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UPGRADED TWO-STEP-SCALING APPROACH TO THE DTB CHARACTERIZATION OF FERRITIC STEELS

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Abstract:

The fracture toughness of ferritic steels in the DTB (ductile-to-brittle) transition temperature region is a stochastic *extrinsic* property known for pronounced experimental data scatter that necessitates statistical approach in the DTB characterization. The novel two-step-scaling (2SS) method, proposed recently for the size effect-modeling across the DTB transition region, is developed based on the weakest-link statistics and the two-parametric Weibull distribution. Specifically, the size sensitivity of the Weibull parameters of scale and shape are built into the appropriate framework. This approach is upgraded in this article to render the comparison with the existing models more transparent. Specifically, the original 2SS method is enhanced by adding a lower limit on fracture toughness, resulting in the translated (three-parameter) Weibull cumulative distribution function. This third Weibull parameter, often dubbed the location parameter, defines a threshold value that limits the accessible fracture toughness domain. The upgraded 2SS approach is compared to two established methods of the DTB fracture toughness assessment, which favorably reflected upon its generality and application flexibility.

Key words: scaling, fracture toughness, size effect, Weibull distribution, location parameter

1. Introduction

The brittle fracture at low temperatures is characterized by pronounced variations of fracture toughness (especially for small specimen) as well as others fracture properties and a statistical approach is a necessity. The Weibull theory is one of the first size-effect theories of the strength of materials that is developed on purely statistical arguments [1, 2]. The Weibull statistics is based on the weakest-link theory that is considered appropriate for modeling of the cleavage fracture of ferritic steels in the DTB (ductile-to-brittle) transition region, addressed in the present study. The plasticity mechanisms and stress redistribution are largely suppressed, which results in catastrophic failure, and, consequently, an inherently statistical nature of the size effect – the kind traditionally described by the Weibull distribution. Landes et al. (e.g., [4]) based their statistical approach on the premise that the cleavage fracture toughness is controlled by the weakest link at the crack front. They used the two-parameter Weibull distribution, W (β, η), which is a frequent choice for the DTB characterization to this day (e.g., [3, 5]). A succinct historical survey of some of the most influential statistical studies of the cleavage fracture toughness of ferritic steels that make use of the Weibull statistics is, as an example, recently compiled in [6].

The novel two-step-scaling (2SS) approach has been developed [3, 7] with a focus on the DTB assessment of the fracture toughness size effect. The present study upgrades that original 2SS approach by introducing a lower limit on fracture toughness in the Weibull CDF (cumulative distribution function), resulting in a three-parameter Weibull distribution, W (β, η, γ). This third Weibull parameter, called the location parameter, defines a threshold value that limits the accessible fracture toughness domain [8].

2. The 2SS procedure revisited

The starting point in the present analysis is the translated Weibull CDF:

$$F(K \mid \beta,\eta,\gamma) = 1-\exp\left[-\left(\frac{K-\gamma}{\eta}\right)^{\beta}\right]; \qquad (K-\gamma)\geq 0;\, \beta,\eta,\gamma \in \Re^{+} \tag{1}$$

where β, η ($= K_0 - K_{\min}$) and γ ($=K_{\min}$=const.) are the Weibull shape, scale and location parameters [9], respectively. In Eq. (1), the symbol K is used for the generic critical value of the stress intensity, while K_0 and $K_{\min}$ stand for the normalization and the threshold values, respectively.

The scaling procedure involves also the W (β, η, γ) probability density function (PDF)

$$f(K \mid \beta,\eta,\gamma) = \frac{\beta}{\eta}\left(\frac{K-\gamma}{\eta}\right)^{\beta-1}\exp\left[-\left(\frac{K-\gamma}{\eta}\right)^{\beta}\right] = \frac{dF(K)}{dK} \tag{2}$$

that represents slope in the F vs. $(K\text{-}\gamma)$ space. Hereinafter, $dK = d(K\text{-}\gamma)$ is used for brevity.

Furthermore, it is of interest to derive the maximum CDF slope, which corresponds to the inflection point (Π) defined by:

$$\left.\frac{d^2F}{dK^2}\right|_{K=K_\Pi} = \left(\frac{\beta}{\eta}\right)^{2}\left(\frac{K_\Pi-\gamma}{\eta}\right)^{\beta-2}\exp\left[-\left(\frac{K_\Pi-\gamma}{\eta}\right)^{\beta}\right]\left[1-\frac{1}{\beta}-\left(\frac{K_\Pi-\gamma}{\eta}\right)^{\beta}\right] = 0 \tag{3}$$

The inflection point definition (3) determines its coordinate in the F vs. $(K\text{-}\gamma)$ space

$$K_\Pi - \gamma = \eta \cdot \left(1-\frac{1}{\beta}\right)^{1/\beta} \tag{4}$$

that corresponds to $f_{\max}$ (5) and represents the mode of the Weibull distribution (1) by definition.

After a straightforward derivation, the Weibull CDF slope (2) at the inflection point (4) that corresponds to the PDF maximum is obtained in the following form:

$$S = \left.\frac{dF(K)}{dK}\right|_{K=K_\Pi} = \frac{1}{\eta}\,\Xi(\beta) = f(K)\big|_{K=K_\Pi} = f_{\max} \tag{5}$$

where

$$\Xi(\beta) = \beta\left(1-\frac{1}{\beta}\right)^{1-1/\beta}\exp\left[-\left(1-\frac{1}{\beta}\right)\right]; \quad \beta > \beta_{\times} \approx 1.35 \tag{6}$$

designates the shape function (as introduced in [3]). The domain definition $(6)_2$ ensures that the Weibull CDF assumes the characteristic sigmoid shape [3, 10].

2.2 The two-step scaling scheme for the three-parameter Weibull CDF

The same basic relationships derived in the preceding section are revisited herein in the scaled space: $F\cdot W^{\xi}$ vs. $(K-\gamma)\cdot W^{\kappa}$ illustrated in Fig. 1e. The motivation is that the gist of present approach to investigating the fracture toughness size effect rests upon the two scaling premises [3]:

(i) The scaling condition along the CDF abscissa (driven by the scaling parameter κ):

$$\eta_* = \eta \cdot W^{\kappa} = \left(K_0 - K_{\min}\right)\cdot W^{\kappa} = const. \tag{7}$$

defining the size-independent Weibull scale parameter η_* in *the scaled space* (Fig. 1c), and

(ii) The scaling condition along the CDF ordinate (driven by the scaling parameter ξ):

$$S_* = S \cdot W^{\xi} = const. \tag{8}$$

defining the common CDF slope S_* in the scaled space (Fig. 1e) that represents the common PDF maximum (Fig. 1f), related to the PDF maxima in the same space (Fig. 1b) by the formula

$$f_{\max} = W^{\kappa-\xi}\ S_* \tag{9}$$

Thus, it is required to re-derive the CDF slope (5), this time in the F–$(K-\gamma)$ space, which yields

$$S_* = \left.\frac{dy}{dx}\right|_{x=x_\Pi} = \frac{1}{\eta_*}\,\Xi(\beta)\,W^{\xi} \tag{10}$$

In the preceding derivation, it is convenient to use the change of variables $y = F\cdot W^{\xi}$ and $x = (K-\gamma)\cdot W^{\kappa}$, which results in the functional dependence of the inflection point coordinate in the scaled space upon the Weibull shape parameter

$$\frac{\left(K_\Pi - \gamma\right)\cdot W^{\kappa}}{\eta_*} = \left(1 - \frac{1}{\beta}\right)^{1/\beta} \tag{11}$$

that is unchanged compared to Eq. $(4)_1$ (by virtue of the first constancy condition (7)).

A couple of observations could be made based on Eq. (10). First, the Weibull scale parameter in the scaled space is size-independent (Fig. 1c) by virtue of the K-scaling condition, $\eta_* = const.$ (7). Second, the CDF slope in the scaled space $F\cdot W^{\xi}$ vs. $(K-\gamma)\cdot W^{\kappa}$ is also size-independent (Fig. 1c) by virtue of the second step scaling condition, $S_* = const.$ (8). Consequently, Eq. (10) implies that

$$\Xi(\beta)\,W^{\xi} = const. \tag{12}$$

The value of shape function Ξ

$$\Xi\left(\beta\,\middle|\,W,\xi\right) = S_*\,\eta_*\,W^{-\xi} \tag{13}$$

can be calculated for each particular specimen size once ξ and S_* are determined.

The pair of scaling parameters (κ, ξ) that govern the two scaling steps (illustrated in Fig. 1) is defined by the constancy conditions (7) and (12):

$$\kappa = \log_{\left(\frac{W_j}{W_i}\right)}\left(\frac{\eta_i}{\eta_j}\right), \quad \xi = \log_{\left(\frac{W_j}{W_i}\right)}\left[\frac{\Xi(\beta_i)}{\Xi(\beta_j)}\right] \tag{14}$$

where indices i, j (=1,2,..) mark the input experimental data sets (e.g., W_1, W_2,...= 25, 50,...).

The shape parameter $\beta(W, \xi)$ can be determined based on Eq. (6) once the value of Ξ $(\beta|W, \xi)$ is known.

Finally, the Weibull CDF can now be written in the following form

$$F\left(K \mid \beta, \eta_*, \gamma\right) = 1 - \exp\left\{ -\left(\frac{(K-\gamma)\cdot W^{\kappa}}{\eta_*} \right)^{\beta(W,\xi)} \right\}; \qquad (K-\gamma) \geq 0;\, \beta, \eta_*, \gamma \in \Re^+ \tag{15}$$

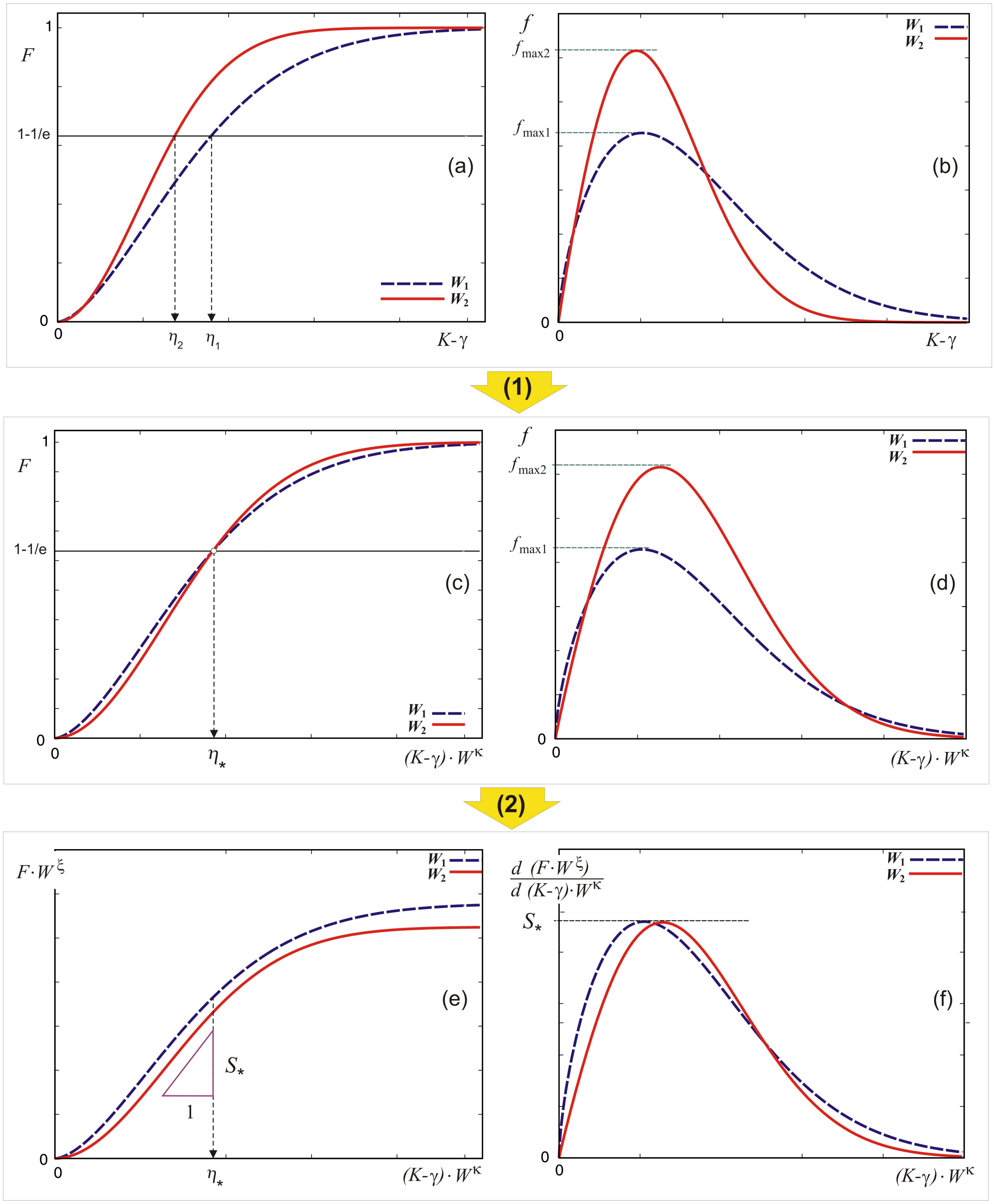

Fig. 1. Schematics of the two scaling steps in the upgraded 2SS procedure (W_1 and W_2 mark sizes of two experimental data sets)

3. Relationship between the novel 2SS method and two established methods for DTB characterization of fracture toughness

The scaling along the abscissa is defined by the parameter κ which ensures that the constancy condition (7) is met. Therefore, in the novel 2SS procedure, κ is an independent fitting parameter determined by the input experimental data sets. Application of the 2SS method requires as an input at least two experimental data sets corresponding to two C(T) specimen size (e.g., W_1 and W_2 shown in Fig. 1). If that is the case, the constancy condition governing the first scaling step (along the abscissa) can be written in the form:

$$\eta_* = \eta_1 \cdot W_1^\kappa = \eta_2 \cdot W_2^\kappa \quad \Rightarrow \quad \left(K_{01} - K_{\min}\right) \cdot W_1^\kappa = \left(K_{02} - K_{\min}\right) \cdot W_2^\kappa \tag{16}$$

The constancy condition written in the form of Eq. (16) will serve for comparison of the 2SS method with two established methods for DTB fracture toughness assessment.

First, it is obvious from Eq. $(16)_1$ that if the Weibull scale parameter (η_2) for the specimen of effective width W_2 is unknown, it can be calculated from the corresponding values of the first specimen as follows:

$$\eta_2 = \eta_1 \cdot \left(\frac{W_1}{W_2}\right)^\kappa \tag{17}$$

The relation (17) is identical to the corresponding expression from the 1-point method [5, 6]

$$K_{B_2} = K_{B_1} \cdot \left(\frac{B_1}{B_2}\right)^{1/\beta}, \quad K_{\min} = 0, \ \beta = const. \tag{18}$$

for the special case $\kappa = 1/\beta$ (bearing in mind that the geometric similarity implies $B_1/B_2=W_1/W_2$). (Importantly, the 2SS procedure can use any characteristic linear dimension of the C(T) specimen, not necessarily the effective width, W. Assuming the geometrical similarity, $B \propto W$, the specimen thickness can replace the width in Eq. (16) without loss of generality.)

Similarly, based on the three-parameter Weibull CDF of cleavage fracture with constant shape parameter ($\beta = 4$), Wallin [8] proposed the following expression

$$K_{B_2} = K_{\min} + (K_{B_1} - K_{\min})\left(\frac{B_1}{B_2}\right)^{1/4} \tag{19}$$

It is obvious that Eq. $(16)_2$ reduces Eq. (19) if the scaling parameter $\kappa = 1/\beta = 1/4$ (since K_B and K_0 depict the the same physical property). It should be emphasized that the assumption of the size-insensitivity of the Weibull shape parameter ($\beta =$ const.) makes the second scaling in the 2SS method unnecessary (i.e., $\xi \equiv 0$ in Eq. (8) and Fig. 1) since the first scaling would result in the overlap of the Weibull CDF in Fig. 1c. This indicates that the 2SS method is both more general and more flexible then both above mentioned methods.

4. Numerical example: Prediction of CDF (K_{Jc}) of 22NiMoCr37 reactor steel at T=-91ºC

The following numerical example is performed using C(T) sample thickness B as the sample size parameter instead of the effective width W to demonstrate that their use is interchangeable in the presence of geometric similarity. The application of the 2SS approach starts with the data fitting of the two input experimental data sets (B = 12.5, 25) mm with the 3-parameter Weibull CDF.

Assuming the threshold $\gamma = K_{\min} = 40$ MPa√m based on the two available experimental data sets [10], the fitting results in the Weibull scale and shape parameters (η and β, respectively) given in Table 1. The Ξ values are calculated by using Eq. (6), once β values are known.

Table 1. The Weibull parameters and the corresponding shape function. The values corresponding to B = 12.5, 50 mm are the inputs used to calculate the extrapolated estimate for B = 100 mm (the bold font)

B	β	η_0	γ	$\eta=\eta_0-\gamma$	Ξ
12.5	2.70	119.	40.	79.0	1.075
50	4.25	92.0	40.	52.0	1.611
100	**5.25**	**82.2**	40.	**42.2**	**1.973**

The pair of the scaling parameters (κ, ξ) is calculated from Eq. (14)

$$\kappa = \log_{\left(\frac{50}{12.5}\right)}\left(\frac{79.0}{52.0}\right) = 0.302\,, \quad \xi = \log_{\left(\frac{50}{12.5}\right)}\left(\frac{1.075}{1.611}\right) = -0.292 \tag{20}$$

The size-independent Weibull scale parameter η_{B*} in the scaled space, $P(K_{Jc}{\cdot}B^{\kappa})$ vs. $K_{Jc}{\cdot}B^{\kappa}$, is calculated by using the B-related form of the constancy condition (7) and the Weibull parameters from Table 1:

$$\eta_{B*} = 79.0\cdot 12.5^{0.302} = 52.0\cdot 50^{0.302} = 169.4 = const. \tag{21}$$

Similarly, the common *CDF* slope (S_{B*}) in the scaled space can be calculated based on Eq. (10) for each particular specimen dimension B

$$S_{B*} = \frac{1}{\eta_*}\Xi\left(\beta\,|\,B\right)\cdot B^{\xi} = \frac{1}{169.4}\cdot 1.075\cdot 12.5^{-0.292} = \frac{1}{169.4}\cdot 1.611\cdot 50.0^{-0.292} = 0.003035 = const. \tag{22}$$

The value of the shape function for the C(T) sample dimension B=100 mm, calculated by using Eq. (13), determines the corresponding Weibull shape parameter based on Fig. 2:

$$\Xi\left(\beta\,|\,B=100, \xi=-0.292\right) = 0.003035\cdot 169.4\cdot 100^{-(-0.292)} = 1.973 \quad \Rightarrow \quad \beta = 5.25 \tag{23}$$

The red solid line in Fig. 1 illustrated the Weibull CDF extrapolation for B = 100 mm and offers the comparison with the experimental data reported in [11].

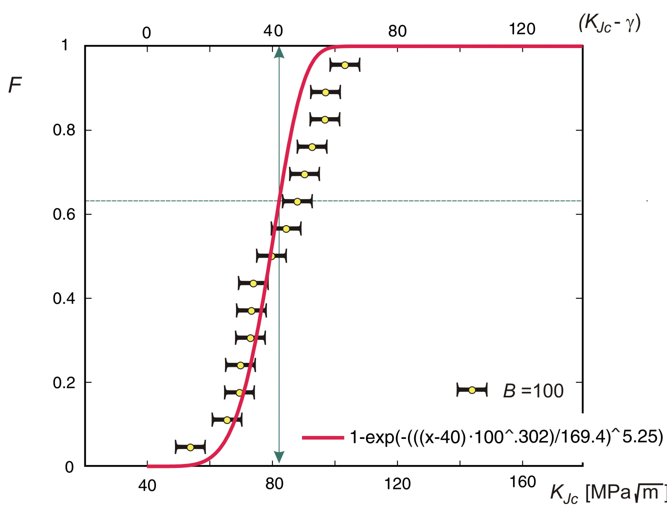

Fig. 2. The output of the 2SS procedure at T = -91ºC obtained based on the inputs presented in Table 1. The estimated K_{Jc} CDF for the C(T) sample sizes B = 100 mm represents an extrapolation of the input data. The symbols of width ±5 MPa√m are centered at the actual experimental data points. The solid line corresponds to 3-parameter Weibull predictions with the assumed fracture-toughness thresholds $\gamma = K_{min}$ = 40 MPa√m.

Finally, the Weibull CDF can now be written in the following form

$$F(K) = 1 - \exp\left\{ -\left(\frac{(K-40)\cdot B^{0.302}}{169.} \right)^{\beta(B,\xi=-0.292)} \right\}; \qquad (K-40) \geq 0;\ \beta \in \Re^{+} \tag{15}$$

The extrapolation results in Fig. 2 are considered satisfactory considering the evident irregularity of the experimental data sets [10] reflecting the inherent stochasticity of fracture toughness in the DTB temperature transition region.

5. Summary

This article is devoted to an upgrade of the novel 2SS approach proposed recently to account for the size effect in the two-parameter Weibull (W (β, η)) CDF of fracture toughness in the DTB transition temperature region. A model modification consists in the addition of a fracture-toughness threshold value (i.e. the Weibull location parameter) which constitutes the transition to the three-parameter Weibull distribution, W (β, η, γ) used extensively by Wallin and coworkers and many other researchers over the last few decades.

The aforementioned upgrade of the 2SS method highlights its relationship with two established models. In comparison, although the 2SS method requires experimental datasets of at least two C(T) sizes while the other two methods need only one, it obviously offers greater analytical flexibility in return. Importantly, it is shown that 2SS method reduces to the above mentioned methods if $\kappa = 1/\beta$ = const. Although these relations deserve further study, it can be affirmed without hesitation that the assumption β = const. is restrictive and its physical justification is somewhat elusive at present. From the standpoint of the 2SS procedure, the size-insensitivity of the Weibull shape parameter makes the second scaling (along the CDF ordinate) unnecessary since CDF curves would overlap into a single curve after the first scaling. Based on the experimental data analysis performed so far, the 2SS approach provides more realistic predictions than the above mentioned methods that are admittedly simpler and require smaller experimental data sets; the latter being a circumstance that should not be taken lightly.

Finally, the upgraded 2SS procedure is applied to an experimental data set available for 22NiMoCr37 ferritic steel extensively utilized as a pressure vessel material in nuclear industry. This experimental data, taken from the EURO fracture toughness data set, correspond to temperature -91ºC that belongs to the DTB transition region. The extrapolation results are considered satisfactory considering the irregularity of the measurement data compiled from two different laboratories, which reflect the inherent stochasticity of fracture toughness.

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