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Procedia Structural Integrity 47 (2023) 589–596

Structural Integrity Procedia

www.elsevier.com/locate/procedia

27th International Conference on Fracture and Structural Integrity (IGF27)

Comparison of two recent approaches to DTB characterization of ferritic steels

Branislav Djordjevic[a,*], Sreten Mastilovic[b], Aleksandar Sedmak[c], Aleksandar Dimic[c], Simon Sedmak[a], Mihajlo Arandjelovic[a]

[a]*Innovation Center of Faculty of Mechanical Engineering, Kraljice Marije 16, Belgrade, Serbia*
[b]*University of Belgrade, Institute for Multidisciplinary Research, Kneza Viseslava 1, Belgrade, Serbia*
[c]*University of Belgrade, Faculty of Mechanical Engineering, Kraljice Marije 16, Belgrade, Serbia*

Abstract

The large scatter of the experimental fracture toughness data, characteristic of all ferritic steels in the ductile-to-brittle transition temperature region, imposed the need to include statistical methods for data processing. Due to the inherent stochasticity, the application of fracture mechanics concepts in the characterization of the DTB transition phenomenon has remained a challenging task over the past 50 years. Various models were developed based on statistical approach to data processing in order to capture the salient features of the phenomenon, but all of them have certain limitations because of the intrinsic complexity of the problem. However, all these models provided a solid basis for the continued development of new approaches in the characterization of DTB. Such two novel models are compared herein. They include size effects and utilize scaling of geometrically similar C(T) specimens, with the aim of obtaining predictions of the fracture toughness. Both proposed models have the weakest link statistics in common. In the present study, the EURO fracture toughness data set for 22NiMoCr37 reactor steel is used and the experimental data obtained at temperature of -60 ºC is selected to demonstrate the accuracy of the estimates. The fracture toughness measure used is the critical value of the stress intensity factor used in the master curve K_{Jc} [MPa √m]. The obtained predictions are in good agreement with the experimental results, taking into account the inherent scatter of the experimental data. The estimate of K_{Jc} cumulative distribution function obtained by extrapolation using the novel two-step-scaling method is sensitive to the statistical size of the input data sets.

* Corresponding author. Tel.: /; fax: /
E-mail address: b.djordjevic88@gmail.com

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Peer-review under responsibility of the IGF27 chairpersons
10.1016/j.prostr.2023.07.065

Keywords: Ductile-to-brittle transition; Fracture toughness; Ferritic steels; Statistical processing.

1. Introduction

The occurrence of the DTB (ductile-to-brittle) transition in ferritic steels has been a research challenge since 1970s. Characterization of this problem within the realm of Fracture Mechanics became inevitable from the pioneering studies based on the LEFM (linear elastic fracture mechanics) to the application of the EPFM (elastic-plastic fracture mechanics) concept. To begin with, it cannot be overemphasized that fracture toughness is not an intrinsic material property. It is sensitive to loading and environmental conditions, type and distribution of material defects, and geometrical factors (e.g., sample shape, thickness, surface roughness) [1, 2]. The pronounced dispersion of experimental data on fracture toughness, characteristic of all ferritic steels in the DTB transition region, necessitated the use of statistical methods for data processing and analytical modeling. That approach, which emerged in the 1970s, can still be found today as the basis for interpreting fracture toughness data in DTB characterization. During these last five decades, an extensive theoretical, experimental and computational literature has been accumulated. Among numerous statistical studies concerned specifically on the cleavage fracture toughness of ferritic steels that make use of the Weibull statistics [3], stand out the empirical approach by Landes and coworkers, the Beremin local model, the Master Curve model of Wallin and others, the Prometey model as outlined, for example, in the recent succinct historical survey [4].

The statistical approach to the problem is based on the idea that the fracture probability increases with increase in the probability of the finding structural defects in the volume of a tested sample or an engineering structure. Also, the increase in volume is generally accompanied by a decrease of stochasticity (data scatter). The research prominence of this research topic has emerged from “the need to extrapolate from laboratory tests to much larger real structures, as well as the recognition that the strength of brittle and quasibrittle structure may be significantly impaired when its size is increased beyond the usual range of dimensions” [5]. Another reason has been the imperative to bridge spatial scales in material modeling and to bind the models of different physical phenomena occurring on different structural scales in order to develop physically sound material models.

The focus of the present case study is on the two new methods of DTB characterization of ferritic steels: (i) the 1-point (1P) method [6, 7] and (ii) the two-step-scaling (2SS) method [8, 9]. The objective is to explore their ability for the fracture toughness assessment in the DTB transition temperature region. The two approaches are briefly summarized in the following section.

2. Two Novel Approaches to Fracture Toughness Assessment in the DTB Transition Region

2.1. The 1P Approach to Size Effect Modeling of Fracture Toughness CDF

This method presented in [6, 7], as an integral part of fracture behavior study [10], demonstrated the possibility of getting Weibull CDF (cumulative distribution function) cleavage fracture predictions for larger C(T) ferritic-steel specimens in the DTB transition temperature region based on the statistical data manipulations of one specimen size dataset. The 1P method tacitly assumes applicability of the weakest-link theory and the two-parameter (β, η) Weibull distribution. The gist of this approach is based on Wallin’s research [11] followed by many similar studies later. The fracture toughness measure K_{Jc} used in the present article represents the critical value of the stress intensity factor used in the master curve. The CDF ($K_{Jc} \mid \beta$, η) predictions for larger C(T) specimen size (B_2) can be written using following equations

$$P\left(K_{Jc} \mid \beta, \eta_2\right) = 1 - \exp\left\{-\left(\frac{K_{Jc}}{\eta_2}\right)^{\beta}\right\} \tag{1}$$

$$\eta_2 = \eta_1 \left(\frac{B_1}{B_2}\right)^{1/\beta} = \eta_1 \left(\frac{W_1}{W_2}\right)^{1/\beta}, \quad \beta = const. \tag{2}$$

$$P_i = \frac{i - 0.3}{n + 0.4} \quad (3)$$

where η and β designate Weibull scale and shape parameters, respectively. Notably, the Weibull parameters η_1 and β = const. are obtained by regression analysis of the experimental data on C(T) specimens with thickness B_1 (width W_1), while η_2 is the Weibull scale parameter for larger specimen (B_2 or W_2) predicted based on Eq. (2). Thus, the 1P method of CDF prediction is based on: (i) regression analysis of one C(T)-size dataset, and (ii) the assumption that the shape parameter is size-independent. In addition to the constancy of β, the key feature of the 1P method is its reliance on a single experimental point (that is, one C(T)-size dataset) for predictions for other C(T) sizes.

2.2. The 2SS Approach to Size Effect Modeling of Fracture Toughness CDF

The objective of the subject size-effect investigation [8, 9] had been the estimation of the Weibull CDF of the fracture toughness in the DTB temperature range. The pertinent equations are rewritten herein by using CDF ($K_{Jc}\,|\,\beta, \eta$). The Weibull CDF can be re-written in the form

$$P\left(K_{Jc} \mid \beta, \eta\right) = 1 - \exp\left\{-\left(\frac{K_{Jc} \cdot W^{\kappa}}{\eta_*}\right)^{\beta(W)}\right\} \quad (4)$$

where W designates the characteristic size (e.g., width in this case) of the C(T) specimen. It cannot be overemphasized that C(T) specimens are geometrically similar (W is proportional to B). Eq. (4) corresponds to the limiting case $\eta_\infty \equiv \lim_{W \to \infty} \eta(W) = 0$ (consult the original article [8] for details). The size-independent Weibull scale parameter η_* in the scaled space, $P(K_{Jc} \cdot W^{\kappa})$ vs. $K_{Jc} \cdot W^{\kappa}$, is defined by the fracture toughness scaling condition illustrated in Fig. 1a:

$$\eta_* = \eta_i \cdot W_i^{\kappa} = const., \quad \forall i = 1,2,... \quad (5)$$

In Eq. (5), i marks the C(T) specimen size class (e.g., W_1=25, W_2=50,...; see Tables 1 and 2).

It should be noted that Eq. (5) reduces to Eq. (2) for the special case $\kappa = 1/\beta$ = const. This is not surprising since the assumption β = const. makes the second scaling in the 2SS method unnecessary (i.e., $\xi \equiv 0$; see [8] for details). This indicates that the 2SS method is more general then the 1P method.

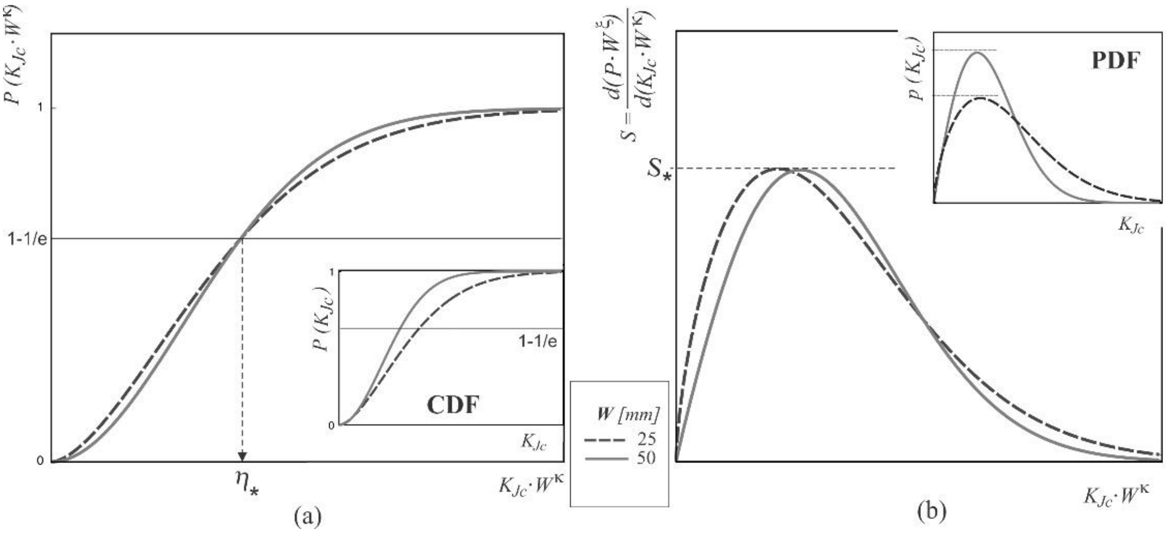


Fig. 1. (a) The outcome of the first scaling is the overlap of the CDF points corresponding to $P(K_{Jc}=\eta)$=1-1/e, which defines the common value of the Weibull scale parameter η_* in the scaled space (note the inset illustration the two CDFs before the scaling). (b) The outcome of the second scaling is the common CDF slope S_* in the scaled space, which scales with the equal PDF maxima. The two scalings are uniquely defined by (κ, ξ).

The entire mapping from the original space, $P(K_{Jc})$ vs. K_{Jc}, to the scaled space, $P(K_{Jc}\cdot W^{\kappa})\cdot W^{\xi}$ vs. $K_{Jc}\cdot W^{\kappa}$,is uniquely defined by a pair of scaling parameters (κ, ξ) that are at the core of the 2SS method. The former is defined by Eq. (5) while the latter is defined by the CDF-scaling condition

$$S_* = S_i \cdot W_i^{\xi} = const., \quad \forall i = 1,2,... \tag{6}$$

that defines the common CDF slope (S_*) in the scaled space (note that S_* scales with the equal PDF maxima (PDF = probability density function of the Weibull distribution marked by p in the inset of Fig. 1b) [8]).

The scale parameters can be calculated from the available experimental dataset *pair* by (*two experimental points* as a minimum) using the following relationships

$$\kappa = \log_{\left(\frac{W_{i+1}}{W_i}\right)}\left(\frac{\eta_i}{\eta_{i+1}}\right), \quad \xi = \log_{\left(\frac{W_{i+1}}{W_i}\right)}\left[\frac{\Xi(\beta_i)}{\Xi(\beta_{i+1})}\right] \tag{7}$$

where index i (=1,2,..) designates the input experimental data sets (e.g., W_1, W_2,...= 25, 50,...; see Tables 1 and 2). The scaling parameters defined by Eqs. $(7)_1$ and $(7)_2$ follow respectively from the constancy conditions (5) and (6) that are at the core of the 2SS method.

Finally, when: (i) the size-independent Weibull scale parameter η_*, (ii) the scaling parameter ξ, and (iii) the corresponding size-independent CDF slope S_* are evaluated; the value of shape function

$$\Xi(\beta) = \beta\, \varpi^{\varpi} e^{-\varpi}, \quad \varpi = 1 - 1/\beta \tag{8}$$

can be calculated for each particular specimen dimension W

$$\Xi(\beta | W, \xi) = S_*\, \eta_*\, W^{-\xi} \tag{9}$$

As defined by Eq. (8) and illustrated by Fig. 2, the shape function provides 1:1 correspondence with the Weibull shape parameter ($\Xi \Leftrightarrow \beta$) under the constraints of the sigmoid shaped CDF [8].

Eqs. (4) through (9) summarize the 2SS method. As stressed in [8], due to the 3-D geometrical similarity of the C(T) specimen ($B \propto W$), it is easy to rewrite them in terms of the C(T) thickness B (similarly to Eq. (2)).

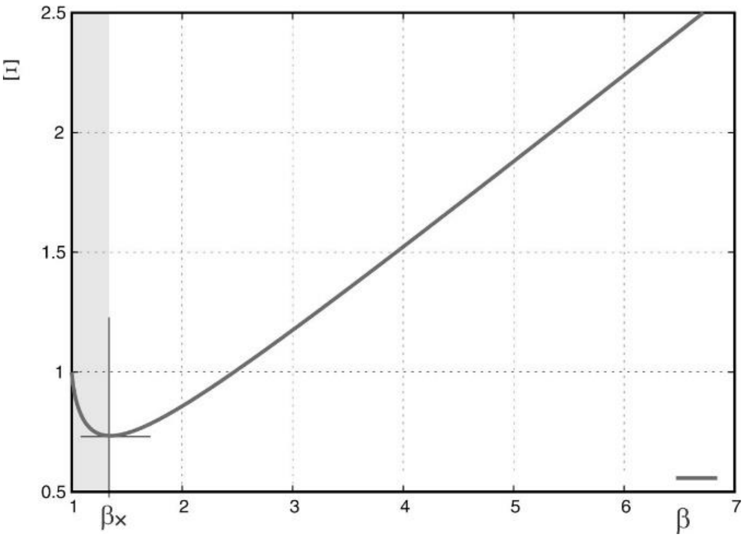


Fig. 2. Dependence of the shape function, defined by Eq. (8), on the Weibull shape parameter β. (The characteristic sigmoid shape is obtained for $\beta > \beta_\times \approx 1.35$ [8]).

3. Predictions of CDF (K_{Jc}) of 22NiMoCr37 reactor steel at low temperature

As note before, the validation of both methods (1P and 2SS) is performed by using K_{Jc} values obtained from [12]. This experimental data is obtained originally from the Euro fracture toughness dataset generated by ten European laboratories in order to provide an experimental data base "sufficiently large to study specimen size and temperature effects on cleavage fracture toughness" in the DTB transition regime [13]. The data quantifies the fracture behavior of the quenched and tempered pressure-vessel reactor steel 22NiMoCr37 frequently used in nuclear power plants [13].

3.1. The estimates of K_{Jc} CDF in the DTB Transition Region by the 1P method

The application of the 1P method starts with the fitting of one C(T)-size experimental dataset obtained at T = -60°C for W_1=2·B_1=25 mm, marked by blue circles in Fig. 3. This fitting procedure (based on the Weibull plot and the regression analysis) results in determination of the Weibull scale and shape parameters (η_1=157. MPa √ m and β=4.80, respectively) using three significant digits. Since β=4.80=const., only the scale parameters η_2 *and* η_3 have been estimated using Eq. (2) (Table 1).

Table 1. The Weibull scale and shape parameters for three different C(T) sizes. The 1P method inputs are parameters corresponding to W = 25 while those corresponding to W = 50, 100 (the bold font) are the outputs.

i	W	η	β = const.
1	25	157.	4.8
2	**50**	**135.9**	**4.8**
3	**100**	**117.6**	**4.8**

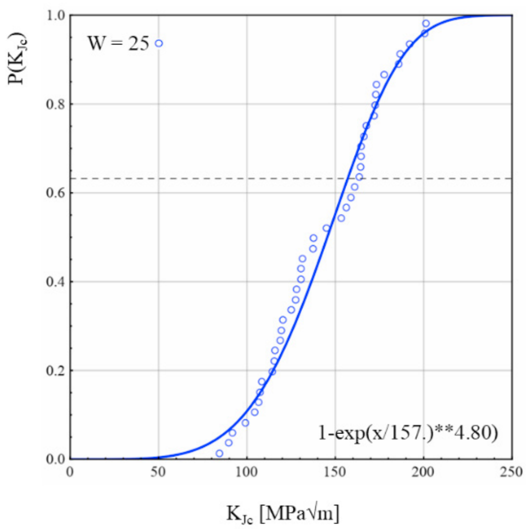
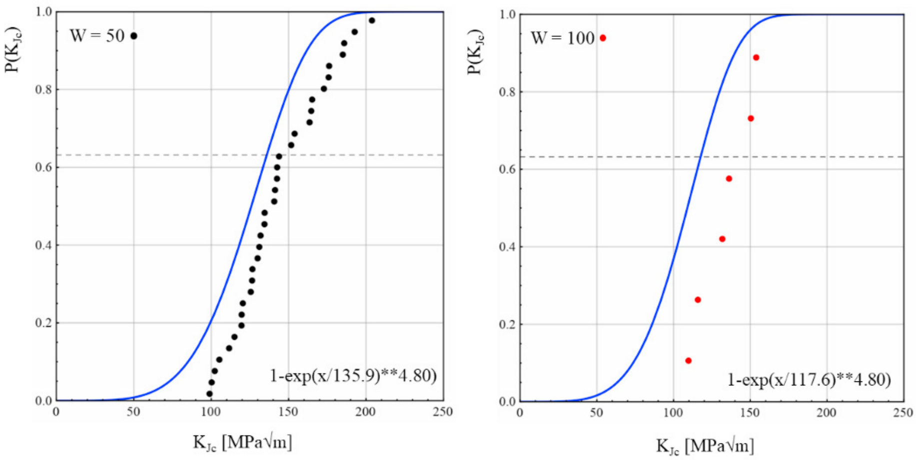


Fig. 3. The inputs for the 1P approach: The experimentally obtained $K_{Jc(exp)}$ CDF (blue dot symbols, n = 44) at T = -60 ºC for the C(T) sample sizes W = 25 and the corresponding Weibull distribution fit (4.80, 157.).

The CDFs estimation for large C(T) specimens size can be drawn using Eq.(1) after shape parameters η were estimated. Fig. 4 illustrates the Weibull CDFs predictions for W = 50,100 (Table 1) and offers the comparison with the experimental data [12] (blue and red circles for C(T)50 and C(T)100, respectively). The estimates shown in Fig. 4 provide conservative CDFs predictions.



(a) (b)

Fig. 4. The output of the 1P approach: an estimated K_{Jc} CDF at T = -60ºC for the C(T) sample sizes W=50,100 (solid lines) based on the W=25 inputs (Fig. 3). The dots correspond to the actual experimental datasets.

3.2. The extrapolation of K_{Jc} CDF in the DTB Transition Region by the 2SS Method

The application of the 2SS approach starts with the data fitting of the two input experimental data sets (W = 25, 50), illustrated by triangle symbols in Fig. 5, with the 2-parameter Weibull CDF. The fitting results in determination of the Weibull scale and shape parameters (η and β, respectively) given in the first two rows of Table 2. (The Weibull parameters are determined by using the Weibull plots and the regression analysis.)

Table 2. The Weibull scale and shape parameters and the corresponding shape function. The values for -60ºC and W = 25, 50 are the inputs used to calculate the extrapolated estimate for W = 100 (the bold font).

i	W	η	β	Ξ
1	25	157.	4.80	1.81
2	50	151.	5.75	2.15
3	**100**	**145.**	**6.85**	**2.55**

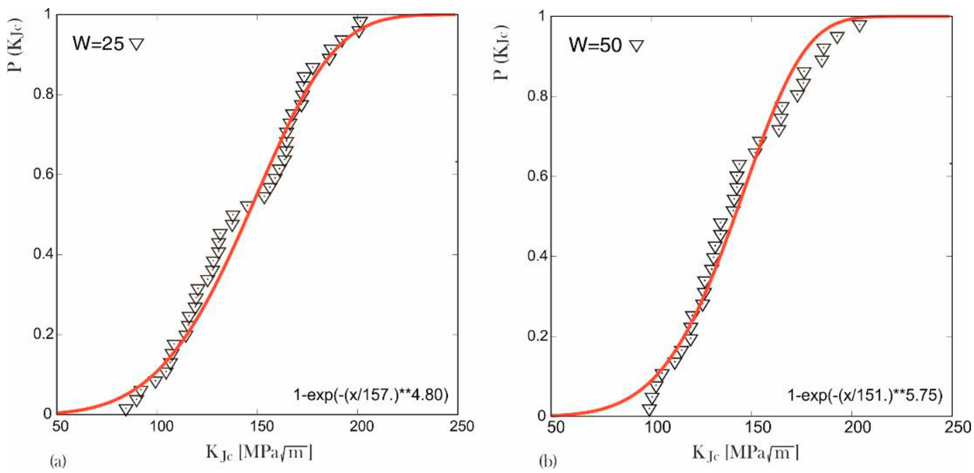


Fig. 5. The inputs for the 2SS Method ("2 points"): The experimentally obtained $K_{Jc(exp)}$ CDF (triangles) at T = -60 ºC for the C(T) sample sizes W = 25, 50 and the corresponding 2-parameter Weibull distribution fits. The C(T) sample corresponding to (a) W = 25 has 44 data points, while (b) W = 50 has 34 data points obtained from two different laboratories (GKSS and SIEMENS [12]).

The values of the shape function Ξ (given in the fifth column of Table 2) are calculated by using Eq. (8), once β values are known. With regards to the data fitting results (η and β) presented, it should be noted that the fitting procedure, in spite of the regression analysis, might allow more subjectivity to an analyst then desirable, which emphasizes the importance of the statistically large and high-quality experimental datasets.

The pair of the scaling parameters (κ, ξ) are calculated from Eq. (7)

$$\kappa = \log_{\left(\frac{50}{25}\right)}\left(\frac{157.}{151.}\right) = 0.0562\,, \quad \xi = \log_{\left(\frac{50}{25}\right)}\left(\frac{1.81}{2.15}\right) = -0.248 \tag{10}$$

for the values of the input parameters given in Table 2.

The size-independent Weibull scale parameter η_* in the scaled space, $P(K_{Jc}\cdot W^{\kappa})$ vs. $K_{Jc}\cdot W^{\kappa}$, is calculated by using the constancy condition (5) and the values from Table 2:

$$\eta_* = 157.\cdot 25^{0.0562} = 151.\cdot 50^{0.0562} = 188. = const. \tag{11}$$

The common (size-independent) *CDF* slope (S_*) in the scaled space can be calculated based on Eq. (9) for each particular specimen dimension W

$$S_* = \frac{1}{\eta_*}\Xi\left(\beta\,|\,W,\xi\right)W^{\xi} = \frac{1}{188.}\cdot 1.81\cdot 25^{-0.248} = \frac{1}{188.}\cdot 2.15\cdot 50^{-0.248} = 0.00433 = const. \tag{12}$$

The shape function value for the C(T) dimension W=100 can be calculated by using Eq. (9)

$$\Xi\left(\beta\,|\,W=100,\xi=-0.248\right) = 0.00433\cdot 188.\cdot 100^{-(-0.248)} = 2.55 \tag{13}$$

The shape function value $\Xi = 2.55$ uniquely determines the Weibull shape parameter $\beta = 6.85$ based on Fig. 2 (in the domain corresponding to the sigmoid shape of the Weibull CDF [8]).

The solid line in Fig. 6 illustrates the Weibull CDF extrapolation for $W = 100$ and offers the comparison with the experimental data (circles) reported in [12]. The extrapolation results in Fig. 6 are satisfactory considering the relatively small number of experimental data points in Fig. 6 as well as the inherent stochasticity of fracture toughness in the DTB temperature transition region.

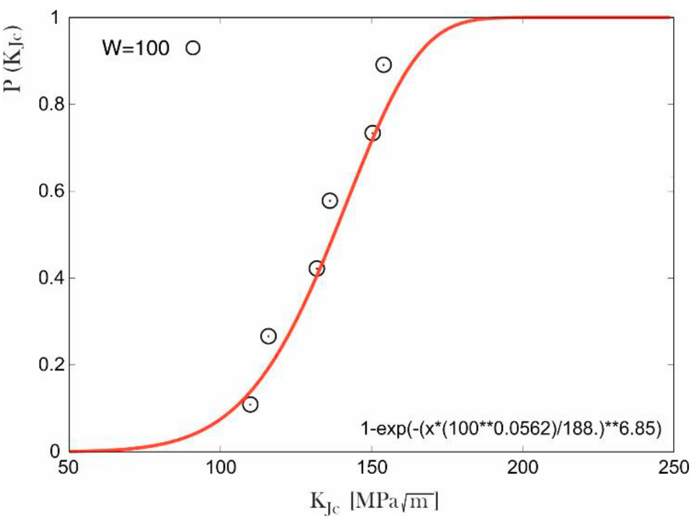


Fig. 6. The output of the 2SS Method: The extrapolated K_{Jc} CDF at T =-60 ºC for the C(T) sample size W=100 (solid line) based on the inputs in Fig. 3. The circles correspond to the actual experimental data set.

4. Summary

The present case study is dedicated to exploration of the ability of the two novel approaches to the DTB characterization of ferritic steels to predict the fracture toughness for structural sizes outside of the experimental data set. The obtained results suggest that the fracture toughness assessment is within the inherent epistemic uncertainty and aleatory variability of the phenomenon. The demonstration procedure also highlights the importance of the statistical sample size (the number of experiments per CT sample size, n) that should be subject of the future work. A comparison of these two approaches suggests that the 1P model is simpler to apply since it requires only one input dataset and simpler mathematics. On the other hand, the Weibull shape parameter is fixed (size-insensitive), which limits flexibility. Fortuitously or not, in the numerical example used herein for model demonstration, the 1P method provided conservative CDF prediction, which is safer from the structural integrity standpoint, but also more expensive during designing. In comparison, the 2SS method requires experimental datasets of at least two C(T) sizes, but offers greater analytical flexibility in return. Thus, the 2SS approach provides more realistic predictions than 1P method, with pronounced trend for optimization during designing.

Importantly, it is shown that 2SS method reduces to the 1P method if $\kappa = 1/\beta$ = const. This deserves further study. Be it as it may, the assumption β = const. makes the second scaling in the 2SS method unnecessary since CDFs would overlap into the master curve after the first scaling.

Finally, it should be noted that the predictions by both algorithms are sensitive to the size n of the statistical sample(s) used as input(s); perhaps more so in the case of the 2SS method.

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