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# Comments on W.S. Lei's discussion of "An engineering methodology for constraint corrections of elastic–plastic fracture toughness – Part II: Effects of specimen geometry and plastic strain on cleavage fracture predictions" by C. Ruggieri, R.G. Savioli and R.H. Dodds

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ABSTRACT

In recent communication to this journal, Lei (2015) raised several questions on previous work by Ruggieri et al. (2015) which extended a modified Weibull stress ($\tilde{\sigma}_w$) model incorporating the influence of plastic strain on cleavage fracture to correct effects of constraint loss in fracture specimens with a diverse range of specimen geometry. This brief note provides further arguments in support of the modified Weibull stress methodology. This short presentation also shows that Lei's conclusions are not necessarily substantial as they follow from incorrect interpretation of the Weibull stress framework.



## 1. Introduction

In recent communication to this journal, Lei [1] raised several questions on our previous work [2] which extended a modified Weibull stress ($\tilde{\sigma}_w$) model incorporating the influence of plastic strain on cleavage fracture to correct effects of constraint loss in fracture specimens with a diverse range of specimen geometry. Using experimentally measured $J_c$-values derived from fracture toughness testing conducted on an A515 Gr 65 pressure vessel steel in the ductile-to-brittle transition (DBT) temperature, we demonstrated convincingly that the modified Weibull stress methodology effectively removes the geometry dependence on $J_c$-values and yields estimates for the reference temperature, $T_0$, from small fracture specimens in good agreement with the corresponding estimates derived from testing of larger crack configurations. We welcome any contribution and discussion on our extension of the Beremin model [3,2]. Nevertheless, Lei's discussion should not be uncritically endorsed. In this brief note, we address the key points of interest raised in Lei's discussion in the approximate order they appear.

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## 2. Estimation of $J_0$ and implications for fracture toughness predictions

### 2.1. Estimation and significance of $J_0$

The Weibull distribution is perhaps the most widely used distribution in reliability and lifetime analysis, including the statistical description of fracture strength related to the weakest link model [4,5]. The general three-parameter Weibull distribution of the random variable $\chi$ has cumulative distribution function (CDF) in the form

$$F(\chi;\,\alpha,\,\beta,\,\gamma) = 1 - \exp\left[-\left(\frac{\chi-\gamma}{\beta-\gamma}\right)^{\alpha}\right], \quad \gamma \leqslant \chi,\ \alpha > 0,\ \beta > 0,\ \gamma \geqslant 0 \tag{1}$$

where $\alpha, \beta$ and $\gamma$ represent the shape, scale and location (threshold) parameters, respectively. When the threshold parameter is known (or assumed) to be zero, the above expression reduces to two-parameter Weibull distribution with parameters $(\alpha,\,\beta)$. A three-parameter distribution can always be transformed into a two-parameter Weibull distribution by simply making $\bar{\chi} = \chi - \gamma$. Throughout this brief note, we refer to the two-parameter Weibull distribution given by

$$F(\bar{\chi};\,\alpha,\,\bar{\beta}) = 1 - \exp\left[-\left(\frac{\bar{\chi}}{\bar{\beta}}\right)^{\alpha}\right], \quad 0 \leqslant \bar{\chi},\ \alpha > 0,\ \bar{\beta} > 0 \tag{2}$$

By making $\chi = \beta$ in the above, the CDF given by Eq. (1) yields $F(\chi = \beta) = 1 - \exp(-1) = 0.632$ for all values of $\beta$. Thus, parameter $\beta$ sets the position of the distribution along the $\chi$-axis and is therefore termed the characteristic value of the distribution [6,7]. Here, it is also understood that when the random variable is described by the fracture toughness value, $J_c$, then $\gamma \equiv J_{min}$ and $\beta = J_0$ as expressed in Eq. (14) of Ref. [2]. Hereafter, we refer to the Weibull distributions defined by Eqs. (1) and (2) in terms of the random variable $J_c$.

Estimation of the Weibull parameters is a key step in accurate applications of Weibull statistics to describe the fracture toughness distribution. Among the various methods for estimating parameters $(\alpha,\,\beta,\,\gamma)$, including the least square procedure and the method of moments, the maximum likelihood estimation (MLE) procedure is often the most versatile and popular method [6]. However, it is well known that the MLE procedure does not always yield consistent and accurate results - the logarithm of the likelihood function (upon which the estimators of the Weibull parameters are determined) is often ill-posed (see, *e.g.*, [8–12]), particularly for small sizes of statistical samples. Indeed, Teimouri and Gupta [13] even report a negative value for the likelihood estimate of the lifetime threshold for an electronic component (*i.e.*, $\gamma < 0$). This behavior associated with the parameter estimation of the three-parameter Weibull distribution has prompted a more practical approach in which a two-parameter Weibull distribution is adopted by either setting the threshold parameter to zero or by assuming a fixed, generally consistent, value for parameter $\gamma$. For example, Johnson et al. [8] suggest using the minimum value of the statistical sample, $\chi_{(1)}$, as the MLE for $\gamma$, whereas Dubey [14] proposes a simple estimator of the form $\gamma = [\chi_{(1)}\chi_{(k)} - \chi_{(j)}^2]/[\chi_{(1)} + \chi_{(k)} - 2\chi_{(j)}]$ in which $\chi_{(k)}$ is any ordered, observable variate such that $\chi_{(1)} < \chi_{(j)} < \sqrt{\chi_{(1)}\chi_{(k)}}$ (see also [6]).

Now, turning attention to the problem of determining the Weibull distribution to describe experimentally measured fracture toughness values, as addressed in Ruggieri et al. [2], the Master Curve methodology [15,16] adopts a threshold value of $J_{min} = 1.7\ \mathrm{kJ/m^2}$ which corresponds to a threshold fracture toughness for $K_{Jc}$ of 20 $\mathrm{MPa}\sqrt{\mathrm{m}}$. While such a threshold value may appear a somewhat arbitrary choice, it is well within the observed minimum values for experimentally measured fracture toughness in ferritic steels. Indeed, Bowman and Shenton [9] analyzed a fracture toughness data set with 26 $K_{Ic}$-values and found an MLE value for the threshold toughness as 28.5 $\mathrm{MPa}\sqrt{\mathrm{m}}$, which is slight below the minimum value of the statistical sample for $K_{Ic}$-values, $K_{Ic(1)} = 29.4\ \mathrm{MPa}\sqrt{\mathrm{m}}$ (we note, however, that Bowman and Shenton [9] used a value of $\alpha = 1.5$ as the shape parameter of the Weibull distribution). More importantly, though, it should be noted that the adopted $J_{min} = 1.7\ \mathrm{kJ/m^2}$ is much smaller than the minimum value of the statistical sample of $J_c$-values for the A515 Gr 65 pressure vessel steel tested by Ruggieri et al. [2]; here, for the SE(B) specimen with $a/W = 0.5$ at $T = -20\,^{\circ}\mathrm{C}$, $J_{c(1)} = 37\ \mathrm{kJ/m^2}$ which clearly indicates the minor role played by $J_{min}$ on the analyses conducted by Ruggieri et al. [2] and, consequently, on $J_0$-estimates.

### 2.2. Multiscale predictions of $J_0$ based on the modified Weibull stress

The toughness scaling model (TSM) based on the modified Weibull stress $(\tilde{\sigma}_w)$ utilized in our previous work [2] to predict effects of specimen geometry on $J_c$-values builds upon the simple axiom that cleavage fracture occurs at a critical value of $\tilde{\sigma}_{w,c}$ for any crack configuration. This enables interpretation of $\tilde{\sigma}_w$ as a macroscopic crack driving force. Under increased remote loading (as measured by $J$), differences in evolution of the Weibull stress reflect the potentially strong variations of near-tip stress fields due to the effects of constraint loss while, at the same time, incorporating statistical effects of the material microstructure on toughness. Here, the Weibull modulus, $m$, describing the Weibull distribution of $\tilde{\sigma}_w$ plays a major role in the process to correlate effects of constraint loss for varying crack configurations and loading modes. Consequently, upon examining the TSM outlined in [2] (and also a number of references therein), it becomes clear that the Weibull scale parameter, $\sigma_u$, is not necessary to correlate $J_c$-values across different specimen geometries and it is actually never calculated in routine applications of the toughness scaling methodology (the character of $\sigma_u$ in the Weibull distribution of $\tilde{\sigma}_w$ is deferred to a later section).

Since the distribution of $\tilde{\sigma}_w$ expressed by Eq. (1) in our previous work [2] is a two-parameter Weibull distribution (see also Eq. (5) below), the TSM could be based on the constraint correlation $\bar{J}_0^{SEB-a/W=0.15} \rightarrow \bar{J}_0^{SEB-a/W=0.5}$ in which $\bar{J}_0 = J_0 - J_{min}$ thereby recovering the two-parameter character of the CDF for $J_c$-values. Observe, however, that this is of limited use for two key reasons: (1) As already hinted before, the adopted $J_{min} = 1.7$ kJ/m$^2$ is much smaller than $J_0$ so that the constraint ratio is $\bar{J}_0^{SEB-a/W=0.15}/\bar{J}_0^{SEB-a/W=0.5} = 1.353$ against $J_0^{SEB-a/W=0.15}/J_0^{SEB-a/W=0.5} = 1.348$ and (2) Perhaps more importantly, the constraint correction lines shown in Fig. 12 of [2] would shift slightly to the left without, nevertheless, affecting the calibrated $m$-value since the critical value of $\tilde{\sigma}_{w,c}$ is essentially unchanged for both crack configurations.

To illustrate this last point, consider a $J_{min} = 6.8$ kJ/m$^2$ which is four times the adopted $J_{min}$-value in the Master Curve methodology [15,16]. Fig. 1 shows the TSM based on this new constraint correlation $\bar{J}_0^{SEB-a/W=0.15} \rightarrow \bar{J}_0^{SEB-a/W=0.5}$ for the parameter calibration analysis conducted by Ruggieri et al. [2] (for comparison, refer also to Fig. 12 in Ref. [2]). The trend is unmistakable. Because the $J_{min}$-value affects *both* the $J_0$-value for the deeply and shallow cracked specimens, the $\tilde{\sigma}_w$-curves for the calibrated Weibull modulus, $m = 11$, still provide the correct constraint ratio within a small error. We make no claim that such behavior would persist for unrealistically large values of $J_{min}$ since there is a nonlinear relationship between $\tilde{\sigma}_w$ and $J$ as Fig. 1 shows. However, for small threshold values, such as the $J_{min}$-value adopted by the Master Curve methodology, the approximation based on $J_0$ rather than $\bar{J}_0$ is quite good thereby justifying its use for convenience.

### 2.3. Confidence limits for $J_0$

In Ruggieri et al. [2], the confidence limits for parameter $J_0$ were determined from the procedure provided by Thoman et al. [17] (see also Mann et al. [6]). Given the statistic $W = \hat{\alpha}\ln(\hat{\beta}/\beta)$, where $\hat{\alpha}$ and $\hat{\beta}$ denote the estimators of $\alpha$ and $\beta$ (refer to previous Eqs. (1) and (2)), we can choose specific values of $W$, such as $W_{1-\eta/2}$ and $W_{\eta/2}$, which satisfy the probability

$$P[W_{1-\eta/2} \leqslant \hat{\alpha}\ln(\hat{\beta}/\beta) \leqslant W_{\eta/2}] = 1 - \eta. \tag{3}$$

Rearranging the inequality yields

$$\frac{\hat{\beta}}{\exp(W_{1-\eta/2}/\hat{\alpha})} \leqslant \beta \leqslant \frac{\hat{\beta}}{\exp(W_{\eta/2}/\hat{\alpha})} \tag{4}$$

which is a $100(1-\eta)\%$ two-sided confidence limit on the scale parameter of the Weibull distribution, $\beta$. The confidence limits for $\bar{J}_0$ follow in a straightforward manner by simply using $\beta = J_0 - J_{min}$ in the above expression.

Here, we note that the statistic $W = \hat{\alpha}\ln(\hat{\beta}/\beta)$ developed by Thoman et al. [17] strictly applies to a two-parameter Weibull distribution. However, as already discussed, since the adopted $J_{min} = 1.7$ kJ/m$^2$ is much smaller than $J_0$, we may take the viewpoint that the same statistic describing the confidence limits for $\bar{J}_0$ can be used to determine the confidence limits for $J_0$ without any consequences to the predicted bounds provided in Ruggieri et al. [2].

When $K_J = \sqrt{EJ/(1-\nu^2)}$, where $E$ and $\nu$ are the elastic modulus and Poisson's ratio, is employed as a macroscopic crack driving force instead of $J$, Eq. (4) can still be used to define the confidence limits for $K_0$. However, since the Weibull parameters $(\alpha, \beta)$ of the Weibull distribution for the $K_{Jc}$-values are now different, it becomes clear that a one-to-one correspondence between the confidence limits for $J_0$ and $K_0$ does not hold. Evidently, it is then necessary or, at least, advisable, when using the methodology, to specify at the onset of the analysis which parameter would be utilized in applications to

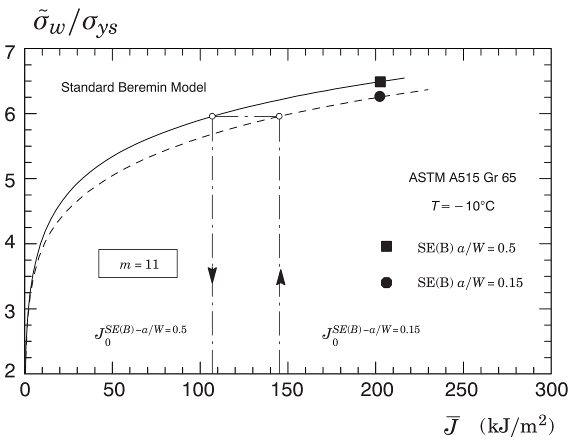


**Fig. 1.** $\tilde{\sigma}_w$ vs. $J$ trajectories for the shallow and deeply-cracked SE(B) specimens at $T = -10$ °C based on the standard Beremin model with $m_0 = 11$ and $J_{min} = 6.8$ kJ/m$^2$.

fracture toughness predictions. Since the central focus of our work reported in [2] was the prediction of specimen geometry effects on experimentally measured $J_c$-values based on the modified Weibull stress model, we did not find very useful bringing this issue into the discussion when predicting the reference temperature, $T_0$.

## 3. Validity of the Weibull stress model

Lei questions the validity of Weibull stress-type models, including the original Beremin model and our proposed modified Weibull stress presented in [2]. This is addressed briefly here. We begin by recalling the distribution of the Weibull stress in the generalized form

$$F(\tilde{\sigma}_w) = 1 - \exp\left[-\left(\frac{\tilde{\sigma}_w}{\tilde{\sigma}_u}\right)^m\right] \tag{5}$$

in which the Weibull modulus, $m$, and parameter $\tilde{\sigma}_u$ define the *shape* and *location* of the distribution.

Now, limiting attention to the standard Beremin model [18] and the modified Weibull stress model incorporating a simplified distribution for the fractured particle developed by Ruggieri and Dodds [3], $\tilde{\sigma}_w$ is given by

$$\tilde{\sigma}_w = \left[\frac{1}{V_0}\int_\Omega \sigma_1^m d\Omega\right]^{1/m} \qquad \text{(Beremin)} \tag{6}$$

and

$$\tilde{\sigma}_w = \left[\frac{1}{V_0}\int_\Omega \left\{1 - \exp\left[-\left(\frac{\sigma_{pf}}{\sigma_{prs}}\right)^{\alpha_p}\right]\right\}\cdot \sigma_1^m d\Omega\right]^{1/m} \qquad \text{(Particle Fracture Distribution)} \tag{7}$$

in which the effect of plastic strain on cleavage fracture probability enters into $\tilde{\sigma}_w$ through the particle fracture stress, $\sigma_{pf}$. Here, $\Omega$ is the volume of the near-tip fracture process zone most often defined as the loci where $\sigma_1 \geqslant \psi\sigma_{ys}$, with $\sigma_{ys}$ denoting the material yield stress and $\psi \approx 2$, and $V_0$ represents a reference volume (see details in [2,3]).

Reading from the above, $\tilde{\sigma}_w$ is unmistakably interpreted as the *random variable* of the Weibull distribution defined by Eq. (5). Thus, when the character of $\tilde{\sigma}_w$ changes, so must the Weibull parameters $(m, \tilde{\sigma}_u)$ in order to maintain the properties of Eq. (5) as a CDF. This is a very important (and fundamental) concept apparently overlooked by Lei in the discussion sent to this journal [1] as well in recent work published elsewhere [19]. As a consequence, the conclusions provided in Lei's discussion are not substantial - they follow from incorrect interpretation of Eq. (5) and associated expressions.

To illustrate this issue, Fig. 2 shows schematically the procedure to determine the Weibull distribution of critical values, $\tilde{\sigma}_{w,c}$, for the deeply-cracked SE(B) specimen at $T = -20\,^\circ$C made of an ASTM A515 Gr 65 steel analyzed by Ruggieri et al. [2] for the standard Beremin model and the modified Weibull stress model incorporating a particle fracture distribution (WL model). Each $J_c$-value defines the corresponding $\tilde{\sigma}_{w,c}$-value determined on the appropriate $\tilde{\sigma}_w$ *vs.* $J$ curve with a fixed value of $m = 11$ (which is the calibrated Weibull modulus for the tested material) as indicated in Fig. 2. For each expression of $\tilde{\sigma}_w$ as presented above, the data set of $\tilde{\sigma}_{w,c}$-values then defines a CDF with parameters $(m, \sigma_u)$ as shown in Fig. 3. Since $\sigma_u$ is the $\tilde{\sigma}_{w,c}$-value corresponding to 63.2%, we have $\sigma_u = 1840$ MPa for the Beremin model and $\sigma_u = 1565$ MPa for the simplified particle distribution (WL) model. These results are an analog of the original work of Beremin [18] in which they report varying $\sigma_u$-values depending on whether plastic strain effects are incorporated into the Weibull stress.

Such behavior can be anticipated by noting that, when the Weibull stress admits alternative definitions, there exists a coupling between $\tilde{\sigma}_w$ and $\tilde{\sigma}_u$ in which case $\tilde{\sigma}_u$ can be considered a material property. To further illustrate the coupling

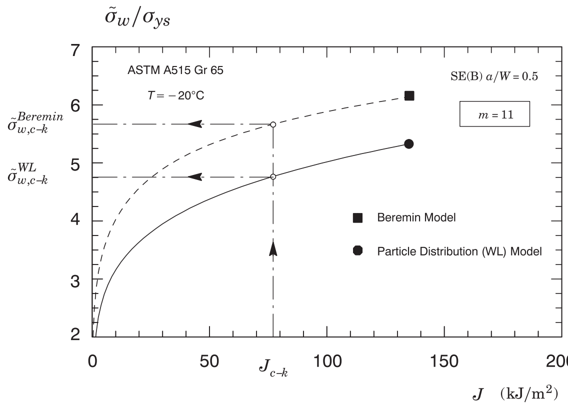


**Fig. 2.** Evolution of $\tilde{\sigma}_w$ with $J$ for the deeply-cracked SE(B) specimen at $T = -20\,^\circ$C and $m = 11$ for the Beremin model and the simplified particle distribution (WL) model derived from the analysis conducted by Ruggieri et al. [2].

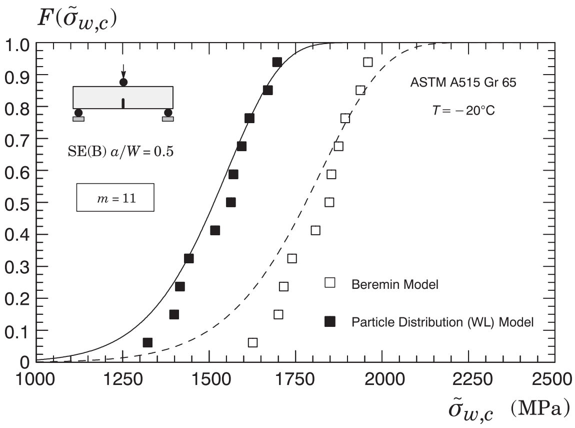


**Fig. 3.** Cumulative Weibull distribution of $\tilde{\sigma}_{w,c}$-values for the SE(B) specimen with $a/W = 0.5$ for the Beremin model and the simplified particle distribution (WL) model with $m = 11$ derived from the analysis conducted by Ruggieri et al. [2].

between $\tilde{\sigma}_w$ and $\tilde{\sigma}_u$, consider the conventional Beremin model described by Eq. (6). Instead of using the simple maximum principal stress as the fracture criterion, we may adopt the coplanar energy release rate criterion [20], as proposed in earlier work of Thiemeir et al. [21], in which a penny-shaped microcrack is assumed so that the fracture criterion now incorporates the effects of *both* the normal and the shear stress acting on the microcrack. Clearly, this "new" Weibull stress so defined will differ from the $\tilde{\sigma}_w$ determined from Eq. (6) such that, for a fixed value of $m$, parameter $\tilde{\sigma}_u$ must be different as well. Similar conclusions can be drawn when a threshold fracture stress, $\sigma_{th}$, is included into the Weibull stress expressed by Eq. (6). Here, replace $\sigma_1$ by $\hat{\sigma}_1 = \sigma_1 - \sigma_{th}$ thereby reducing the magnitude of $\tilde{\sigma}_w$ for a fixed value of $J$ and, consequently, affecting the $\sigma_u$-value of the corresponding Weibull distribution with a fixed $m$-value.

## 4. Conclusions

This brief note provides further arguments in support of the modified Weibull stress model and the associated approach adopted in Ruggieri et al. [2]. While application of the modified Weibull stress methodology predicted accurately the fracture toughness distribution for an A515 Gr 65 pressure vessel steel tested in the ductile-to-brittle transition region, it is clear from the work conducted by Ruggieri et al. [2] that additional studies are needed to further assess the robustness of the methodology in engineering fracture analysis. A simple and yet effective calibration of the Weibull stress parameters, specifically the key parameter $m$, still remains a key issue and challenging procedure. An investigation along this line is currently in progress.

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