Weibull Modulus of Cleavage Fracture Toughness of Ferritic Steels

W.-S. LEI, G. QIAN, Z. YU, and P. ZHANG

The ordinary Weibull distribution function has been commonly accepted for empirical characterization of cleavage fracture toughness of nuclear reactor and containment pressure vessel steels. However, this method lacks a fundamental basis. This work adopts the standardized Weibull distribution function to analyze cleavage fracture toughness of ferritic steels measured from different sized fracture mechanics specimens at different temperatures to estimate the Weibull modulus. The toughness data of five different nuclear reactor and containment vessel steels are analyzed. The estimations obtained the Weibull modulus (m) in the range of 1.83 to 2.55 and strong temperature dependence of the threshold cleavage fracture toughness $K_{\min}$, as opposed to the constant values of $m_K = 4$ and $K_{\min} = 20$ MPam$^{1/2}$ given in ASTM E1921-19. The goodness of fit test by the one-sample Kolmogorov–Smirnov (K–S) test validated Weibull distribution function for describing the toughness distribution.

https://doi.org/10.1007/s11661-021-06169-w

I. INTRODUCTION

FERRITIC steels are the materials of choice for fabricating nuclear reactor and containment pressure vessels. As defined by ASTM E1921-19,[1] ferritic steels are typically carbon, low-alloy, and high-alloy grades, with bainite, tempered bainite, tempered martensite, and ferrite and pearlite as typical microstructures. Due to their body-centered-cubic crystal structures, all ferritic steels possess ductile-to-brittle transition temperature (DBTT) fracture toughness characteristics. In the lower shelf and the DBTT regime, the cleavage fracture toughness exhibits a large variation and significant specimen size dependence. As the most critical component of a nuclear power plant, nuclear reactor and containment pressure vessels are designed against catastrophic failure at a very low failure probability in the order of 10^{-6} to 10^{-7}. Since it is impossible to directly test or duplicate such a low probability failure event on the full-size scale at an affordable cost, a probabilistic design methodology is demanded. This calls for a statistical assessment of cleavage fracture toughness data as an essential step. According to a critical review by Lei[2] and the work by Qian *et al.*[3], major efforts on statistical modeling of cleavage fracture toughness fall into the empirical approach[4–7] and the fracture mechanism-based approach.[7–11] The empirical approach adopts the following ordinary Weibull distribution function to fit the cleavage fracture toughness data of ferritic steels.

$$P(K_{Jc}, B) = 1 - \exp\left[-\left(\frac{K_{Jc} - K_{\min}}{K_0}\right)^{m_K}\right] \qquad [1]$$

where P (K_{JC}, B) is the cumulative failure probability corresponding to the fracture toughness K_{JC} of specimen with thickness B, K_0 is scale parameter for normalization, and m_K is the Weibull modulus. The fracture mechanism-based approach has yet obtained an explicit solution to the cumulative failure probability as a function of cleavage fracture toughness. The following two-parameter Weibull statistical model of the fracture toughness K_{Ic} with a modulus of 4 formulated by Margolin *et al.*[7] Beremin[8] and Wallin[9] is disproved[2,10,11]:

$$P(K_{Jc}, B) = 1 - \exp\left[-\frac{B}{B_0}\left(\frac{K_{Jc}}{K_0}\right)^4\right] \qquad [2]$$

where B_0 is reference thickness for normalization. As a consequence, there lacks a valid theoretical basis or rationale for the following three-parameter Weibull distribution of fracture toughness K_{Ic} with a modulus of 4 and a threshold toughness of $K_{\min} = 20\,\text{MPa}\sqrt{m}$, which was arbitrarily extended from Eq. [2] by Wallin[9] and later on adopted in the Master Curve approach[1] for specimens of a given thickness at a

W.-S. LEI, Z. YU, and P. ZHANG are with the School of Materials Engineering, Shanghai University of Engineering Science, 333 Long Teng Rd., Shanghai 201620, P.R. China. Contact e-mail: leiws2008@gmail.com G. QIAN is with the State Key Laboratory of Nonlinear Mechanics (LNM), Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, P.R. China.
Manuscript submitted October 4, 2020, accepted January 28, 2021.
Article published online February 27, 2021

specific temperature for ferritic steels with yield strengths between 275 and 825 MPa in DBTT regime.

$$P(K_{Jc}, B) = 1 - \exp\left[-\frac{B}{B_0}\left(\frac{K_{Jc} - K_{\min}}{K_0 - K_{\min}}\right)^4\right] \quad [3]$$

The lack of a valid theoretical basis implies that Eq. [3] is essentially an application of the ordinary empirical Weibull distribution function Eq. [1]. The only difference is that Weibull modulus m_K and threshold toughness $K_{\min}$ are determined by goodness of fit in the empirical approach, while here they are assigned to specific values with debatable rationale. Therefore, further studies are necessary to justify the adopted values of Weibull modulus $m_K = 4$ and threshold toughness $K_{\min} = 20\,\text{MPa}\sqrt{m}$ for ferritic steels with the specified yield strengths (275 to 825 MPa). In view of the foregoing, this work aims to explore an approach to estimating the Weibull modulus of cleavage fracture toughness. In the following, the method will be introduced first. Then several groups of cleavage fracture toughness data of nuclear vessel steels will be analyzed. This is followed by the one-sample Kolmogorov–Smirnov (K–S) test as a goodness of fit test to compare the proposed approach and the Master Curve approach.

II. METHOD

A. *Description*

By assuming μ_K and σ_K as the mean and standard deviation of fracture toughness K_{Jc}, the standardized toughness parameter Z is introduced as follows:

$$Z = \frac{K_{Jc} - \mu_K}{\sigma_K} \quad [4]$$

Refer to Eq. [1], μ_K and σ_K are given by

$$\mu_K = K_{\min} + K_0 \Gamma(1 + 1/m_K) \quad [5]$$

$$\sigma_K = K_0 \sqrt{\Gamma(1 + 2/m_K) - [\Gamma(1 + 1/m_K)]^2} \quad [6]$$

where $\Gamma(m_K) = \int_0^\infty e^{-x} x^{m_K - 1} dx$ is the Gamma function.

Accordingly,

$$\frac{K_{Jc} - K_{\min}}{K_0} = \Gamma(1 + 1/m_K) + Z \cdot \sqrt{\Gamma(1 + 2/m_K) - [\Gamma(1 + 1/m_K)]^2} \quad [7]$$

Now the three-parameter Weibull distribution in Eq. [1] reduces to the standardized format with a single parameter (m_K):

$$P(Z, m_K) = 1 - \exp\left\{-\left[\left(\Gamma(1 + 1/m_K) + Z \cdot \sqrt{\Gamma(1 + 2/m_K) - (\Gamma(1 + 1/m_K))^2}\right)^{m_K}\right]\right\} \quad [8]$$

Equation [8] is rewritten as:

$$P(Z, m_K) = 1 - \exp\left[-\left(\frac{Z - Z_{\min}}{Z_0}\right)^{m_K}\right] \quad [9]$$

The corresponding probability density function is

$$f(Z, m_K) = \frac{m_K}{Z_0}\left(\frac{Z - Z_{\min}}{Z_0}\right)^{m_K - 1} \exp\left[-\left(\frac{Z - Z_{\min}}{Z_0}\right)^{m_K}\right] \quad [10]$$

with

$$Z_{\min} = -\frac{\Gamma(1 + 1/m_K)}{\sqrt{\Gamma(1 + 2/m_K) - [\Gamma(1 + 1/m_K)]^2}} \quad [11]$$

$$Z_0 = \frac{1}{\sqrt{\Gamma(1 + 2/m_K) - [\Gamma(1 + 1/m_K)]^2}} \quad [12]$$

For a given set of fracture toughness data $K_{Jc,i} (i = 1, 2, \ldots, n)$, in order to convert them into the standardized format $Z_i (i = 1, 2, \ldots, n)$, the population mean ($\mu_K$) and standard deviation (σ_K) are estimated by the sample average $\hat{\mu}_K$ and standard deviation $\hat{\sigma}_K$ as below

$$\hat{\mu}_K = \frac{\sum_{i=1}^n K_{Jc,i}}{n} \quad [13]$$

$$\hat{\sigma}_K = \sqrt{\frac{1}{(n - 1.5)}\sum_{i=1}^n \left(K_{Jc,i} - \hat{\mu}_K\right)^2} \quad [14]$$

Note that Eq. [14] is slightly different with the following common expression for sample standard deviation:

$$\hat{\sigma}_K = \sqrt{\frac{1}{n - 1}\sum_{i=1}^n \left(K_{Jc,i} - \hat{\mu}_K\right)^2} \quad [15]$$

This is based on the following considerations: Unlike that Eq. [13] is an unbiased estimator of the population mean μ_K, Eq. [15] is a biased estimator of the population standard deviation σ_K. An approximate formula for the unbiased estimator of the population standard deviation σ_K for non-normal distributions is[12]:

$$\hat{\sigma}_K = \sqrt{\frac{1}{n - 1.5 - 0.25\gamma_2}\sum_{i=1}^n \left(K_{Jc,i} - \hat{\mu}_K\right)^2} \quad [16]$$

where γ_2 denotes the population excess kurtosis. For Weibull distribution with a modulus m_K, there is

$$\gamma_2 = \frac{-3\left[\Gamma\left(1 + \frac{1}{m_K}\right)\right]^4 + 6\Gamma\left(1 + \frac{2}{m_K}\right)\left[\Gamma\left(1 + \frac{1}{m_K}\right)\right]^2 - 4\Gamma\left(1 + \frac{3}{m_K}\right)\Gamma\left(1 + \frac{1}{m_K}\right) + \Gamma\left(1 + \frac{4}{m_K}\right)}{\left\{\Gamma\left(1 + \frac{2}{m_K}\right) - \left[\Gamma\left(1 + \frac{1}{m_K}\right)\right]^2\right\}^2} \quad [17]$$

As shown in Figure 1, for $1.5 \le m_K \le 6$, there is $-0.29 \le \gamma_2 \le 1.11$. Within this range, with specimen number $n = 10$, the difference in the value of $\hat{\sigma}_K$ is 0.4 to 2.1 pct between Eqs. [14] and [16] and is 2.5 to 5.7 pct

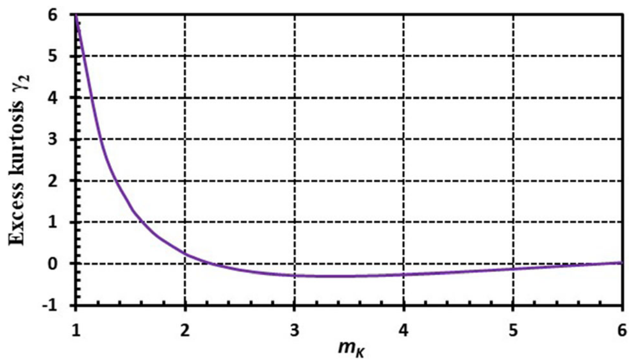


Fig. 1—Variation of excess kurtosis γ_2 with Weibull modulus m_K.

between Eqs. [15] and [16]. With specimen number $n = 20$, the corresponding difference reduces to < 0.01 and ~ 1.3 pct, respectively.

Since both $Z_{\min}$ and Z_0 are functions of m_K, the logarithmic likelihood function of Weibull parameters $(m_K, Z_{\min}, Z_0)$ for the samples $Z_1, Z_2, \ldots, Z_n$ depends only on m_K as below

$$L(m_K, Z_{\min}, Z_0) = n \ln\left(\frac{m_K}{Z_0}\right) + (m_K - 1)\sum_{i=1}^{n} \ln\left(\frac{Z_i - Z_{\min}}{Z_0}\right) - \sum_{i=1}^{n}\left(\frac{Z_i - Z_{\min}}{Z_0}\right)^{m_K} \quad [18]$$

Now the maximum likelihood estimation reduces to search for the value of the single parameter m_K that maximizes the likelihood function $L(m_K, Z_{\min}, Z_0)$.

Once the estimated value of m_K, $\hat{m}_K$, is known, $K_{\min}$ and K_0 are estimated as below due to Eqs. [5] and [6]:

$$\hat{K}_0 = \frac{\hat{\sigma}_K}{\sqrt{\Gamma(1 + 2/\hat{m}_K) - [\Gamma(1 + 1/\hat{m}_K)]^2}} \quad [19]$$

$$\hat{K}_{\min} = \hat{\mu}_K - \hat{K}_0 \cdot \Gamma(1 + 1/\hat{m}_K) \quad [20]$$

B. *Significance of the Standardized Weibull Distribution Function*

The purpose of this section is to demonstrate the validity of the proposed method with $m_K = 4$ as an example. Equation [9] implies that for different fracture toughness data sets, such as those measured at different temperatures and with different specimen geometries, the values of $K_{\min}$ and K_0 may vary. But so long as the Weibull modulus m_K remains constant as a material property, all the data sets will fall onto a same curve described by Eq. [9]. With all the data measured at different temperatures and with different specimen geometries as inputs, the Weibull modulus estimate should be more accurate than one single data set at one temperature for a given specimen size. As an example, Figure 2(a) shows three distributions of fracture

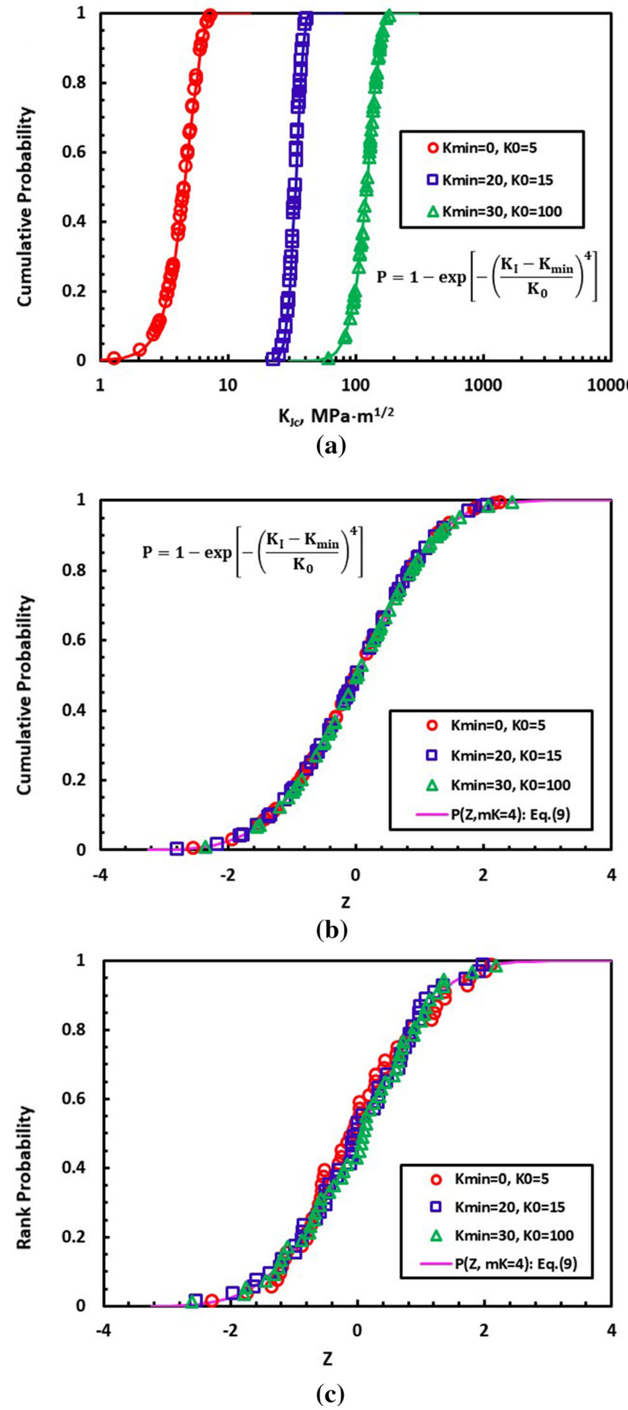


Fig. 2—Three cleavage fracture toughness distributions all with $m_K = 4$ but different K_0 and K_{min}: (*a*) Raw toughness data, (*b*) the standardized formats with population mean and standard deviation, (*c*) the standardized formats with sample average and standard deviation, (*d*) $\hat{m}_K$ *vs* number of data sets, (*e*) maximum likelihood estimation with all three data sets as input.

toughness K_{JC} all with $m_K = 4$ but different values of K_{min} and K_0, which are arbitrarily assumed as examples. 50 data points are randomly generated on each prescribed distribution as often used in Monte Carlo simulation.[2,9] The corresponding population mean and standard deviation are also shown in brackets according to Eqs. [5] and [6]:

A. $m_K = 4, K_{\min} = 0, K_0 = 5\,\mathrm{MPam}^{1/2}$ $\left(\mu_K = 4.53\,\mathrm{MPam}^{1/2}, \sigma_K = 1.27\,\mathrm{MPam}^{1/2}\right)$

B. $m_K = 4, K_{\min} = 20\,\mathrm{MPam}^{1/2}, K_0 = 15\,\mathrm{MPam}^{1/2}$ $\left(\mu_K = 33.60\,\mathrm{MPam}^{1/2}, \sigma_K = 3.81\,\mathrm{MPam}^{1/2}\right)$

C. $m_K = 4, K_{\min} = 30\,\mathrm{MPam}^{1/2}, K_0 = 100\,\mathrm{MPam}^{1/2}$ $\left(\mu_K = 120.64\,\mathrm{MPam}^{1/2}, \sigma_K = 25.43\,\mathrm{MPam}^{1/2}\right)$

With the known population mean and standard deviation and exact cumulative probability of the 50 data points in each distribution, Figure 2(a) is transformed into the standardized format in Figure 2(b). It shows that all the 150 data points from three distributions fall exactly onto a single master curve defined by Eq. [9].

However, in a real experiment, the exact cumulative probability of each measured data point, the population mean, and population standard deviation are all unknown. Therefore, the rank probability, the sample average and standard deviation in Eqs. [13] and [14] are adopted as corresponding estimators. The accuracies of these three estimators are affected by the number of samples. Figure 2(c) shows the corresponding standardized distributions with the rank probability calculated by

$$P_i = (i - 0.3)/(n + 0.4) \qquad [21]$$

where n is the total number of samples in one data set. In this example, $n = 50$. i is the sequential number of the ith data point when all the data are ranked in an ascending order, $i = 1, 2, \ldots, n$. Regardless of the minor deviations, it is obvious that all the three sets of data points closely fall onto the theoretical curve $P(Z, m_K)$ according to Eq. [9]. When using the one-sample Kolmogorov–Smirnov (K–S) test for goodness of fit test, the standardized data sets converted in both ways in Figures 2(b) and (c) follow the Weibull distribution $P(Z, m_K = 4)$ as defined by Eq. [9]. In order to evaluate the minor deviation of using the rank probability to approximate the true probability and adopting the sample average and standard deviation to estimate the population average and standard deviation, the root-mean-square error (RMSE) is calculated for each case for comparison. RMSE is defined in Eq. [22] and it measures the differences between the values of probability P calculated by a prescribed distribution function and the observed values. It is often used for either testing the goodness of fit of a prescribed distribution function to different data sets or comparing the errors of different distribution functions for a particular variable. A lower value of RMSE corresponds to a more precise model.

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(\hat{P}_i - P_i\right)^2} \qquad [22]$$

where $\hat{P}_i$ is the predicted failure probability based on a prescribed distribution such as Eq. [9], P_i is the probability value corresponding to the standardized value Z_i of each toughness datum $K_{Jc,i}$ (i = 1, 2,..., n), which is often estimated by the rank probability based on Eq. [21], n is the total number of toughness data points.

For each of the three data sets, when the true probability of each datum is known and the population mean and standard deviation are adopted for standardization as shown in Figure 2(b), RMSE = 0 is obtained. While when the rank probability of each datum and the sample mean and standard deviation are adopted for standardization as shown in Figure 2(c), $RMSE = 0.04, 0.03, 0.04$ is obtained, respectively. It tells that while Figure 2(c) is less accurate than Figure 2(b) in terms of data fitting with the standardized Weibull distribution $P(Z, m_K = 4)$, the RMSE value is still low.

To show the effect of sample number on the bias of estimation using Eq. [18], m_K is estimated with the following data conditions as input:

(A) 50 data points in each data;
(B) 100 data points of any two data sets;
(C) all 150 data of three data sets.

The results are summarized in Figure 2(d). A single data set yields $\hat{m}_K = 3.0, 4.7, 4.95$; Any two data sets

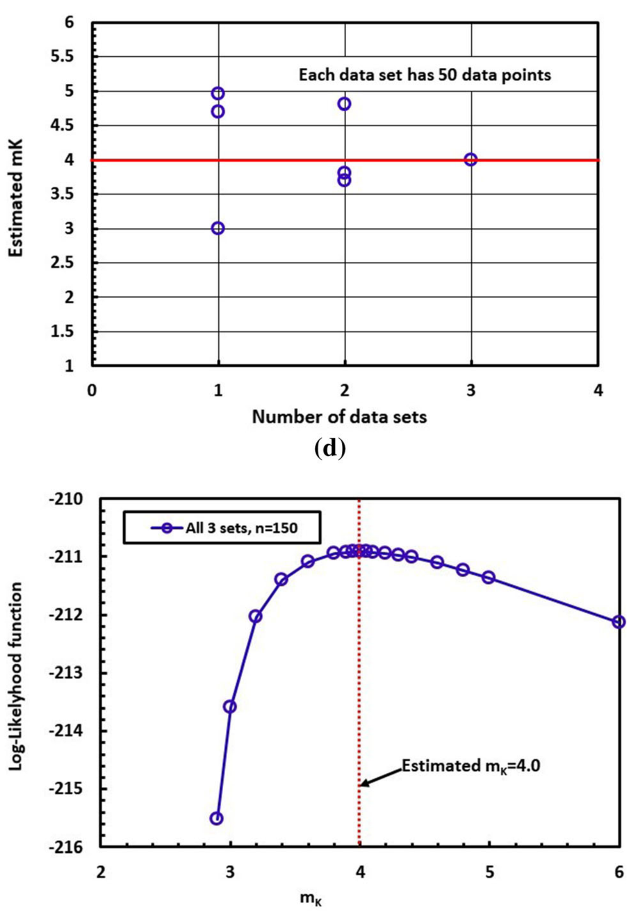


Fig. 2—continued.

lead to $\hat{m}_K = 3.7, 3.8, 4.8$; All the 150 data points give $\hat{m}_K = 4.0$. Figure 2(e) shows the result of maximum likelihood estimation with all 150 data as input.

III. STATISTICAL ANALYSIS OF CLEAVAGE FRACTURE TOUGHNESS DATA

Several groups of cleavage fracture toughness data of nuclear reactor or containment vessel steels are analyzed using the statistical method to assess potential effects of temperature and specimen size on Weibull modulus m_K. All the toughness data are measured with the ratio of crack length to specimen width of approximately 0.5 conforming to fracture toughness measurement requirements regardless of specimen size and are given in a table in related references.

A. *Cleavage Fracture Toughness of SA738Gr.B Steel*

The effect of temperature on Weibull modulus m_K is evaluated for a given specimen size. Zhang *et al.*[13] reported the experimental results of cleavage fracture toughness of SA738Gr.B steel measured with 1T-CT specimens at four different temperatures namely, 133 K, 143 K, 153 K, and 163 K. SA738Gr.B is a bainistic steel used for manufacturing nuclear containment vessels that serve as the third and final barrier for leakage prevention of radioactive materials after the nuclear fuel shell and the first-circuit pressure boundary. Each temperature is controlled within $\pm$ 3 K using a regulated liquid nitrogen flow in an insulated chamber equipped with PID controller. The standard 25.4 mm thick 1T-CT fracture toughness specimens are prepared along the T–L direction from a 60 mm thick SA738Gr.B plate. Taking the upper surface of the CT specimen as the sampling reference location, the specimens are extracted from four region namely, at surface, at 1/8 plate thickness, at 1/4 plate thickness, and at 1/2 plate thickness for the specimens to be tested at 133 K, 143 K, 153 K, and 163 K in sequence. The fracture toughness measurements according to ASTM E1921[1] are reported in table format in Reference 13. In total, there are 116 data points at all four temperatures including: 28 at 133 K, 30 at 143 K, 46 at 153 K, and 12 at 163 K. All the measured K_{Jc} values are below the limit value K_{Jc}(limit) specified by the ASTM E1921 standard[1] and were valadiated by SEM fractographic analysis. Figure 3(a) shows the experimental data, and Figure 3(b) shows the result of maximum likelihood estimation. It is determined that $\hat{m}_K = 1.9$. Figure 3(c) presents the standardized distribution of cleavage fracture toughness. The solid line is the fitting curve using Eq. [9] with $\hat{m}_K = 1.9$. For individual data set at each temperature, the values of $\hat{m}_K$ are 1.6 (133 K), 1.42 (143 K), 2.05 (153 K) and 1.03 (163 K).

B. *Cleavage Fracture Toughness of A533B Cl.1 Steel*

The examples of A533B Cl.1 steel mainly intend to evaluate the effect of specimen size on Weibull modulus m_K at a same temperature.

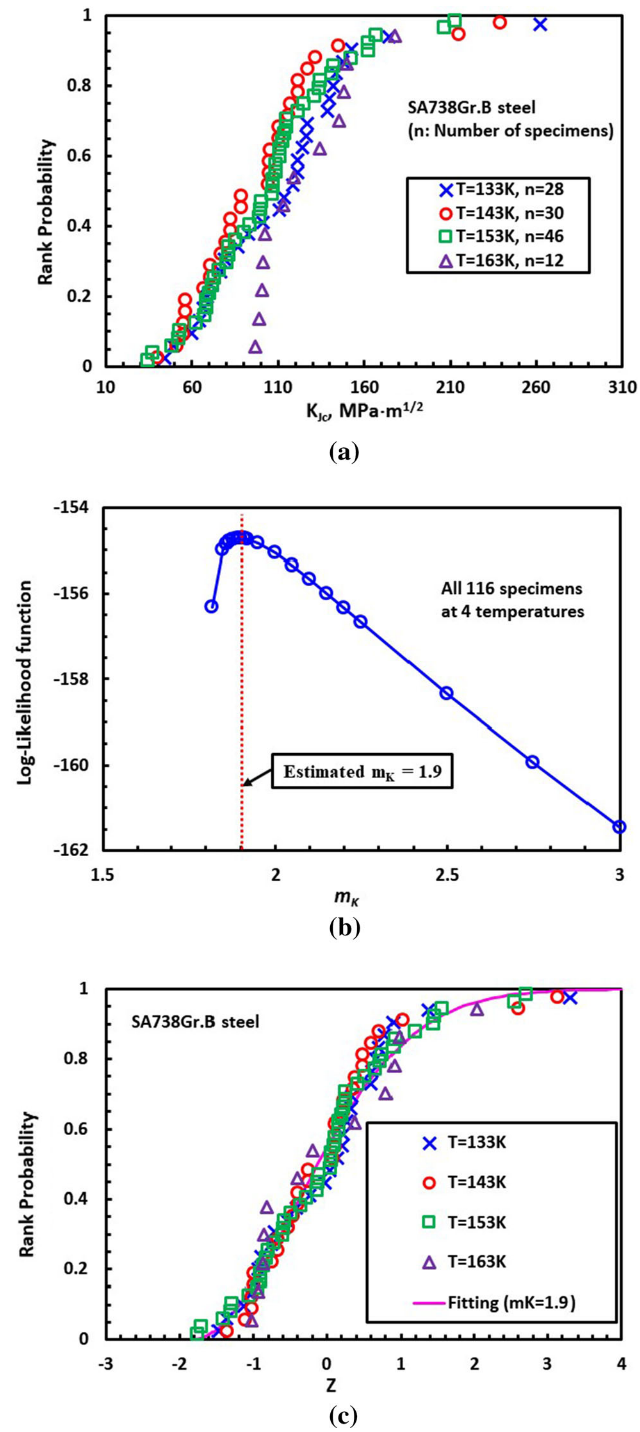


Fig. 3—(*a*) Experimental data of cleavage fracture toughness K_{JC} of SA738Gr.B steel measured with 1T-CT specimens at different temperatures (data listed in Ref. [13]), (*b*) maximum likelihood estimate of Weibull modulus m_K using all 116 experimental data, (*c*) comparison of experimental K_{JC} distribution with estimation.

Williams *et al.*[14] reported cleavage fracture toughness data of A533B Cl.1 steel (HSST Plate 13) measured on 12.5 mm thick (0.5 T), standard 25 mm thick (1 T) and 50 mm thick (2 T) CT specimens at 123 K. Figure 4 summarizes the experimental data and analysis. It is determined that $\hat{m}_K = 1.83$.

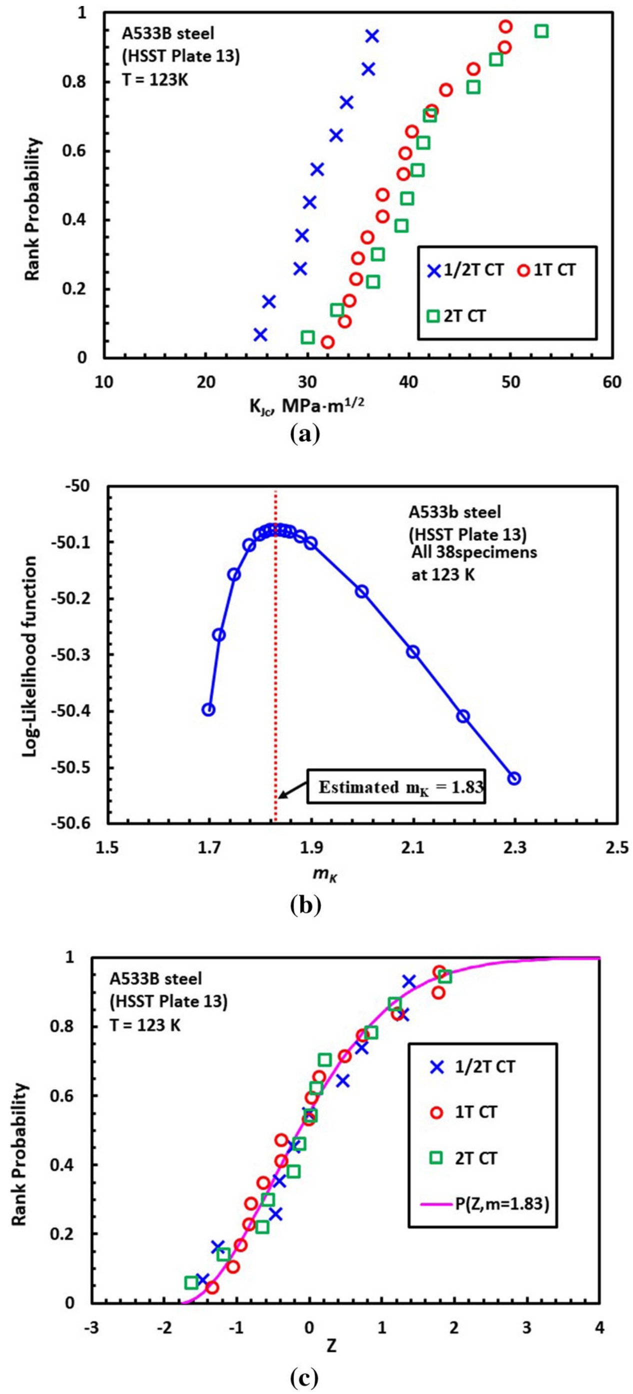


Fig. 4—(*a*) Experimental data of cleavage fracture toughness K_{JC} of A533B Cl.1 steel measured with 0.5 T, 1 T and 2 T specimens at 123 K (data listed in Ref. 14], (*b*) maximum likelihood estimate of Weibull modulus m_K using all 38 experimental data, (*c*) comparison of experimental K_{JC} distribution with estimation.

Onizawa *et al.*[15] compared cleavage fracture toughness measured from 10 pre-cracked Charpy (PCCv) specimens of 10 × 10 × 55 (mm) size, with 5 mm crack length, and 12 standard 25 mm thick (1T) CT specimens at two temperatures (193 K and 223 K). Both types of specimens are side- grooved by 10 pct of thickness on each side of the specimen after pre-cracking. The materials are an old version (designated as

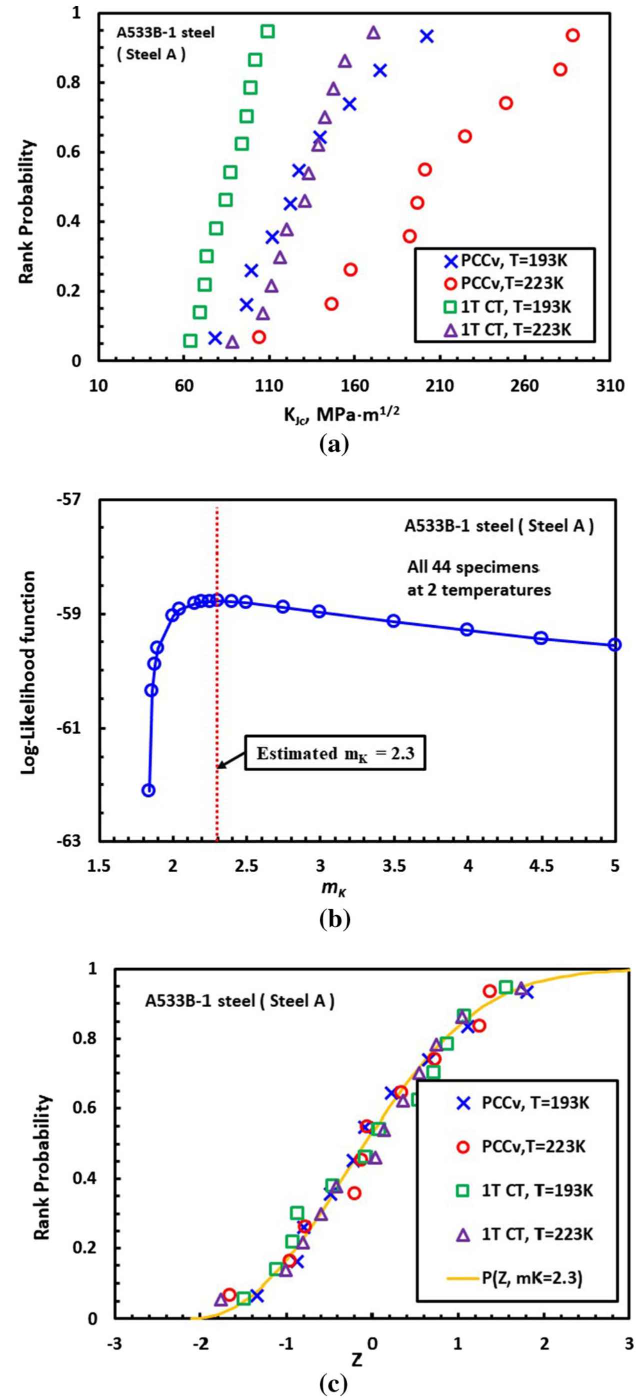


Fig. 5—(*a*) Experimental data of cleavage fracture toughness K_{JC} of A533B-1 steel (Steel A) at different temperatures (data listed in Ref. 15), (*b*) maximum likelihood estimate of Weibull modulus m_K using all 44 experimental data, (*c*) comparison of experimental K_{JC} distribution with estimation.

“Steel A”) and a modern version (designated as “Steel B”) of A533B-1 steel. Figures 5 and 6 summarize the experimental data and analysis for both steels. It is determined that $\hat{m}_K = 2.3$ for Steel A and $\hat{m}_K = 2.55$ for Steel B. The results seem to support the suggestion of using the less expensive side-grooved pre-cracked Charpy specimens to replace the standard 1T CT

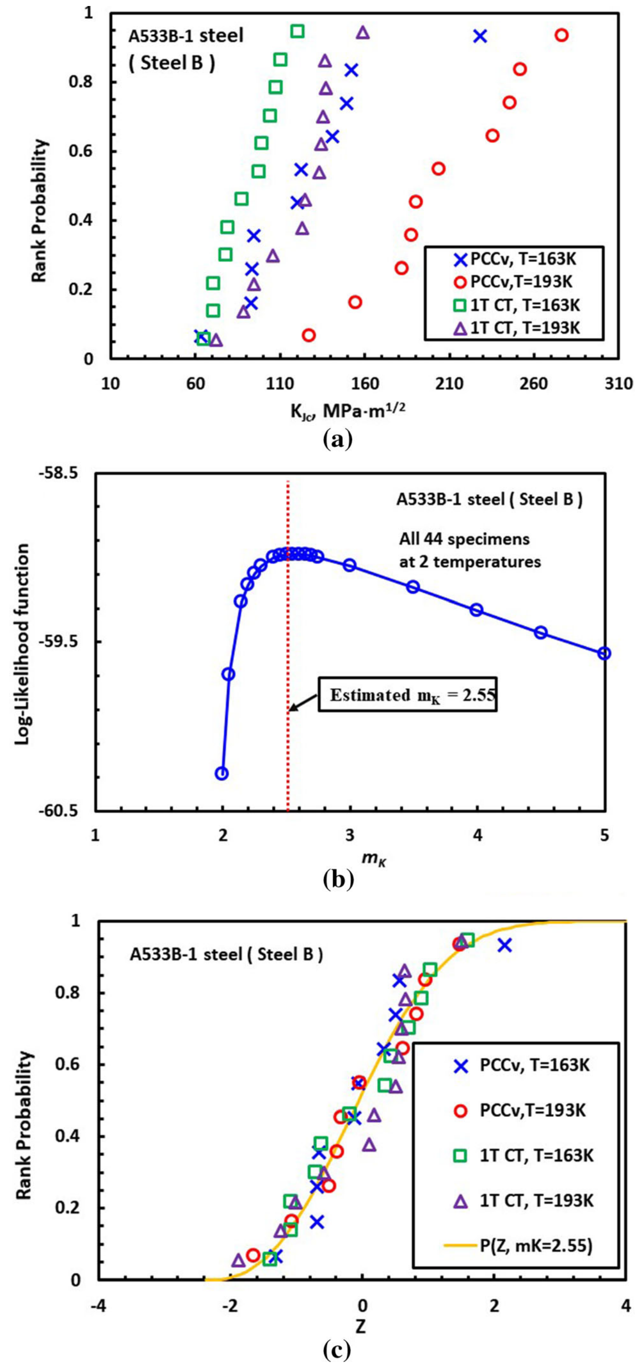


Fig. 6—(*a*) Experimental data of cleavage fracture toughness K_{JC} of A533B-1 steel (Steel B) at different temperatures (data listed in Ref. 15], (*b*) maximum likelihood estimate of Weibull modulus m_K using all 44 experimental data, (*c*) comparison of experimental K_{JC} distribution with estimation.

specimens for Weibull modulus m_K assessment of cleavage fracture toughness.[15]

C. *Cleavage Fracture Toughness of DIN 22NiMoCr37 Steel*

To evaluate the combined effects of temperature and specimen size on cleavage fracture toughness distribution characteristics, previously published fracture

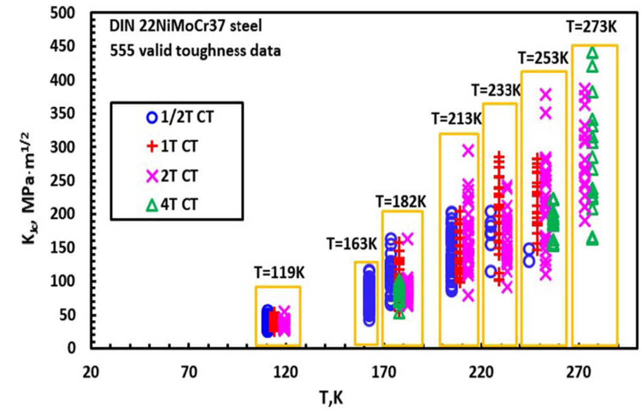


Fig. 7—All 555 valid data points of cleavage fracture toughness (Data listed in Ref. 16).

toughness data of a DIN 22NiMoCr37 steel are analyzed. The Euro fracture toughness dataset of a quenched and tempered RPV steel DIN 22NiMoCr37 is developed in the project ‘‘Fracture Toughness of Steel in the Ductile to Brittle Transition Regime’’ sponsored by ‘‘Measurement and Testing Programme (MAT1-CT-940080)’’ of the European Commission.[16] This steel is similar to steel type A508 Cl.3 and is widely used in nuclear power plants. About 800 fracture toughness tests were performed using 12.5 mm (1/2 T), 25 mm (1 T), 50 mm (2 T), and 100 mm (4 T) thick compact tension (CT) fracture toughness specimens. Refer to Reference 16 for the internet link to download the dataset. Figure 7 shows all the 555 valid data points of cleavage fracture toughness. Table I summarizes the number of valid cleavage fracture toughness measurements for different sized specimens at different temperatures. Note that the 7 data points at 233 K and 2 data points at 253 K are not included in the following analysis.

First, the toughness data from same sized specimens but at different temperatures will be analyzed together to explore temperature effect. Next, all the toughness data in Table I will be analyzed together to understand the specimen size effect as well. Figure 8 summarizes the results of maximum likelihood estimation in each case. The values of $\hat{m}_K = 2.9, 2.4, 2.15, 3$ are estimated for 1/2 T, 1 T, 2 T and 4 T CT specimens in sequence. When all the 555 data points of cleavage fracture toughness measured from different sized CT specimens in Figure 7 are used for maximum likelihood estimation, $\hat{m}_K = 2.5$ is determined.

Figure 9(a) shows all 170 data of cleavage fracture toughness measured with 1/2 T CT specimens (excluding the 7 data points at 233 K and 2 data points at 253 K). Figure 9(b) shows the standardized distribution of cleavage fracture toughness.

Figure 10(a) shows all 161 data points of cleavage fracture toughness measured from 1T CT specimens. Figure 10(b) shows the standardized distribution of cleavage fracture toughness.

Figure 11(a) shows all 170 data points of cleavage fracture toughness measured from 2 T CT specimens.

Table I. Number (n) of Valid Cleavage Fracture Toughness Measurements for Different Sized Specimens at Different Temperatures

	Specimen Size and Configuration			
Test Temperature (K)	½ T (12.5 mm) CT	1 T (25 mm) CT	2 T (50 mm) CT	4 T (100 mm) CT
119	35	39	32	
163	55			
182	31	34	30	14
213	49	34	30	
233	7	32	30	
253	2	22	30	15
273			18	16

Figure 11(b) shows the standardized distribution of cleavage fracture toughness.

Figure 12(a) shows all 45 data points of cleavage fracture toughness measured from 4 T CT specimens. Figure 12(b) shows the standardized distribution of cleavage fracture toughness.

When all the 555 data points of cleavage fracture toughness measured from different sized CT specimens in Figure 7 are used for maximum likelihood estimation, $\hat{m}_K = 2.5$ is determined. Figure 13 is the corresponding standardized distribution of cleavage fracture toughness.

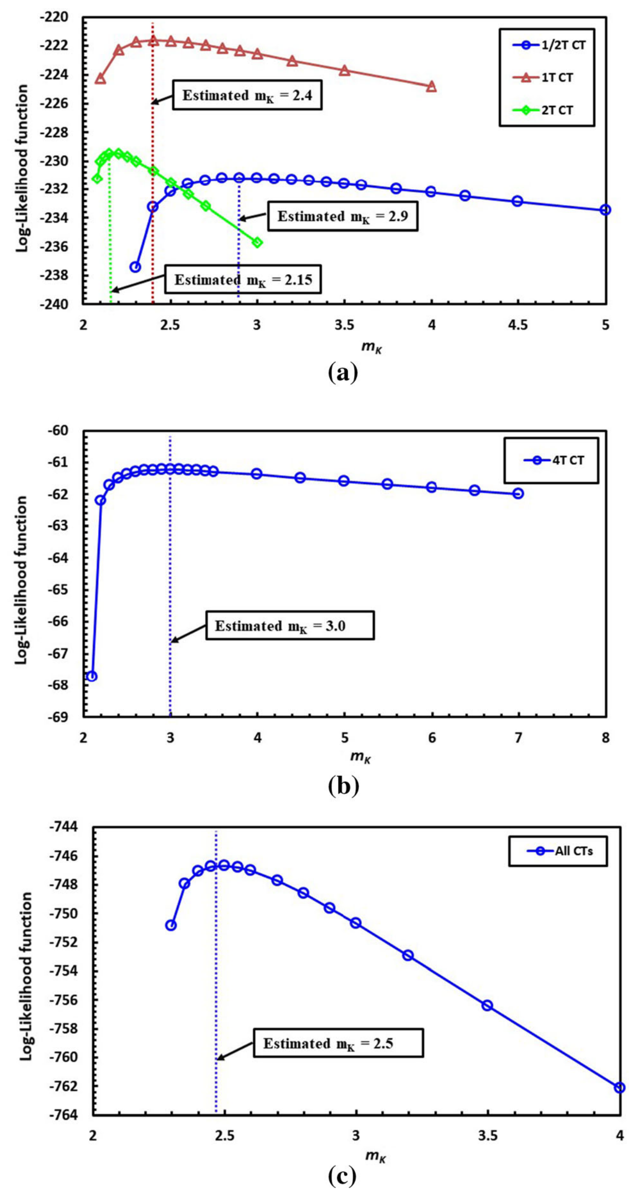


Fig. 8—Results of maximum likelyhoold estimation: (*a*) 1/2 T CT, 1 T CT and 2 T CT specimens; (*b*) 4T CT specimens; (*c*) all CT specimens.

IV. DISCUSSIONS

A. *Temperature Dependence of K_{min} and K_0*

The estimated Weibull modulus $\hat{m}_K$ falls in the range of 1.83 to 2.55 for the toughness data as a single group for each steel and 1.03 to 3 for the toughness data measured at each temperature or with a same specimen size. It does not show a strong tendency of either temperature or specimen size dependence. With the estimated Weibull modulus $\hat{m}_K$ as input, the threshold toughness $K_{\min}$ and the scale parameter K_0 are estimated *via* Eqs. [19] and [20] and are summarized in Figure 14. While there are relatively large scatters of the data, particularly for K_0, The results suggest a strong temperature dependence of both $K_{\min}$ and K_0 while less sensitivity to specimen size. This large scatter is possibly due to the sample size and the microstructural inhomogeneity of steels.

B. *Goodness of Fit Test*

As highlighted in the Section I, it is a popular empirical assumption rather than a strict theoretical inference that cleavage fracture toughness of ferritic steels follows the Weibull distribution. This work develops an approach to including more toughness data measured from different sized specimens and at different temperatures for Weibull parameters estimation. This empirical assumption is validated by all the examples shown. To evaluate this work from a statistical standpoint, the one-sample Kolmogorov–Smirnov (K–S) test is used as goodness of fit test. First, calculate the test statistic D, which is the maximum deviation between the

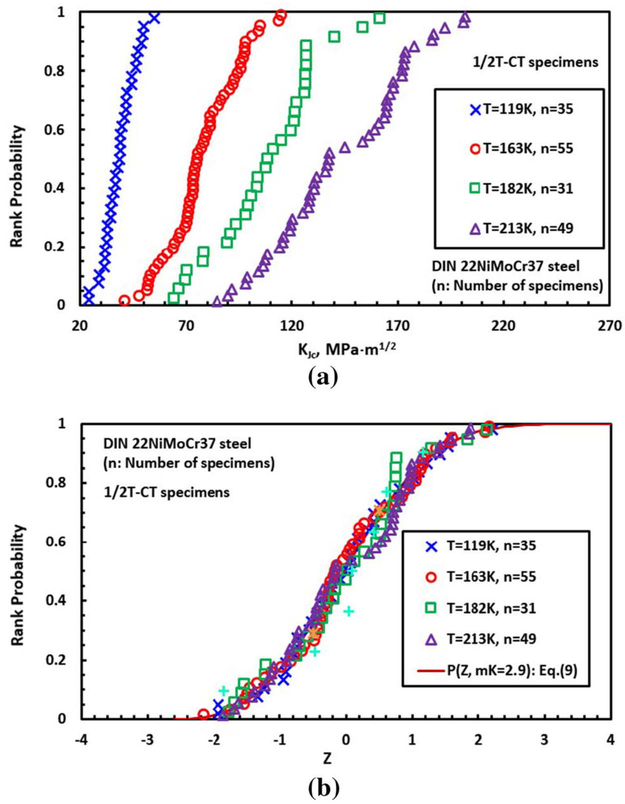


Fig. 9—Cleavage fracture toughness of 1/2 T CT specimens: (*a*) experimental data (Data listed in Ref. [16]), (*b*) standardized distribution of cleavage fracture toughness.

rank probability $P(i)$ according to Eq. [23] and the cumulative probability P calculated with Eq. [1] and the estimated Weibull parameters, as below:

$$D = Max|P(i) - P| \quad [23]$$

Second, find the critical value of the test statistic D corresponding to a given sample number (n) at a significance level of $\alpha = 0.05$, $KS_{0.05}$. If $D < KS_{0.05}$, the measured data follow the estimated Weibull distribution. The values of $KS_{0.05}$ can be found in literature, *e.g.*,.[17]

Figure 15 summarizes the results of goodness of fit test on the Weibull distribution functions determined by the proposed approach for all the steels .

It is clear that all the test statistic D values are below the critical value $KS_{0.05}$. This suggests that at 95 pct confidence level, the fracture toughness data for different steels follow Weibull distributions with the parameters estimated by the maximum likelyhood method for the standardized Weibull distrbution.

The one-sample Kolmogorov–Smirnov (K–S) test can be also used to assess the Master Curve approach for the same data sets. To do this, the scale parameter K_0 in Eq. [3] is estimated as follows at each temperature:

First, at each temperature, the fracture toughness for different thicknesses are converted into the standard fracture toughness by Eq. [24] with the reference thickness $B_0 = 25\,\text{mm}$:

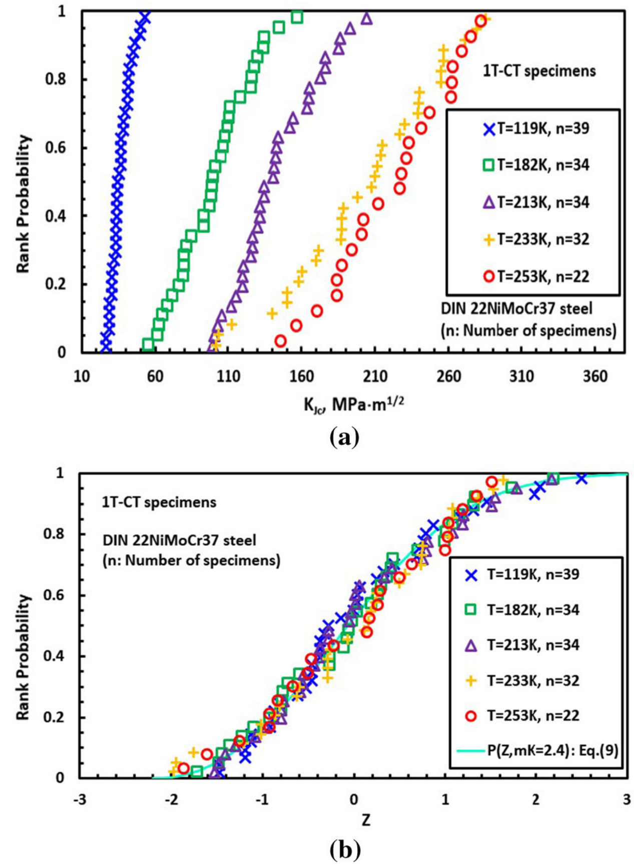


Fig. 10—Cleavage fracture toughness of 1 T CT specimens: (*a*) experimental data (Data listed in Ref. [16]), (*b*) standardized distribution of cleavage fracture toughness.

$$K_{J_C(1TCT)} = 20 + (K_{Jc} - 20) \cdot \left(\frac{B}{B_0}\right)^{1/4} \quad [24]$$

Second, K_0 at each temperature is estimated by

$$K_0 = \left[\sum_{i=1}^{n} \frac{(K_{Jc} - 20)^4}{r - 0.3}\right]^{1/4} \quad [25]$$

where n is the total number of specimens tested at a same temperature, and r is the number of specimens corresponding to brittle fracture.

Accordingly, the cumulative probability P is calculated by Eq. [3] for the Master Curve approach with $B_0 = 25\,\text{mm}$, $K_{\min} = 20\,\text{MPa}\sqrt{m}$ and K_0 from Eq. [25]. This allows to calculate the test statistic D as the maximum deviation between the rank probability $P(i)$ according to Eq. [21] and the cumulative probability P by the Master Curve approach.

Figure 16 summarizes the results of goodness of test on the Weibull distribution functions determined by the Master Curve approach for all the steels. It is found that some of the test statistic D values are above the critical value $KS_{0.05}$. This tells that at 95 pct confidence level, the fracture toughness data for different steels do not always follow the Weibull distribution functions with the

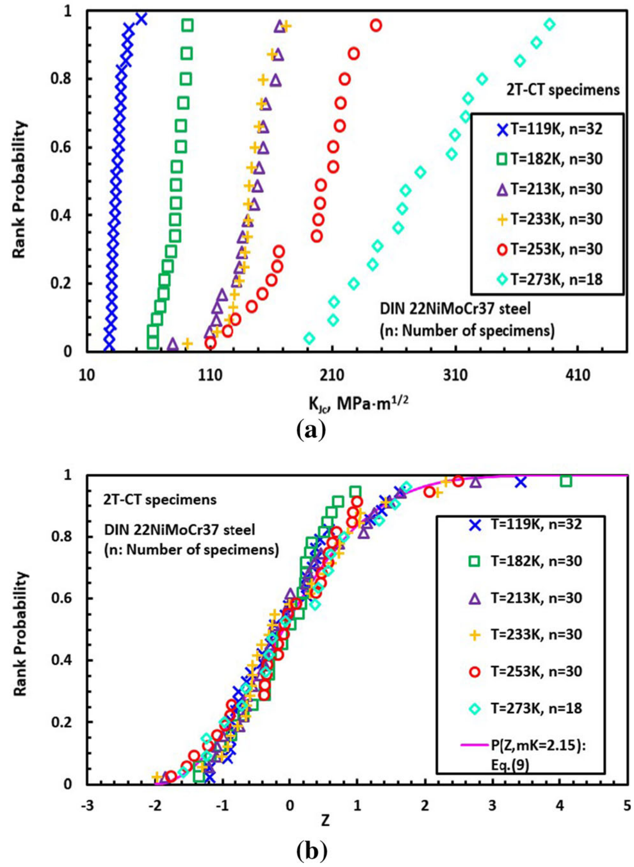


Fig. 11—Cleavage fracture toughness of 2 T CT specimens: (*a*) experimental data (Data listed in Ref. [16]), (*b*) standardized distribution of cleavage fracture toughness.

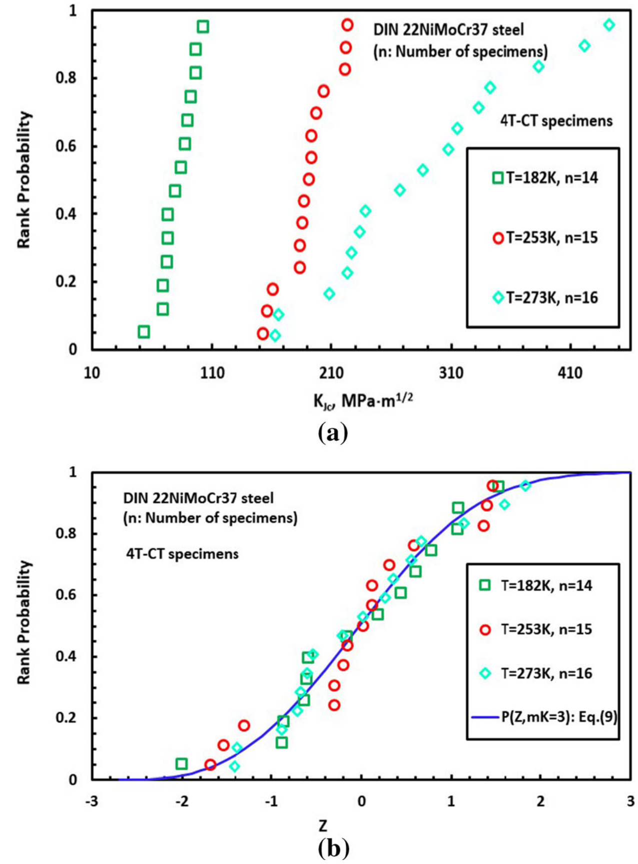


Fig. 12—Cleavage fracture toughness of 4 T CT specimens: (*a*) experimental data (Data listed in Ref. [16]), (*b*) standardized distribution of cleavage fracture toughness.

parameters ($m_K = 4$, $K_{\min} = 20\,\text{MPa}\sqrt{m}$) determined by the Master Curve approach.

The one-sample Kolmogorov–Smirnov (K–S) test provides an alternative way to illustrate the limitations of the Master Curve (MC) approach, which have been identified by other researchers.[13,18,19] As stated by Lucon and Scibetta,[18] the conventional Master Curve approach is only intended and applicable for macroscopically homogeneous ferritic steels. However, certain deterministic inhomogeneities, such as the locations to extract specimens within a steel plate,[13] may be unavoidable for thick section ferritic steels. For inhomogeneous materials, the bi-modal and multi-modal Master Curve approaches have been proposed,[18] which still assume $m_K = 4$ and $K_{\min} = 20\ \text{MPam}^{1/2}$ with 3 or more parameters for the bi-modal or multi-modal Weibull distributions. However, no specific criterion is given to identify a data set as inhomogeneous. In addition, calibration of a bi-modal and multi-modal Weibull distribution is more complicated than that of the conventional Master Curve distribution. For example, the bi-modal Master Curve approach is expressed as follows:

$$P(K_{J_C}, 1CT) = 1 - p_a \cdot \exp\left[-\left(\frac{K_{Jc} - 20}{K_{01} - 20}\right)^4\right] - (1 - p_a) \cdot \exp\left[-\left(\frac{K_{Jc} - 20}{K_{02} - 20}\right)^4\right] \quad [26]$$

Equation [26] involves two scale parameters (K_{01} and K_{02}) and the probability p_a of the data set belonging to distribution a (the probability of the data set belonging to distribution b is $p_b = 1 - p_a$). Recently, Meshii[19] reported the fracture toughness of ferritic CrMo steel JIS SCM440 measured at temperatures from 213 K to 373 K, in which the yield strength varies from 410 to 523 MPa. It is concluded that while this steel satisfies the prerequisites of ASTM E 1921-19 standard, the Master Curve approach fails to characterize its fracture toughness temperature dependence.

A one-to-one comparion of the proposed method and the Master Curve approach is made for all the cited steels to inspect the difference between the rank probability at the measured fracture toughness and the corresponding cumulative probability estimated by the proposed approach and the Master Curve approach.

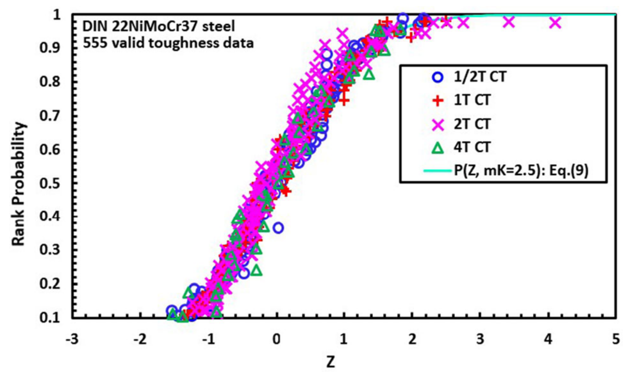


Fig. 13—Standardized distribution of cleavage fracture toughness of all CT specimens.

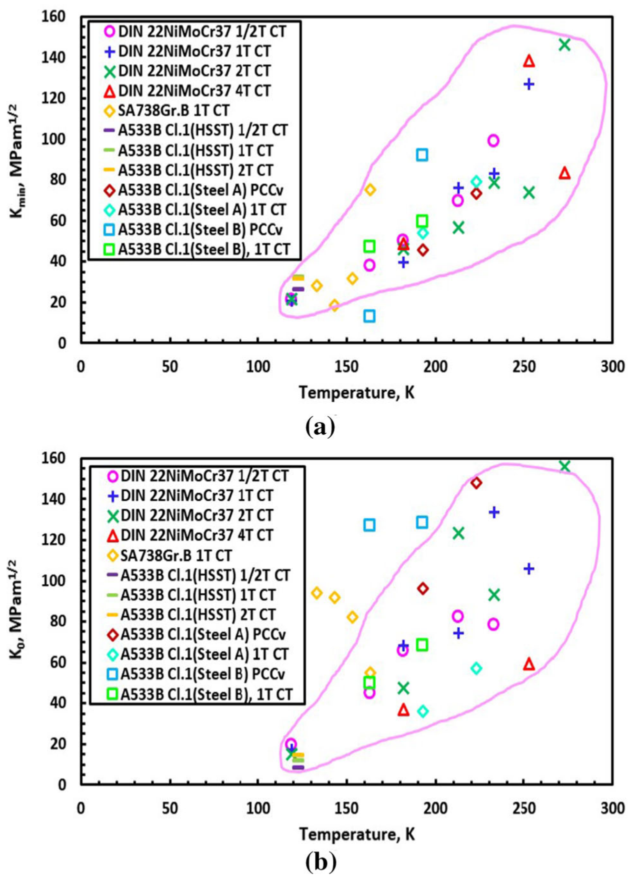


Fig. 14—Summary of (*a*) estimated $K_{\min}$ and (*b*) K_0 of different steels.

Figure 17 shows some typical scenarios as examples. The following observations can be made:

A. The proposed approach. For each steel, all the toughness data fit well with Eq. [1] for Weibull distribution with a same value of Weibull modulus determined by maximum likelihood estimation of the standardized ordinary Weibull distribution, while the threshold toughness $K_{\min}$ and the scale parameter K_0 may vary with specimen size and tempewrature.

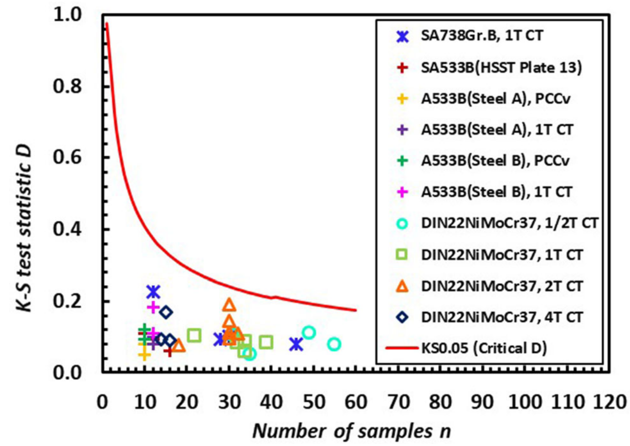


Fig. 15—Results of Kolmogorov–Smirnov (K–S) test of the proposed method.

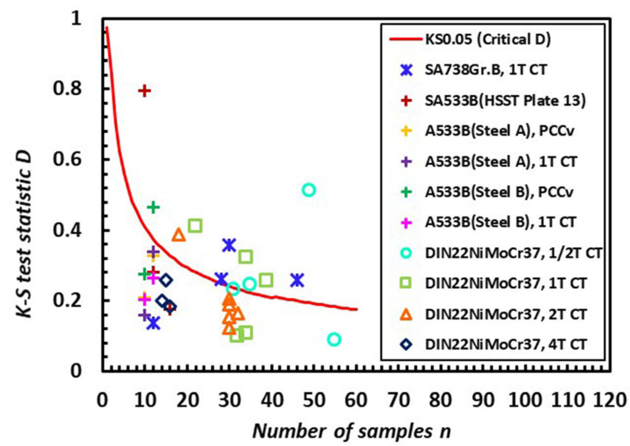
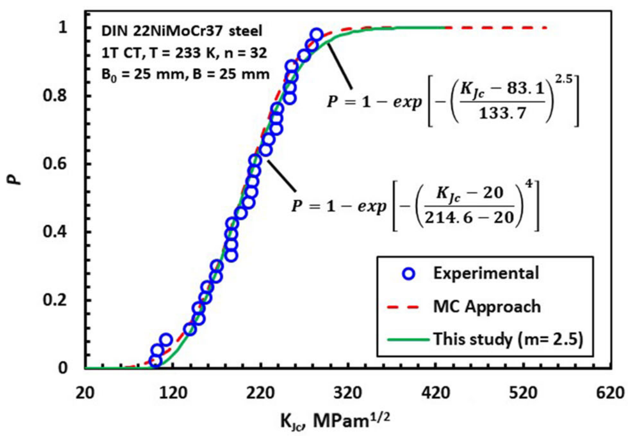


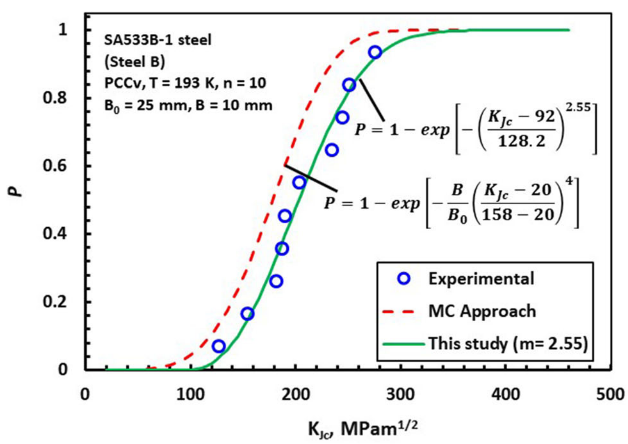
Fig. 16—Results of Kolmogorov–Smirnov (K–S) test of the Master Curve approach.

B. The Master Curve approach. Depending on the specimen size and test temperature, the conventional Master Curve approach results in the following different types of predictions: (i). The prediction fits well with the experimental results within the whole toughness range (Figure 17(a)); (ii). The predicton overestimates the failure probability within the whole toughness range (Figure 17(b)); (iii). The prediction underestimates the failure probability within the whole toughness range (Figure 17(c)); (iv). The prediction overestimates the failure probability in some toughness range but underestimates the failure probability in the other range (Figure 17(d)). This is consistent with the observations from Figure 16.

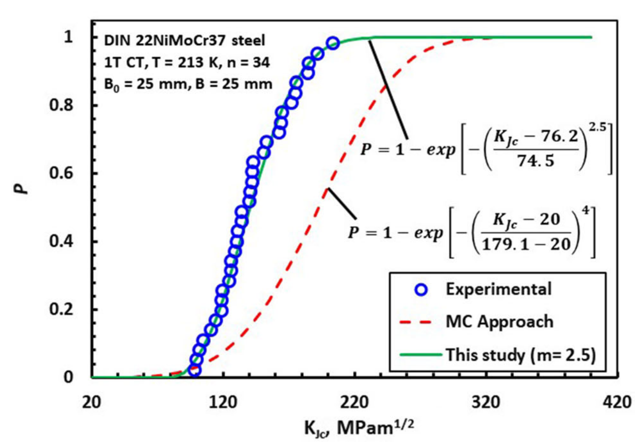
In a review of the history and technical basis of the Master Curve approach, Kirk[20] confirms that the original proposal of the Weibull modulus $m_K = 4$ is based on Eq. [2] derived from the micromechanical model[7–9] and that of the threshold toughness of $K_{\min} = 20\,\text{MPa}\sqrt{m}$ is based on Monte Carlo simulation of the expected confidence bounds in accord with experimental



(a)



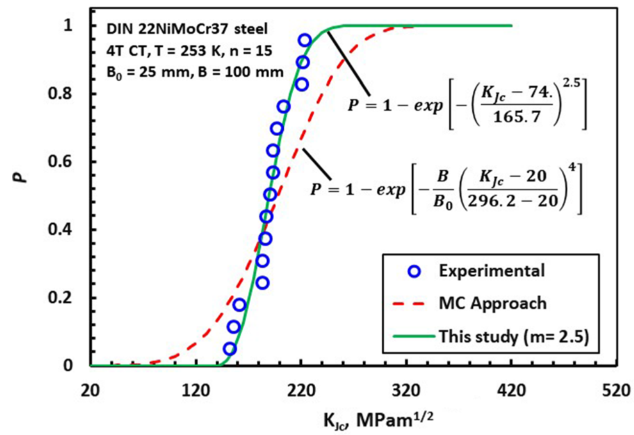
(b)



(c)

Fig. 17—Typical scenarios of data fitting by the Master Curve (MC) approach and comparision with the proposed approach: (*a*) close esimate by MC, (*b*) overestimate by MC; (*c*) underestimate by MC, (*d*) inconsistent estimate by MC.

evidence then available in 1984.[9] These references support the argument in Section I that it lacks rigorous theoretical basis to assign $m_K = 4$ as a constant. This work clearly shows that m_K is more likely in the range of 2 to 2.5. However, it remains a task to make a proper simplification of the threshold toughness of $K_{\min}$ with its



(d)

Fig. 17—continued.

temperature dependence and to explicitly express the specimen size effect on toughness.

V. CONCLUSION

1. The maximum likelihood estimation of the standardized Weibull distribution of cleavage fracture toughnes resulted in Weibull modulus of 1.8 to 2.5 and revealed strong temperature dependence of the threshold toughness and the scale parameter while a less sensitivity to specimen size.
2. The one-sample Kolmogorov–Smirnov (K–S) test based goodness of fit test validated the practice of using the standardized Weibull statistics to characterize cleavage fracture toughness and estimate Weibull modulus, rather than assuming a constant value as prescribed by ASTM E1921-19.

ACKNOWLEDGMENTS

GQ is grateful to the funding of National Natural Science Foundation of China (Grant Nos. 11872364, 11932020) and Chinese Academy of Science (CAS) Pioneer Hundred Talents Program.

REFERENCES

1. ASTM E 1921-19: Standard test method for determination of reference temperature, T0, for ferritic steels in the transition range, ASTM International, 2019.
2. W.-S. Lei: *Mech. Mater*., 2016, vol. 101, pp. 81–92.
3. G. Qian W.-S. Lei, Z. Tong, and Z. Yu: *Materials,* 2019, vol. 12, paper # 982. https://doi.org/10.3390/ma12060982.
4. J.D. Landes and D.H. Shaffer: Statistical characterization of fracture in the transition region. In: *fracture mechanics: twelfth conference*. *ASTM STP 700,* Philadephia: American Society for Testing and Materials, 1980, pp. 368–82.
5. J.D. Landes and D.E. McCabe:Effect of section size on trnsition temperature behavior of structural steels in *Fracture Mechanics: 15th Symposium, ASTM STP 833*, R.J. Sanford, ed., American Society for Testing and Materials, Philadephia, 1984, pp. 378–392.

6. D.E. McCabe: A Comparison of Weibull and β_{Ic} analyses of transition range data. Presented at the 23rd National Symposium on Fracture Mechanics, College Station, TX, 18-20, June, 1991. http://www.iaea.org/inis/collection/NCLCollectionStore/_Public/23/021/23021397.pdf.
7. B. Margolin, A. Gulenko and V. Shvetsova: Fracture toughness prediction for RPV steels with various degree of embrittlement. Transactions of the 17th International Conference on Structural Mechanics in Reactor Technology (SMiRT 17) Prague, Czech Republic, August 17 –22, 2003, Paper # G03-4. 7 pages.
8. F.M. Beremin: *Metall. Trans. A*, 1983, vol. 14A, pp. 2277–87.
9. K. Wallin: *Eng. Fract. Mech.*, 1984, vol. 19, pp. 1085–93.
10. W.-S. Lei: *Mech. Mater.*, 2016, vol. 93, pp. 184–98.
11. W.-S. Lei: *Philos. Mag.* 2016, vol. 96, pp. 3586-3631.
12. D.C. Montgomery and G.C. Runger: *Applied Statistics and Probability for Engineers*, 3rd ed., Wiley, Hoboken, 2003.
13. Y.L. Zhang, H. Hui, J.B. Zhang, Z.Q. Zhou, X. Hu, and X. Cong: *Int. J. Pres. Ves. Pip.*, 2020, vol. 182, pp. 104033-1–104033-10.
14. P.T. Williams, T.L. Dickson, and S. Yin: Fracture Analysis of Vessels — Oak Ridge FAVOR v04.1, Computer Code: Theory and Implementation of Algorithms, Methods, and Correlations (NUREG/CR-6854, ORNL/TM-2004/244). https://www.nrc.gov/reading-rm/doc-collections/nuregs/contract/cr6854/.
15. K. Onizawa, T. Tobita, and M. Suzuki: Investigation on the evaluation of cleavage fracture toughness using PCCv specimens in the ductile-brittle transition range of reactor pressure vessel steels (Contract Research), Report of Japan Atomic Energy Research Institute #JAERI-Research-97-081, 1997. http://www.iaea.org/inis/collection/NCLCollectionStore/_Public/29/019/29019931.pdf.
16. J. Heerens and D. Hellmann: *Eng. Fract. Mech.*, 2002, vol. 69, pp. 421–49.
17. H.C. Kaner, S.G. Mohanty, and J.C. Lyons: *Psychol. Bull.*, 1980, vol. 88 (2), pp. 498–501, https://doi.org/10.1037/0033-2909.88.2.498.
18. E. Lucon and M. Scibetta: Application of Advanced Master Curve Approaches to the EURO Fracture Toughness Data Set. In: *S. Kalluri, M. McGaw, and A. Neimitz (Eds.), STP1526-EB Fatigue and Fracture Mechanics: 37th Volume*, Philadephia: ASTM International, 2011, pp. 116-129. doi: https://doi.org/10.1520/STP49283S.
19. T. Meshii: *Theor. Appl. Fract. Mech.*, 2019, vol. 100, pp. 354–61.
20. M.T. Kirk, The technical basis for application of the Master Curve to the assessment of nuclear reactor pressure vessel integrity, United States Nuclear Regulatory Commission, The Agency-wide Documents Access and Management System (ADAMS), ML093540004, 2002. https://www.nrc.gov/docs/ML0935/ML093540004.pdf.