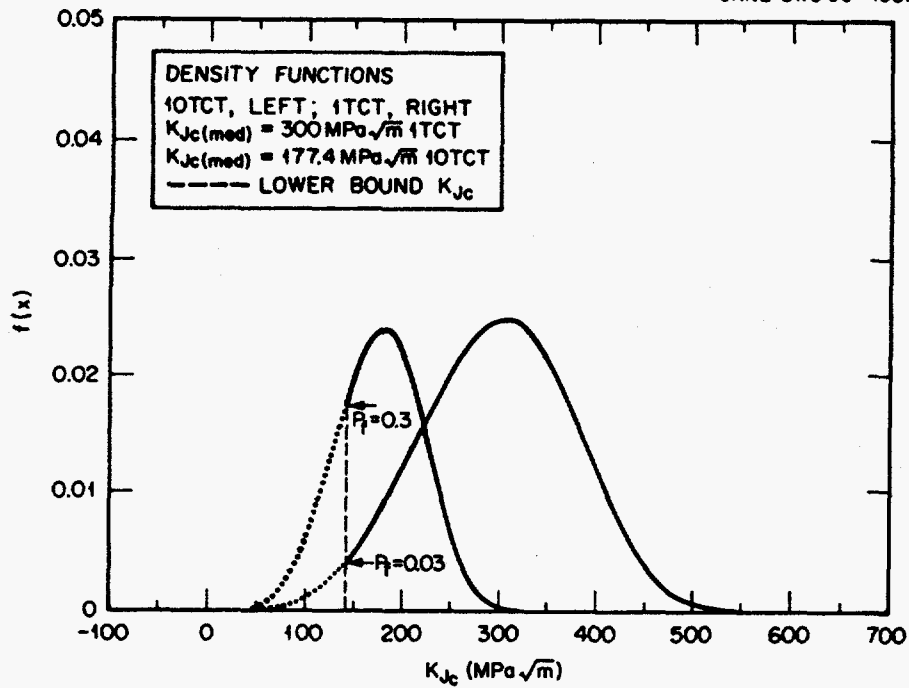


FIG. 3--Density function distributions for 1T C(T) and 10T C(T) specimens showing the effect of a true lower bound on distribution shape.

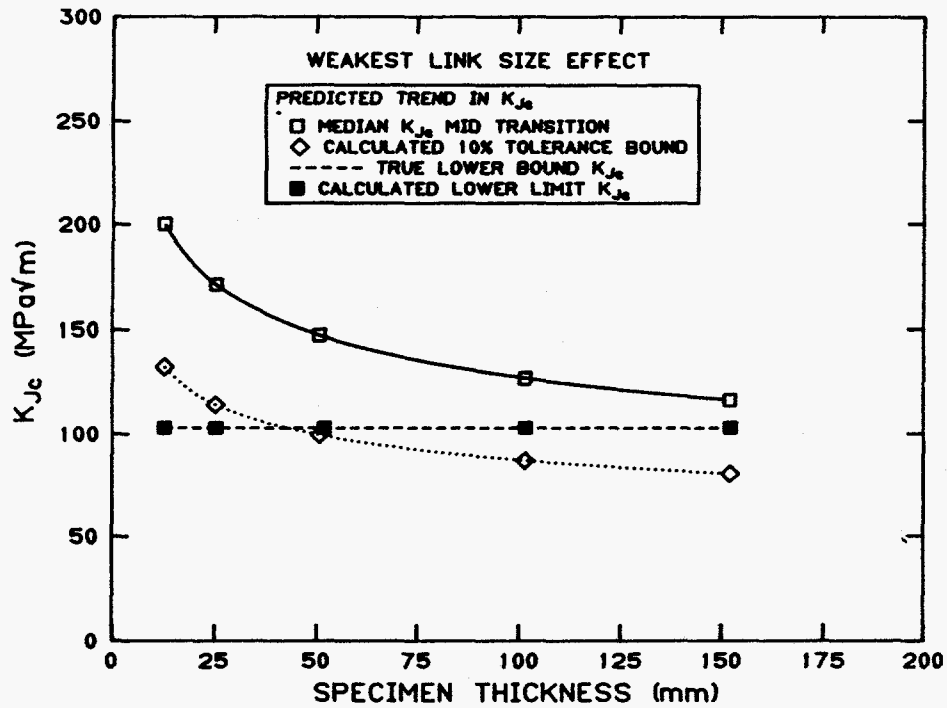


FIG. 4--Three toughness versus specimen size trends showing  $K_{Jc}$  median trend by weakest link (open squares),  $K_{Jc}$  10% tolerance bound trend by weakest link (open diamonds), and lower-bound  $K_{Jc}$  (dashed line).

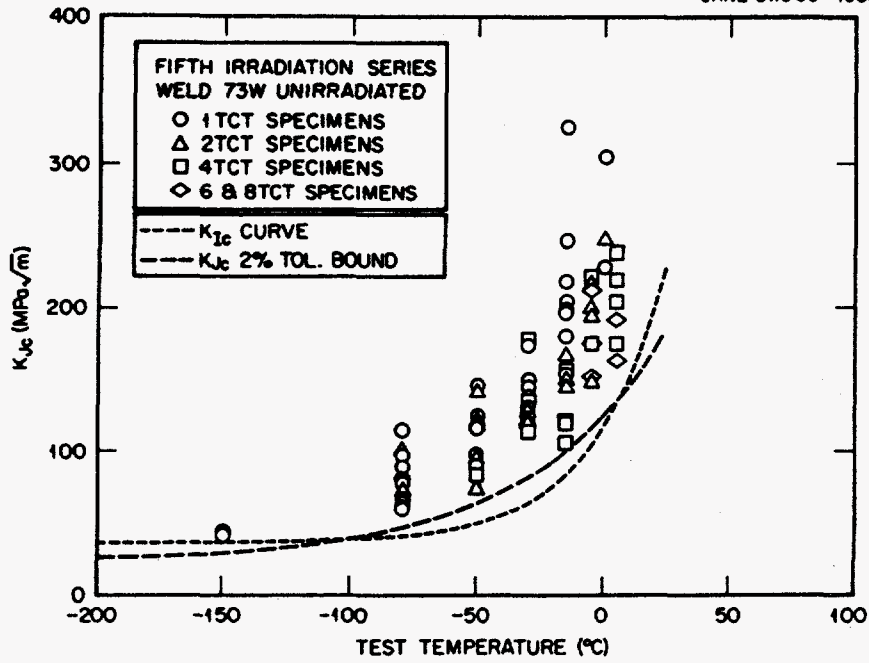


FIG. 5--Unadjusted data, American Society of Mechanical Engineers lower-bound  $K_{Ic}$  curve (dotted), and 2% tolerance bound curve (dashed), for weld 73W (A 533 grade B) of the Heavy-Section Steel Irradiation Program Fifth Irradiation Series.

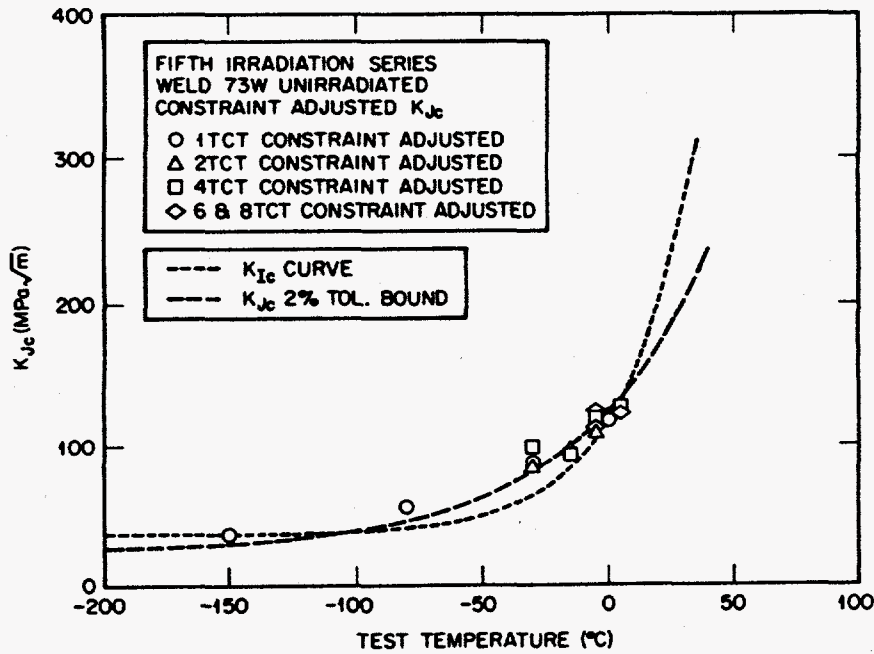


FIG. 6--American Society of Mechanical Engineers  $K_{Ic}$  curve (dotted), 2% tolerance bound curve (dashed), and procedurally adjusted lower-bound estimates (data) for Heavy-Section Steel Irradiation Program weld 73W.

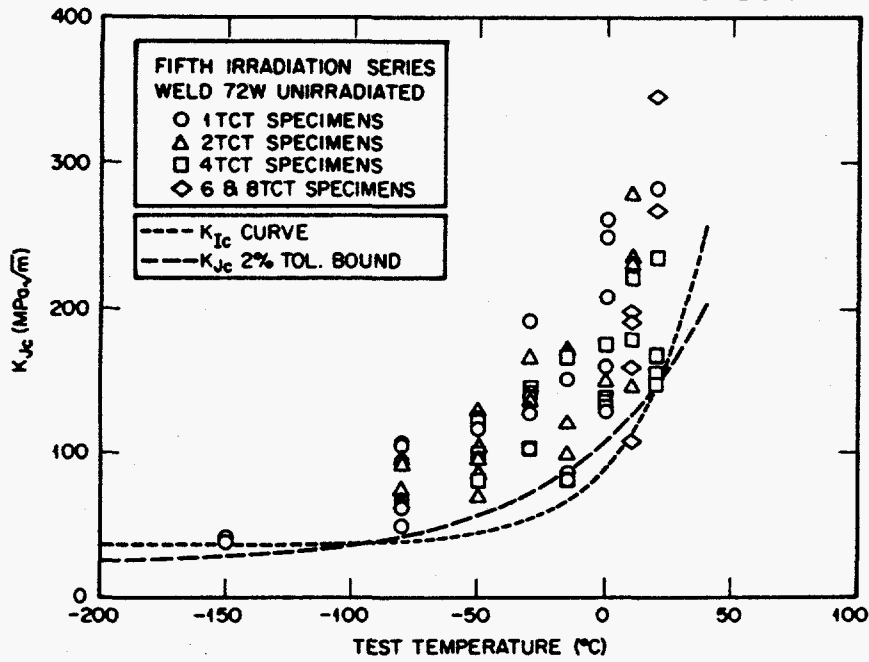


FIG. 7--Unadjusted data, American Society of Mechanical Engineers lower-bound  $K_{Ic}$  curve (dotted), and 2% tolerance bound curve (dashed) for Weld 72W of the Heavy-Section Steel Irradiation Program Fifth Irradiation Series.

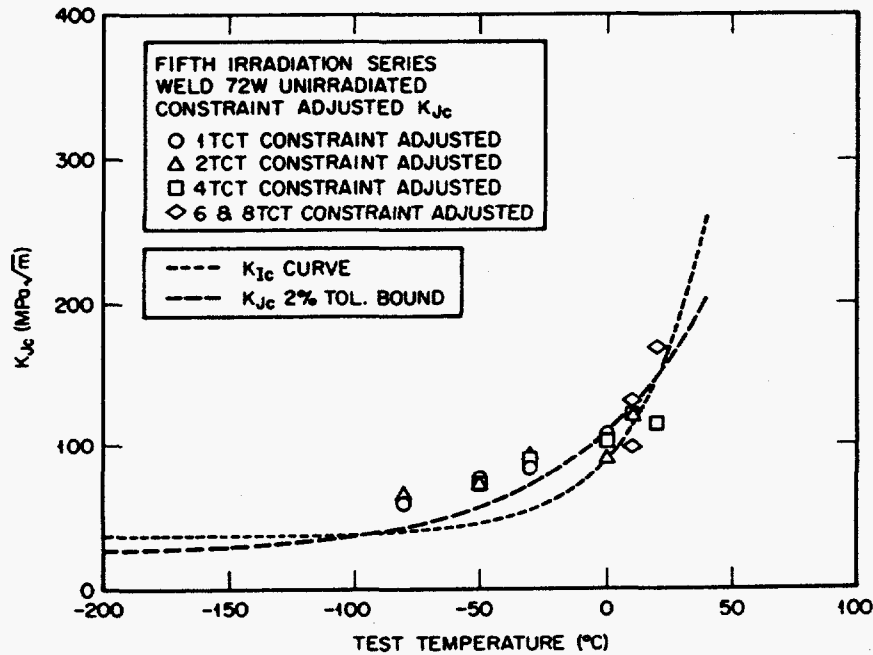


FIG. 8--American Society of Mechanical Engineers  $K_{Ic}$  curve (dotted), 2% tolerance bound curve (dashed), and procedurally adjusted lower-bound estimates (data) for Heavy-Section Steel Irradiation Program weld 72W.

Figures 9 and 10 present the same comparison for both materials in the irradiated condition. In this case, 72W and 73W data were combined because the two materials ended up with the same irradiated  $RT_{NDT}$  temperature. The adjusted data of Fig. 10 are quite similar to those of Fig. 6, both of which tend to favor the 2% tolerance bound curve.

## CONCLUSIONS

This paper proposes a method of analysis that represents a best effort at predicting lower-bound fracture toughness  $K_{Jc}$  values when the supporting data are sparse. Order statistics can be used to estimate a  $K_{Jc}$  toughness value that is near to lower bound when the data sample is small. The resulting  $K_{Jc}$  estimate can be adjusted for specimen size to large flaw size equivalence. A constraint model is used to truncate the statistical weakest-link size effect trend at a size where constraint will cease to increase with increased crack size. This model is of most value in the middle-to-high toughness part of the transition range, where the weakest-link size effect begins to vanish. The lower-bound  $K_{Jc}$  estimate may or may not be precisely the same as lower-bound  $K_{Jc}$  but, at the same time, it is preferred as an estimate of that value as opposed to the alternative use of impact tests with an assumed correlation to the universal  $K_{Jc}$  lower-bound curve.

The methodology presented is flexible in terms of the value of  $\alpha_0$  and/or confidence limits selected and can be adjusted to various levels of conservatism chosen at the discretion of the user. The levels chosen for this paper were selected to follow the transition  $K_{Jc}$  lower-bound curve. However, this practice is not proposed to replace the more rigorous statistical practices.<sup>3</sup> The applications are for circumstances where source information is sparse or for engineering applications where the conditions are such that the weakest-link theory cannot properly model the fracture toughness/size effect trend.

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<sup>3</sup>Test Method for the Determination of Reference Temperature,  $T_{00}$ , for Ferritic Steels in the Transition Range, Appendix C, Draft 12, American Society for Testing and Materials, January 31, 1996.

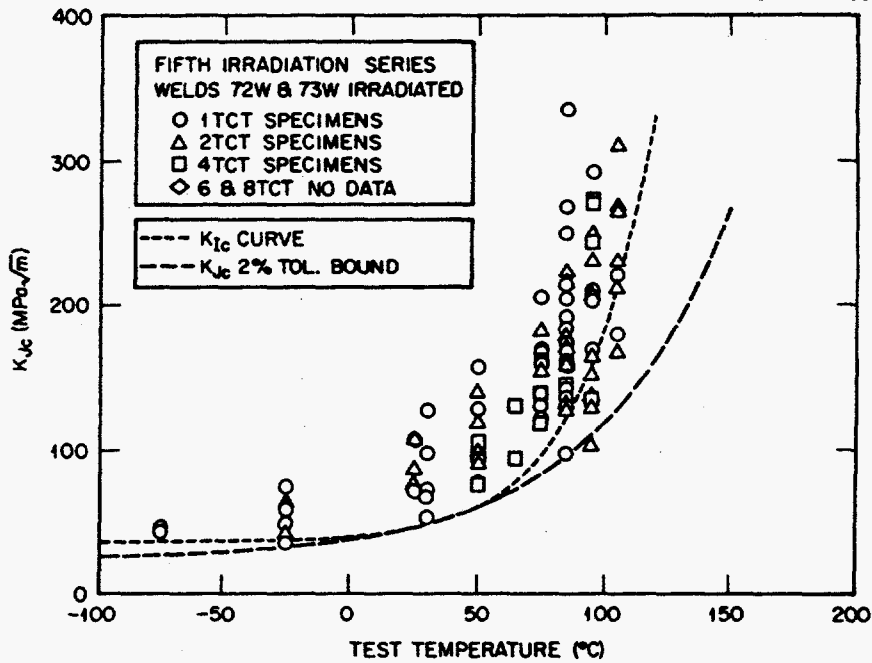


FIG. 9--Unadjusted data, lower-bound  $K_{Ic}$  curve (dotted), and 2% tolerance bound curve (dashed) for Heavy-Section Steel Irradiation Program welds 72W and 73W irradiated to a fast neutron fluence of  $1.5 \times 10^{19} \text{ n/cm}^2 (>1 \text{ MeV})$ .

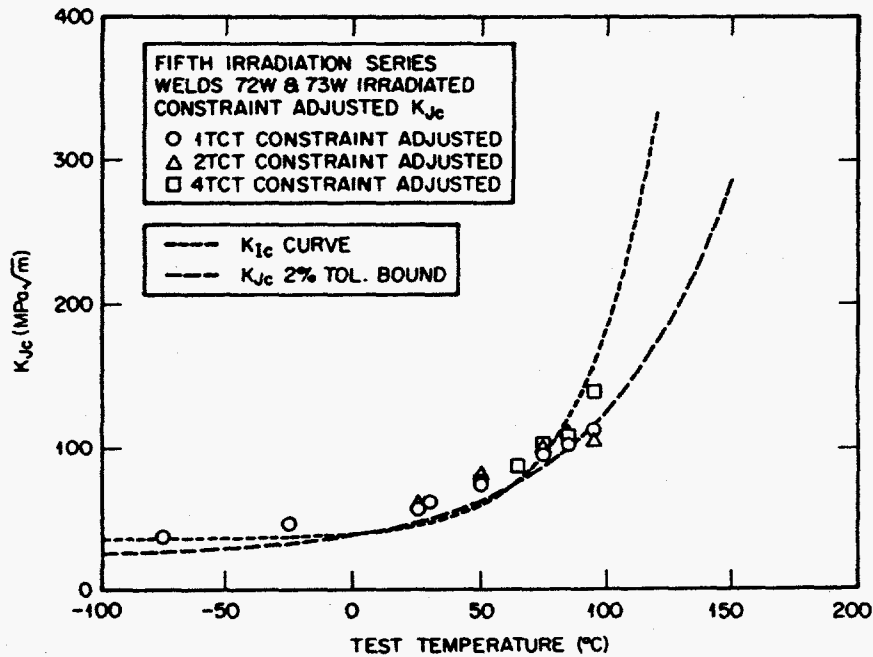


FIG. 10--American Society of Mechanical Engineers  $K_{Ic}$  curve (dotted), 2% tolerance bound curve (dashed), and procedurally adjusted to lower-bound data for Heavy-Section Steel Irradiation Program welds 72W and 73W irradiated to a fast neutron fluence of  $1.5 \times 10^{19} \text{ n/cm}^2 (>1 \text{ MeV})$ .



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