A geometry and temperature dependent regression model for statistical analysis of fracture toughness in notched specimens

A. Álvarez-Vázquez[a,*], M. Muñiz-Calvente[a], A. Fernández-Canteli[a], M. J. Lamela[a], Enrique Castillo[b,c]

[a]Department of Construction and Manufacturing Engineering, University of Oviedo, 33204 Gijón, Spain
[b]Royal Academy of Engineering of Spain, don Pedro 10, 28005 Madrid, Spain
[c]Royal Academy of Sciences of Spain, Valverde 24, 28005 Madrid, Spain

Abstract

In this work, a novel methodology for fracture characterization of metallic notched components including the effect of notch root radius and temperature is proposed based on the brittle-to-ductile transition curve. To this aim, two different regression models are derived, either by considering temperature as an influencing variable or combined with the notch radius effect. In the former case, the compatibility condition between the statistical distributions of the fracture toughness for a given temperature and of the temperature for a given fracture toughness is applied. This allows the $K_c - T$ field to be analytically defined proving that both distributions are interrelated and cannot be arbitrarily defined. The second regression model is based on the Theory of the critical distances by converting the experimental data at different notch radii to a reference value. In this way the so-called notch or apparent fracture toughness is calculated in a probabilistic manner for any combination of notch radii and temperature. The proposed methodology is applied to the results of a large experimental campaign on a S355J2 steel involving different temperatures and notch root radii conditions confirming its utility and suitability.

Keywords: Compatibility condition, Notched components, Stress intensity factor, Temperature effect, Theory of critical distances.

1. Introduction and motivation

The fracture characterization of structural and mechanical components is usually confronted with the presence of notches and notched-type defects due to manufacturing and mechanical design details, as rivets, holes and fillets, or in-service defects, such as corrosion pits and impact indentations, among others. As a result, local stress concentration raise around those notches causing premature failures of specimen or components under service conditions, such as those due to fatigue crack growth when they are subject to cyclic loading (see Yen and Dolan [1] and Glinka and Newport [2]). Additionally, the structural and mechanical components under real service conditions are also concerned with other surrounding effects, such as for instance the temperature. In fact, temperature represents one of the variables most influencing the fracture resistance properties of materials, particularly of metals, in which the predominant fracture mechanism may evolve from ductile to brittle depending on the particular value of the temperature (see Ritchie *et al.* [3] and Pineau [4]). Nevertheless, despite the possible concurrent effect of the mentioned influencing factors, well-established methodologies, currently applied for fracture characterization, continue treating them separably each other.

*Corresponding author
E-mail address: alvarezvadrian@uniovi.es ().

Nomenclature

β	shape Weibull parameter
δ	scale Weibull parameter
λ	location Weibull parameter
ρ	notch root radius
ρ_0	reference value of notch root radius
K_c	fracture toughness
K_c^N	notch fracture toughness
$K_{\min}$	minimum value of the fracture toughness
L	critical distance parameter
p	probability
Q_ρ	notch factor
$q_{\max}(x)$	extreme value distribution for maxima values
$q_{\min}(x)$	extreme value distribution for minima values
T	temperature
T_0	reference temperature

Usually, those methodologies modelling the notch-effect referred to the root radius ρ provide a deterministic value of the fracture resistance value for a given notch radius, despite of the non-negligible scatter exhibited by the notch fracture toughness for fixed notch radii (see Anderson [5] and Wallin [6]), as illustrated in Figure 1. Thus, these methods are focused on fitting the mean value of the notch fracture toughness for any notch radii, instead of providing its statistical distribution to allow realistic probabilistic failure prediction to be performed according to the structural integrity concept.

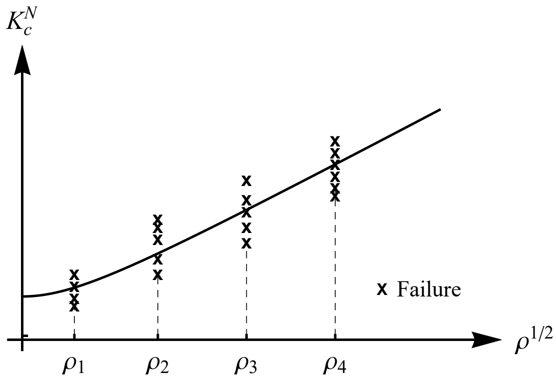

Figure 1: A schematic example of experimental notch fracture toughness scatter for different values of notch radii.

From a theoretical viewpoint, failure of notched components is addressed by categorizing them as cracked ones, leading to over-conservative predictions since the fracture resistance properties of notches are higher than that of cracks. These predictions have been improved by defining the so-called notch or apparent fracture toughness K_c^N instead of the conventional fracture toughness K_c, as defined according to the two classical failure criteria paradigms: local and global (see Pluvinage [7], Bao and Jin [8], Gómez and Elices [9, 10], Cicero *et al.* [11], Ayatollahi and Torabi [12], Ayatollahi *et al.* [13, 14] and Radaj [15]). After the early contributions of Neuber [16] and Peterson [17], the theory of critical distances (TCD) developed by Taylor [18] is one of the most celebrated and successfully applied in a large variety of materials (see Cicero *et al.* [19], Cicero *et al.* [20], Negru *et al.* [21, 22] and Justo *et al.* [23]).

In parallel, the effect of the temperature on the fracture resistance properties in metallic materials has been widely studied during the last decades. Currently, this effect on the fracture toughness K_c is referred to the three main zones, that is, lower or cleavage (LS), intermediate or transition (IS) and upper or ductile shelves (US), of the so-called brittle-to-ductile transition curve (see Anderson [5]), as can be seen in Figure 2. Most of the proposed methodologies are focused on the LS and IS regions, such as the master curve method developed by Wallin [6, 24, 25], in which the fracture toughness K_c is assumed to follow a minimal Weibull distribution, thus providing a probabilistic definition of the $K_c - T$ field results though assuming universally fixed values of the Weibull parameters for certain types of materials and failure.

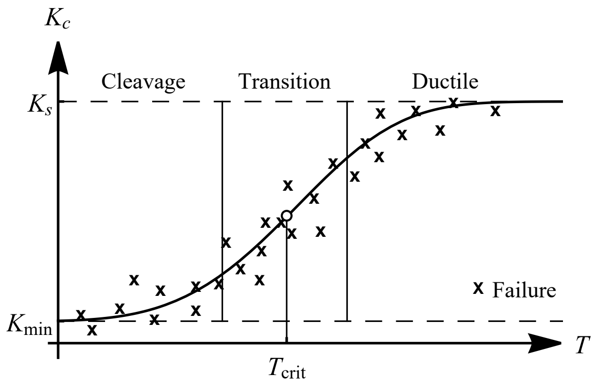

Figure 2: A schematic example of brittle-to-ductile transition curve for a metallic material indicating the lower, intermediate and upper shelves.

Further advance and improvement of the master curve method would be of great interest in practical design, for instance trough development of suitable innovative methodologies, in particular, those enabling the fracture assessment under simultaneous participation of intervening factors or conditions, such as temperature and notch radius. Additionally, a pending aspiration of material scientists and engineers, which represents a critical paradigm in the characterization of materials, would be to guarantee the uniqueness and equivalence material characterization from different test conditions (specimen size and shape, test type, etc.). This would even permit the joint evaluation of experimental results from different test conditions (specimen size and shape, test type, etc.). Once this aim is achieved, transferability of this basic material characterization to the components design could be ensured.

To this aim, a novel probabilistic methodology is proposed for modelling the effects of both notch and temperature conditions acting simultaneously on the fracture resistance properties at lower and intermediate shelves. The model is derived from the compatibility condition between the statistical distribution of the fracture toughness for a given temperature and that of the temperature for a given fracture toughness of the brittle-to-ductile transition curve. This yields the unique possible solution according with the theory of the functional equations. Additionally, the theory of critical distances (TCD) is used to allow the influence of the notch radius to be taken into account. In this way, the notch fracture toughness is analytically derived and the brittle-to-ductile transition curve is extended to any other notch radius condition. As a result, the transition curve is defined in a probabilistic way for any temperature and notch radius condition in a probabilistic way, overcoming current deterministic approaches, in which both effects are treated separately each other. The compatibility condition also shows that the statistical distribution of the fracture toughness for a given temperature, and that of the temperature for a given fracture toughness, may not be independently and arbitrarily defined due to their mutual dependency. This is an important premise to take into account in the derivation of any regression model, which intend to consider both effects.

This proposal enhances the previous work of the authors (see Muñiz-Calvente *et al.* [26]) where the temperature effect was assumed to act as a scale change in the distribution of the fracture toughness of the material since the proposed methodology represents a more robust solution as the former assumption, which is replaced by other more general statistical conditions now considered.

Additionally, the work also attempts to become a reference guideline in the derivation of mathematical models dealing with both temperature and notch radius effects based strictly on a more general formulation founded on statistical and physical considerations, that is, avoiding particular solutions only valid for a particular family of materials.

The paper is organised as follows. In Section 2, some conditions indispensable for deriving valid mathematical models handling simultaneously both temperature and notch effects, are presented. Section 3 describes the proposed methodology, distinguishing two possible versions depending on the external effects considered: a) temperature and b) notch effect and temperature. Then, in order to illustrate how the proposed methodology can be used in practice for modelling both effects, an experimental campaign is used in Section 4 involving several temperatures and radii. Finally, Section 5 discusses the advantages and limitations of the proposed methodology, and Section 6 outlines the main conclusions of this work.

2. Feasible conditions

2.1 Dimensional analysis of the problem

The dimensional analysis, based on the Buckingham's Theorem [27], represents a powerful tool to consider in the derivation of mathematical models taking advantage of working with dimensionless variables. The involved variables when modelling the effect of both temperature and notch geometry on the fracture toughness are summarized in the following set:

$$\nu \equiv \{K_c, K_{\min}, T, T_0, \rho, \rho_0, p\}. \tag{1}$$

The Buckingham's theorem states that the system of physical equations as a function of the initial set of seven dimensional variables can be reduced, without loss of generality, to an equivalent one as a function of four dimensionless variables. By selecting $K_{\min}, T_0$ and ρ_0 as the normalizing ones, the following ratios[1] result:

$$K_c^* = \log\left(\frac{K_c}{K_{\min}}\right); \; T^* = \log\left(\frac{T}{T_0}\right); \; \rho^* = \frac{\rho}{\rho_0}, \tag{2}$$

from which the probability of failure p can be then written as:

$$p = f(K_c^*, T^*, \rho^*). \tag{3}$$

2.2 Physically valid formulas

An additional and necessary condition to be applied in the derivation of the model arises from the concept of physically valid formulas concept, closely related with the dimensional analysis, namely that an equation relating dimensional variables at both sides must satisfy that unit changes due to location or scale transformation at the one side must be conveniently replicated at the other side.

For example, it is crucial to select properly the log-normal distribution for modelling temperatures, as occurs in the work of Moskovic [28] about the fracture toughness, since this distribution is not stable with respect to changes in location, while the temperature variable is allowed to. For this reason, if the units are transformed from Celsius to Fahrenheit, implying location and scale changes, the log-normal distribution must also be transformed into a new one that does not turn out to be from the same family. As a consequence, as a function of the units selected from measuring the sample temperature, the parameters of the distribution will be different, as indicated in Castillo *et al.*

[1] The asterisk notation indicates a dimensionless variable.

[29] and Castillo *et al.* [30]. Examples of valid distributions when dealing with temperatures are provided by the generalized the extreme value family (Weibull, Gumbel and Fréchet) and the extended normal distribution.

Consequently, the use of the generalized extreme value family of distributions together with dimensionless variables in the proposed model in this paper guarantees this important feasible condition to be fulfilled.

3. The proposed methodology

In this section, the derivation of the proposed methodology is presented. Initially, the temperature effect on the fracture toughness for a constant value of the notch radius is handled, and then the analysis is extended by including the notch radius as an additional variable.

3.1 The regression model for constant notch radii ρ

The analysis of the brittle-to-ductile transition process for a constant notch radius in the lower and intermediate shelves allows some interesting physical properties to be identified:

1. The lower and intermediate shelves in the brittle-to-ductile transition curve are concave from above.

2. The fracture toughness K_c is identified as the critical value of the stress intensity factor K_{I}, i.e. the minimum one at which the fracture occurs according to the weakest link principle. Thus, only minimal Weibull and Gumbel distributions are justified for this random variable.

3. The critical value of the fracture toughness with respect to the temperature is identified with the largest value of it at which the transition from brittle to ductile behaviour takes place, that is, the prediction of the turning temperature in the $K_c - T$ field constitutes a problem of maxima value, for that reason, only maximal Weibull and Gumbel distributions must be considered.

Accordingly, the analytical definition of the $K_c - T$ field comprises the simultaneous definition of the two extremal distributions, i.e. $F(K_c^*|T^*)$ referred to the fracture toughness for a given temperature and $F(T^*|K_c^*)$ referred to the temperature for a given fracture toughness. This implies that these distributions are not independent interrelated each other which is a fact ignored by previous models describing the $K_c - T$ field. The interrelation condition can be established through the compatibility condition at both participating distributions $F(K_c^*|T^*)$ and $F(T^*|K_c^*)$ in the $K_c - T$ field, as originally proposed by Castillo and Fernández-Canteli [31] for modelling the fatigue lifetime prediction through the $\Delta\sigma - N$ field (assuming minima-minima distributions) or the crack growth curves in the $a - N$ field (assuming maxima-minima distributions).

In the present case, the critical conditions for the $K_c^* - T^*$ field are represented by the minimum distribution for the fracture toughness, K_c^*, and the maximum distribution for temperature T^* while the material behaviour evolves from brittle to ductile behaviour. Accordingly, the compatibility condition between both distributions is defined as

$$F_{K_c^*|T^*}(K_c^*|T^*) = F_{T^*|K_c^*}(T^*|K_c^*), \tag{4}$$

where $F_{K_c^*|T^*}(K_c^*, T^*)$ and $F_{T^*|K_c^*}(T^*, K_c^*)$ are the cdf of K_c^* given T^* and T^* given K_c^*, referred to as extreme value distributions for minima and for maxima, respectively. Thus, by assuming a family of location and scale parameters, the following compatibility condition in Eq. (4) results (see Castillo *et al.* [32]):

$$1 - q_{\min}\left(\frac{K_c^* - \lambda_1(T^*)}{\delta_1(T^*)}\right) = q_{\max}\left(\frac{T^* - \lambda_2(K_c^*)}{\delta_2(K_c^*)}\right), \tag{5}$$

where $q_{\min}$ and $q_{\max}$ represent the two distributions for minima and maxima respectively, in an equivalent formulation as the proposed by Castillo and Fernández-Canteli [31] for modelling the $a - N$ crack growth curves. In Eq. (5),

$\lambda_1(T^*), \lambda_2(K_c^*)$ and $\delta_1(T^*), \delta_2(K_c^*)$ are the location and scale parameters as a function of temperature and fracture toughness, respectively.

Figure 3 illustrates schematically the compatibility condition in the $K_c^* - T^*$ field for both distributions evidencing the coincidence of the areas of the frequency distributions for a given percentile curve.

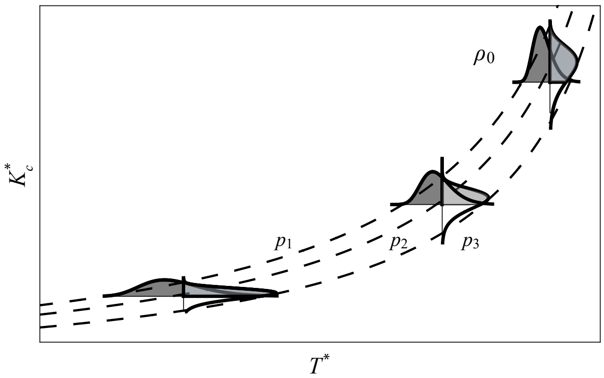

Figure 3: Illustration of the compatibility condition showing equal areas (probabilities) of the two intersecting densities of $K_c^*|T^*$ and $T^*|K_c^*$.

The solution of the functional equation (5) for the unknown functions $\lambda_1(T^*), \lambda_2(K_c^*), \delta_1(T^*)$ and $\delta_2(K_c^*)$ provides the unique possible functional expression of the $K_c^* - T^*$ field, which satisfies the compatibility condition comprising both minima and maxima event conditions. To this end, substituting the Weibull distributions for maxima and minima, that is,

$$q_{\min}(x) = 1 - \exp[-(x)^{\beta}], \text{ and } q_{\max}(x) = \exp[x^{\beta}], \tag{6}$$

into the compatibility condition Eq. (5) and solving the resulting functional equation, provides the final Weibull model for the $K_c^* - T^*$ field:

$$F(K_c^*, T^*; \lambda, \delta, \beta) = \exp\left[-\left(-\frac{(B-T^*)(K_c^*-C)-\lambda}{\delta}\right)^{\beta}\right], \tag{7}$$

where (λ, δ, β) are the parameters of the Weibull distribution. The solution of the compatibility condition confirms that only hyperbolic and straight percentile lines are the only possible solution to define the $K_c^* - T^*$ field, though only the first option satisfies the physical properties required to the brittle-to-ductile transition curve in the LS and IS zones, as previously mentioned. The result corroborates that any other model different from those solved will violate the compatibility condition and the extremal conditions the random variables must compulsory satisfy.

The resulting asymptotes of the model, i.e. C and B, deserve particular attention. On the one hand, the horizontal asymptote C indicates that fracture will not occur below a certain minimum value, $K_{\min}$, as shown in Figure 2. On the other hand, the vertical asymptote B establishes the limit of applicability of the model, which can be interpreted as the turning point or the transition temperature T_{crit} (see Figure 2). Both results are relevant for practical design.

Finally, the quantile function $F^{-1}(p; T^*)$ can be applied to obtain the regression p-percentile family of curves in the Weibull-Weibull Eq. (7) when the interest is focused on the explicit definition of the fracture toughness as a function of temperature:

$$K_c^*(T^*) = F^{-1}(p;T^*) = \frac{\lambda - \delta(-\log p)^{1/\beta}}{B - T^*} + C. \tag{8}$$

3.2 The regression model for varying notch radii ρ

Once the methodology for defining the $K_c^* - T^*$ field for constant notch radius has been established, the model extension implying the notch radius acting as an additional variable is straightforward by resorting to the theory of critical distances.

The TCD represents one of the most celebrated models to derive the local failure criteria for notched components. To be more precisely, this methodology comprises not only one model but a group of models, denoted Point, Line, Surface and Volume methods. The theoretical stress distribution around the notch tip can be approached by the expression proposed by Creager and Paris [33]:

$$\sigma(r) = \frac{K_I}{\sqrt{\pi}} \frac{2(r+\rho)}{(2r+\rho)^{3/2}}, \tag{9}$$

which is only valid if the notch radius $\rho << a$, being K_{I} the stress intensity factor. Taking this into account, the line method allows a simpler expression for the notch fracture toughness K_c^N to be derived (see Taylor [18]):

$$K_c^N(\rho;L) = K_c\sqrt{1+\frac{\rho}{4L}}, \tag{10}$$

where L is the critical distance parameter and K_c is the fracture toughness for the cracked specimens, i.e. $\rho = 0$. Accordingly, the notch fracture toughness K_c^N results as the fracture toughness of the material K_c multiplied by a factor given by the TCD approach as a function of ρ and L.

In a more general set, the transformation between two different notch radii ρ_1 and ρ_2 due to the TCD approach is defined as:

$$\left.\begin{aligned} K_c^N(\rho_1;L) &= K_c\sqrt{1+\frac{\rho_1}{4L}} \\ K_c^N(\rho_2;L) &= K_c\sqrt{1+\frac{\rho_2}{4L}} \end{aligned}\right\} \Rightarrow \frac{K_c^N(\rho_2;L)}{K_c^N(\rho_1;L)} = \sqrt{\frac{4L+\rho_2}{4L+\rho_1}}, \tag{11}$$

which can be rewritten as follows:

$$K_c^N(\rho_2;L) = Q_\rho(\rho_1,\rho_2)K_c^N(\rho_1;L), \tag{12}$$

where

$$Q_\rho(\rho_1,\rho_2) = \sqrt{\frac{4L+\rho_2}{4L+\rho_1}}, \tag{13}$$

represents a transformation factor allowing the values of the notch fracture toughness for different values of the notch radius to be interrelated.

As suggested by Muñiz-Calvente *et al.* [26], the TCD method can be successfully applied to transform the results of the fracture resistance for a given notch radii $(K_{c\ 1}^{N}, ..., K_{c\ n}^{N})$ into the corresponding values for the cracked condition $(K_{c1}, ..., K_{cn})$, that is, for a reference value of $\rho = 0$ at each tested temperature:

$$K_c = K_c^N(\rho;L)Q_\rho(0,\rho) = K_c^N(\rho;L)\sqrt{\frac{4L}{4L+\rho}}. \tag{14}$$

In this way, the experimental data in the $K_c - T - \rho$ field can now be transformed to a master field $K_c - T$ for $\rho = 0$ where the compatibility condition is conveniently applied for a constant value of the notch radius as already described in previous section. Once the master field has been defined, the TCD can again

$$p = \exp\left[-\left(-\frac{(B-T)(K_c^N Q_\rho(0,\rho) - C) - \lambda}{\delta}\right)^\beta\right], \tag{15}$$

to derive univocally the notch fracture toughness K_c^N corresponding to any other notch radius ρ, that is,

$$p = \exp\left[-\left(-\frac{K_c^N - \lambda_{\rho,T}(\rho,T)}{\delta_{\rho,T}(\rho,T)}\right)^\beta\right], \tag{16}$$

where the model parameters λ and δ are now including the notch effect according to the following expressions:

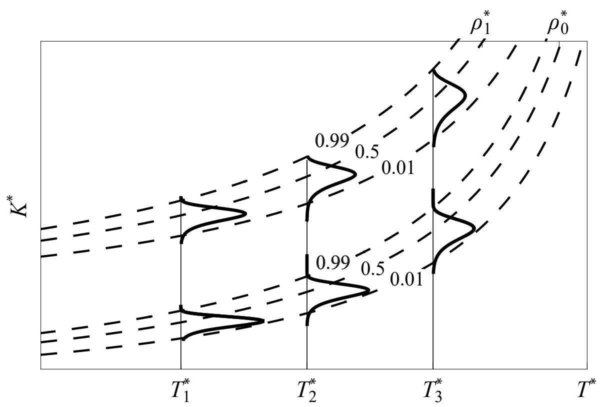

Figure 4: Schematic illustration of the $K_c^N - T$ field for two different notch radii, indicating the evolution of the notch fracture toughness densities for various given values of temperature.

$$\lambda_{\rho,T}(\rho,T) = \left[C + \frac{\lambda}{B - T^*}\right]\sqrt{1 + \frac{\rho}{4L}},$$
$$\delta_{\rho,T}(\rho,T) = \frac{\delta}{B - T^*}\sqrt{1 + \frac{\rho}{4L}}. \tag{17}$$

The resulting $K_c - T$ fields for two different notch radius, at both lower and intermediate shelves, are schematically represented by three percentile curves in Figure 4. Note that the percentile curves are shifted vertically implying change of both location and scale parameters.

Thus, the explicit analytical definition of the notch fracture toughness K_c^N for any notch radius is obtained in terms of the quantile function of the Weibull-Weibull model,

$$K_c^N(\rho,T;p) = \left[\frac{\lambda - \delta(-\log p)^{1/\beta}}{B - T} + C\right]\sqrt{1 + \frac{\rho}{4L}}. \tag{18}$$

Note that the proposed model, in contrast to current methodologies only focused on the mean values (see Figure 1), provides the analytical expression of the $K_c^N - \rho^{1/2}$ field in a probabilistic manner for a given temperature according to Eq. (18), as shown in Figure 5, which represents a relevant feature in practical design.

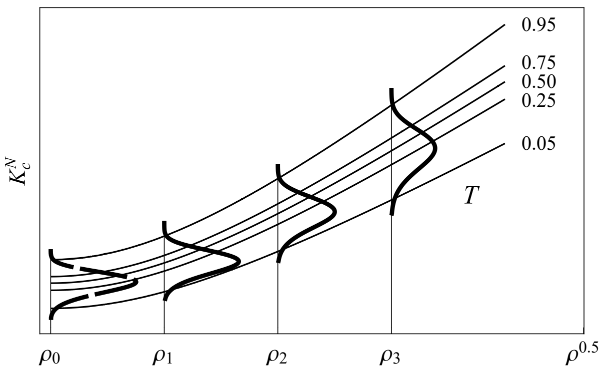

Figure 5: Schematic illustration of the percentile curves in the $K_c^N - \rho^{0.5}$ field for a given temperature.

As a result, the pdf and cdf of the notch fracture toughness can be obtained for any notch radius and given temperature, as can be seen in Figure 6, where both location and scale parameters of the Weibull distribution are calculated according to Eq. (17).

3.3 Parameter estimation

When both temperature and notch effects are considered, the parameter estimation in the proposed methodology is performed in the following steps:

a) *Collecting experimental data*. The general set of experimental notch fracture toughness data, collected from different combinations of notch radius and temperatures, is expressed as follows:

$$\left\{\left(K^N_{c_{ijk}}, T_j; \rho_k\right) | i = 1,...,n; j = 1,...,m; k = 1,...,r\right\}, \tag{19}$$

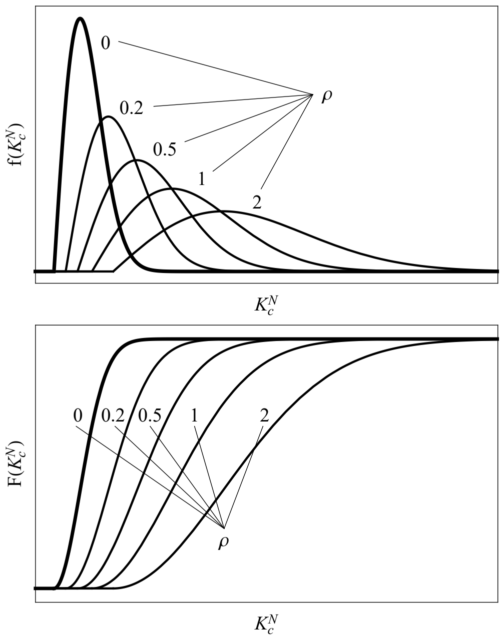

Figure 6: Pdf and cdf of the notch fracture toughness for different notch radius and a given temperature.

where $K^N_{c_{ijk}}$ represents the i-th value of the experimental fracture toughness resulting at temperature T_j and notch radius ρ_k.

b) *Estimation of the K_c, L parameter*. The parameters of the TCD in Eq. (10) for describing the notch effect on the fracture toughness K_c^N can be estimated for each j-th temperature value based on the Least Squares (LS) method, that is,

$$\min_{(K_c,\ldots,K_{c_m},L,\ldots,L_m)} \left\{ \sum_{j=1}^{m} \left[\sum_{i=1}^{n} \left(K^N_{c_{ijk}} - K_{c_j}\sqrt{1+\frac{\rho_k}{4L_j}} \right) \right]^2 \right\}. \tag{20}$$

c) *Conversion of the experimental data from ρ to ρ_0*. Once the parameters of the TCD method are known, the experimental random samples $(K^N_{c_{1jk}},\ldots,K^N_{c_{njk}})$ at notch radius ρ_k and temperature T_j are transformed into their equivalences $(K_{c_{1j}},\ldots,K_{c_{nj}})$ referred to notch radius ρ_0 at temperature T_j, according to Eq. (14), that is,

$$K_{c_{ij}} = K^N_{c_{ijk}}(\rho_k; L_j) Q_\rho(0,\rho_k). \tag{21}$$

As a result, the $K_c^N - T$ field can now be transformed to its equivalent $K_c - T$ field for applying the compatibility condition.

d) *Estimation of B, C parameters*. According to Castillo *et al.* [34], Castillo and Hadi [35, 36] and Castillo and Fernández-Canteli [31, 37], the parameter estimation of the asymptotes of the Weibull-Weibull model is performed by minimizing the following condition:

$$\min_{(\mu,B,C)} \left(K_{c_{ij}} - C - \frac{\mu}{B - T_j} \right)^2, \tag{22}$$

where μ represents the mean of the temperature variable.

e) *Estimation of the Weibull parameters* λ, β, δ. According to the normalized variable V^* defined as follows:

$$V_i^* = (K_{c_{ij}} - C)(B - T_j), \tag{23}$$

which results from the application of the compatibility condition to the $K_c^* - T^*$ field, all data points are pooled together into a single Weibull cdf representing the $p - V^*$ field. The corresponding Weibull parameters can be estimated using some of the standard estimation techniques for extreme value family of distributions (see Castillo [38] and Castillo *et al.* [39]), such as the probability paper method.

4. Example of practical application

In this section, the extensive experimental campaign of Madrazo *et al.* [40] on the fracture characterization including different combinations of notch radii and temperatures is used to illustrate the suitability of the proposed methodology described in Section 3 to asses the fracture toughness under the effect of both variables.

4.1 Description of the experimental program

The experimental program consists in 102 tests carried out on compact tension (CT) specimens of steel S355J2 with six different notch radii (0.00,0.15,0.25,0.50,1.00 and 2.00 mm.) at different temperatures (-196, -150, -120 and -100º C). Further details about the material, tensile strength, specimen geometry, testing temperature and critical load-bearing results are found in the original work of Madrazo *et al.* [40]. Of particular interest are those considerations related with the definition of the notch fracture toughness K_c^N from the experimental results of the fracture toughness K_c based on cracked specimen formulation outlined in the international standard ASTM E1820 [41].

The selected temperatures extend not only along the ductile-to-brittle transition shelf but also over the lower one, since the fracture behaviour under notch geometries behaves in a more ductile way than that observed under cracked conditions. As a result, the final fracture at the lower shelf may be preceded by a certain ductile behaviour followed by final cleavage fracture with single initiation point.

4.2 Applicability of the proposed methodology

As described in Section 3.3, the first step to apply the proposed methodology consists in fitting the experimental results for different notch radii in the $K_c^N - \rho^{1/2}$ field for each temperature in an independent way, according to the TCD. In this way, the optimal values for K_c and L are provided by minimizing Eq. (20) using the least squares method, allowing the experimental values of the notch fracture toughness to be transformed into the corresponding ones for smooth specimen condition, as listed in Table 1. Figure 8 illustrates the predictions resulting from this deterministic method for each of the different temperatures tested.

Once the TCD parameters are estimated, the original experimental results samples of the notch fracture toughness for each notch radius and temperature are transformed into the equivalent fracture toughness values for the reference notch radius ρ_0 in accordance to Eq. (21). As a result, the compatibility condition can be conveniently applied and the transformed experimental points be plotted in the $K_c - T$ field. Accordingly, the estimation of the asymptotes can

Table 1: Parameter estimates for the TCD method in the analysis of the experimental data for feritic steel S355J2 from Madrazo *et al.* [40].

T	Parameters	
	L	K_c
[º C]	[mm]	[MPa·mm$^{0.5}$]
-196	0.028	32.276
-150	0.0096	61.452
-120	0.014	132.629
-100	0.078	296.546

now be performed by minimizing Eq. (22), providing the following estimates:

$$C = 2.2 \times 10^{-14}, \;\; B = 7.047. \tag{24}$$

From Eq. (24), the normalized variable V^* is defined in such a way that all experimental data can be pooled together into one single Weibull cdf by applying a plotting position scheme, providing the following parameter estimates:

$$\lambda = 6.85, \;\; \delta = 2.76, \;\; \beta = 7.55. \tag{25}$$

Figure 7 illustrates the final estimation of the $K_c - T$ field showing some representative percentile curves after fitting the experimental values of the notch fracture toughness transformed into the equivalent ones for $\rho = 0$. The practical interest of the methodology is that any experimental result from different temperatures and notch geometry conditions can be conveniently pooled into a single cdf representing the $p - V^*$ field, which can now be contemplated as the most general master curve of the material.

Note that the $K_c^N - \rho^{1/2}$ field can be straightforwardly obtained from the $K_c - T$ field, as shown in Figure 8 for the experimental data at an exemplary $T = -196^{\circ}$ C. The inherent scatter of the experimental data can now be conveniently estimated to achieve more reliable failure predictions using the theory of critical distances. This is an additional contribution provided by the proposed methodology in contrast with current deterministic methods used in practical structural and mechanical design.

5. Discussion

Though only the second regression model for considering both effects was illustrated, the first regression method focused solely on the temperature effect could also be used as an alternative definition to the $K_c - T$ field in the conventional the master curve method. In this case, the experimental results of different samples of ferritic steels are pooled together in one single $K_c - T$ field according to the proposed methodology, which ensures compatibility between both minimal and maximal statistical distributions, respectively, of the variables being involved, K_c and T, in contrast to other current probabilistic master curve proposals.

A relaxation of the proposed regression models can alternatively be envisaged to the Weibull-Weibull model by considering Gumbel distribution according to the extreme value theory while maintaining the physical considerations concerning fracture toughness and temperature variables, as mentioned in Section 3 (see Castillo *et al.* [42] and Castillo and Fernández-Canteli [31]).

Finally, it is also worth mentioning that the notch fracture toughness, as well-known, is also dependent of the specimen thickness, i.e. on the specific constraint conditions prevailing (see Wallin [43]). Since only the experimental results from the research of Cicero *et al.* [44] were used in the model assessment, in which the specimen width was

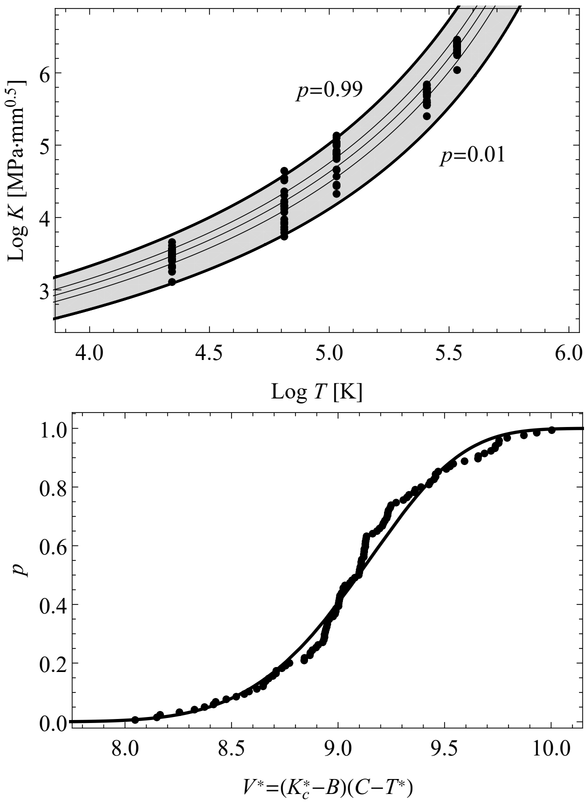

Figure 7: Predicted $K_c - T$ field for some representative percentiles ($p = 0.01, 0.25, 0.50, 0.75, 0.99$) (above) and estimated Weibull cdf in $p - V^*$ field (below) for S355J2 experimental data from Madrazo *et al.* [40].

maintained throughout constant, such a scenario is not considered here. Furthermore, it must be also mentioned that the proposed methodology to model notch effects is only applicable to U-notches whereas V-geometries cannot be handled.

6. Conclusions

- A methodology to predict the probability of failure of notched components under different temperature conditions both in lower and intermediate shelves is proposed. The model is based on statistical conditions, namely, compatibility and those related to the extreme value theory. The resulting functional equations provides the unique possible solution for the probabilistic $K_c - T$ field.

- The compatibility condition implies that the statistical distribution of the fracture toughness for given temperature, $K_c^*|T^*$, and the temperature for a given fracture toughness, $T^*|K_c^*$, in the $K_c - T$ field can neither arbitrarily nor independently be chosen. They are mutually dependent each other, which represents a requirement to be necessarily considered in the derivation of nay valid methodology for definition of the $K_c - T$ field.

- A probabilistic approach, alternative to the deterministic application of the theory of critical distances, is derived, which allows the statistical distributions of the notch fracture toughness to be defined for any value of the notch root radius ($K_c^N - \rho^{1/2}$ field) and given temperature ($K_c^N - T$ field).

- The proposed methodology takes into account the concurrent effect of notch radius and temperature in the prediction of the fracture resistance properties, providing a probabilistic definition of the global $K_c^N - \rho^{1/2} - T - p$ field.

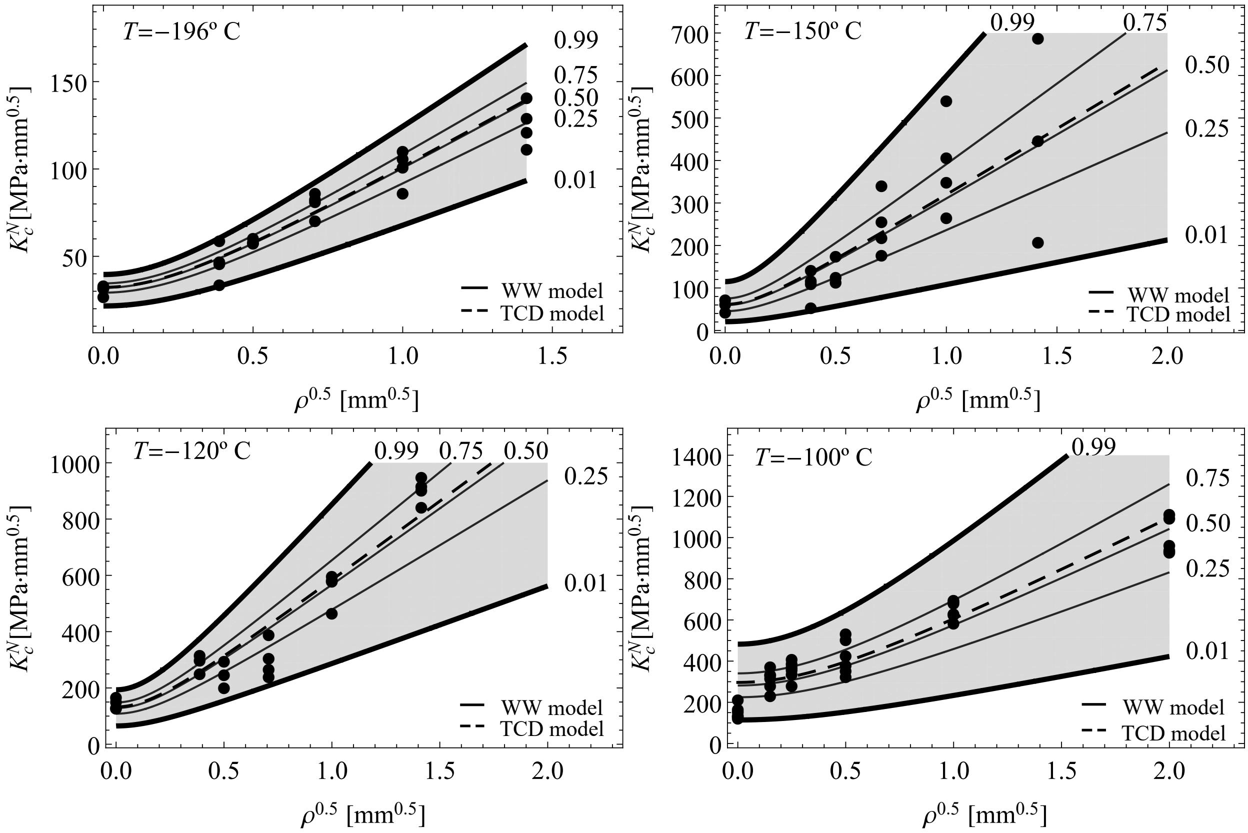

Figure 8: Estimated predictions of the percentile curves for the $K_c^N - \rho^{0.5}$ field as derived from the combination of the Weibull-Weibull (WW) and theory of critical distances (TCD) models for S355J2 experimental data from Madrazo *et al.* [40].

– The compatibility condition allows the experimental results from different temperatures and notch radii conditions to be pooled together into one single cdf pertaining to the Weibull distribution, representing a general master curve of the material.

– The experimental results of an external campaign, including several temperatures and notch radii conditions, are used for confirming the suitability of the proposed methodology in the characterization of metallic materials.

– General guidelines are suggested for derivation of methodologies to model the lower and intermediate shelves of brittle-to-ductile transition curve. They are solely founded on statistical and physical conditions related to the fracture process avoiding particular solutions about the resulting parameters of the models being used.

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References

[1] C. S. Yen and T. J. Dolan. A critical review of the criteria for notch-sensitivity in fatigue of metals. In *Univeristy of Illinois Bulletin*, number 398. University of Ollinois Engineering Experiment Station, Illinois, Urbana, 1952.

[2] G. Glinka and A. Newport. Universal features of elastic notch-tip stress fields. *Int J Fatigue*, 9(3):143 – 150, 1987.

[3] R. O. Ritchie, J. F. Knott, and J. R. Rice. On the relationship betwen critical tensile stress and fracture toughness in mild steel. *1. Mech. Phys. Solids*, 21:395–410, 1973.

[4] A. Pineau. Review of fracture micromechanisms and a local approach to predicting crack resistance in low strength steels. In D. Francois, editor, *Advances in Fracture Reseach, 5th International Conference on Fracture*, volume 2, pages 553–577, 1981.

[5] T. L. Anderson. *Fracture Mechanics. Fundamentals and Applications*. CRC Press, 4 edition, 2017.

[6] K. Wallin. The scatter in K_{IC} results. *Eng Fract Mech*, 19:1085–1093, 1984.

[7] G. Pluvinage. Fatigue and fracture emanating from notch; the use of the notch stress intensity factor. *Nucl Eng Des*, 185:173–84, 1998.

[8] Y. Bao and Z. Jin. Size effects and a mean-strength criterion for ceramics. *Fatigue Fract Eng Mater Struct*, 8:829—-35, 1993.

[9] F. J. Gómez and M. Elices. A fracture criterion for sharp V-notched samples. *Int J Fract*, 123:163—-175, 2003.

[10] F. J. Gómez and M. Elices. Fracture of components with V-shaped notches. *Eng Fract Mech*, 70:1913—-1927, 2003.

[11] S. Cicero, F. Gutiérrez-Solana, and J.A. Álvarez. Structural integrity assessment of components subjected to low constraint conditions. *Eng Fract Mech*, 10:3038–59, 2008.

[12] M.R. Ayatollahi and A. R. Torabi. A criterion for brittle fracture in U-notched components under mixed mode loading. *Eng Fract Mech*, 76(12):1883 – 1896, 2009.

[13] M.R. Ayatollahi, M. Dehghany, and M. Nejati. Fracture analysis of V-notched components – effects of first non-singular stress term. *Int J Solids Struct*, 48(10):1579 – 1589, 2011.

[14] M.R. Ayatollahi, A. R. Torabi, and P. Azizi. Experimental and theoretical assessment of brittle fracture in engineering components containing a sharp V-notch. *Exp Mech*, 51:919 – 932, 2011.

[15] D. Radaj. State-of-the-art review on extended stress intensity factor concepts. *Fatigue Fract Eng M*, 37(1):1–28, 2014.

[16] H. Neuber. *Theory of notch stresses: principles for exact calculation of strength with reference to structural form and material*, volume 4547. USAEC Office of Technical Information, 1961.

[17] R. E. Peterson. Notch sensitivity. In G. Sines and J. L. Waisman, editors, *Metal Fatigue*, pages 293–306. McGraw-Hill, New York, 1959.

[18] D. Taylor. *The Theory of Critical Distances. A New Perspective in Fracture Mechanics*. Elsevier Science, London, 1 edition, 2007.

[19] S. Cicero, V. Madrazo, I. A. Carrascal, and R. Cicero. Assessment of notched structural components using failure assessment diagrams and the theory of critical distances. *Eng Fract Mech*, 16:2809—-25, 2011.

[20] S. Cicero, V. Madrazo, and T. García. The notch master curve: a proposal of master curve for ferritic-pearlitic steels in notched conditions. *Eng Fract Mech*, 16:2809—-25, 2011.

[21] R. Negru, L. Marsavina, H. Filipescu, C. Căplescu, and T. Voiconi. Assessment of brittle fracture for PUR materials using local strain energy density and theory of critical distances. *Theor Appl Fract Mec*, 2015.

[22] R. Negru, L. Marsavina, T. Voiconi, E. Linul, H. Filipescu, and G. Belgiu. Application of TCD for brittle fracture of notched PUR materials. *Theor Appl Fract Mec*, 2015.

[23] J. Justo, J. Castro, S. Cicero, M.A. Sánchez-Carro, and R. Husillos. Notch effect on the fracture of several rocks: Application of the theory of critical distances. *Theor Appl Fract Mec*, 90:251 – 258, 2017.

[24] K. Wallin. The master curve method: a new concept for brittle fracture. *Int J Mater Prod Tec*, 14:342 – 354, 1999.

[25] K. Wallin. Master curve analysis of the "euro" fracture toughness dataset. *Eng Fract Mech*, 69(4):451 – 481, 2002.

[26] M. Muñiz-Calvente, A. Álvarez Vázquez, S. Cicero, J. Correia, A. M. P. de Jesus, S. Blasón, A. Fernández-Canteli, and F. Berto. Study of the influence of notch radii and temperature on the probability of failure: a methodology to perform a combined assessment. *Fatigue Fract Eng Mater Struct*, 42(12):2663–2673, 2019.

[27] E. Buckingham. The principle of similitude. *Nature*, 96:396–397, 1915.

[28] R. Moskovic. Statistical analysis of censored fracture toughness data in the ductile to brittle transition temperature region. *Eng Fract Mech*, 44(1):21 – 41, 1993.

[29] E. Castillo, A. Calviño, M. Nogal, and H. K. Lo. On the probabilistic and physical consistency of traffic random variables and models. *Comput-Aided Civ Infrastruct Eng*, 29:496–517, 2014.

[30] E. Castillo, J. O'Connor, and M. Nogal. On the physical and probabilistic consistency of some engineering random models. *Structural Safety*, 51:1–12, 2014.

[31] E. Castillo and A. Fernández-Canteli. *A Unified Statistical Methodology for Modeling Fatigue Damage*. Springer Netherlands, 1 edition, 2009.

[32] E. Castillo, A. Fernández-Canteli, C. Castillo, and C.M. Mozos. A new probabilistic model for crack propagation under fatigue loads and its connection with wöhler fields. *Int J Fatigue*, 32(4):744 – 753, 2010.

[33] M. Creager and P. C. Paris. Elastic field equations for blunt cracks with reference to stress corrosion cracking. *Int J Fract Mech*, 4:247—-52, 1967.

[34] E. Castillo, A. Fernández-Canteli, V. Esslinger, and Thürliman. Statistical models for fatigue analysis of wires, strands and cables. In *IABSE Proceedings*, volume 82, pages 1–140, 1985.

[35] E. Castillo and A. S. Hadi. Modeling lifetime data with application to fatigue models. *J Am Stat Assoc*, 90(431):1041–1054, 1995.

[36] E. Castillo, A. Fernández-Canteli, and A. S. Hadi. On fitting a fatigue model to data. *Int J Fatigue*, 21(1):97–106, 1999.

[37] E. Castillo and A. Fernández-Canteli. A general regression model for lifetime evaluation and prediction. *Int J Fract*, 107(2):117–137, 2001.

[38] E. Castillo. *Extreme Value Theory in Engineering*. Academic Press, 1 edition, 1988.

[39] E. Castillo, Ali S. Hadi, N. Balakrishnan, and J. M. Sarabia. *Extreme Value and Related Models with Applications in Engineering and Science*. Wiley Series in Probability and Statistics, 1 edition, 2004.

[40] V. Madrazo, S. Cicero, and T. García. Assessment of notched structural steel components using failure assessment diagrams and the theory of critical distances. *Eng Fail Anal*, 36:104–120, 2014.

[41] ASTM 1820-11. Standard test method for measurement of fracture toughness. Technical report, American Society for Testing and Materials, Philadelphia, 2011.

[42] E. Castillo, M. López-Aenlle, A. Ramos, A. Fernández-Canteli, R. Kieselbach, and V. Esslinger. Specimen length effect on parameter estimation in modelling fatigue strength by weibull distribution. *Int J Fatigue*, 28(9):1047 – 1058, 2006.

[43] K. Wallin. The size effect in K_{IC} results. *Eng Fract Mech*, 19:1085–1093, 1984.
[44] S. Cicero, T. García, V. Madrazo, I.A. Carrascal, and E. Ruiz. Analysis of notch effect in load bearing capacity, apparent fracture toughness and fracture micromechanisms of ferritic–pearlitic steels. *Eng Fail Anal*, 44:250 – 271, 2014.
[45] M. Muñiz-Calvente, V. N. Shlyannikov, T. Meshii, W. Giner, and A. Fernández-Canteli. Joint evaluation of fracture results from distinct test conditions, implying loading, specimen size and geometry. pages 720–727, Catania (Italy), 20–24 June 2016. XXI European Conference on Fracture, Procedia Engineering.