Measurement uncertainty of plane-strain fracture toughness K_{IC} testing by the Monte Carlo Method

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Daniel Antonio Kapper Fabricio
http://orcid.org/0000-0001-6365-8625
Professor
Instituto Federal de Santa Catarina – IFSC
Campus Chapecó – Santa Catarina – Brasil
Doutorando
Universidade Federal do Rio Grande do Sul – UFRGS
Programa de Pós-Graduação em Engenharia de Minas, Metalúrgica e de Materiais
Porto Alegre – Rio Grande do Sul – Brasil
daniel.fabricio@ifsc.edu.br, danielkapper@gmail.com

Lisiane Trevisan
Professora
Instituto Federal de Educação, Ciência e Tecnologia do Rio Grande do Sul – IFRS
Campus Farroupilha – Rio Grande do Sul – Brasil
Doutora
Universidade Federal do Rio Grande do Sul – UFRGS
Programa de Pós-Graduação em Engenharia de Minas, Metalúrgica e de Materiais
Porto Alegre – Rio Grande do Sul - Brasil
lisiane.trevisan@farroupilha.ifrs.edu.br

Afonso Reguly
Professor-Titular
Universidade Federal do Rio Grande do Sul – UFRGS
Programa de Pós-Graduação em Engenharia de Minas, Metalúrgica e de Materiais
Porto Alegre – Rio Grande do Sul – Brasil
reguly@ufrgs.br

Carla Schwengber ten Caten
Professor-Associado
Universidade Federal do Rio Grande do Sul – UFRGS
Programa de Pós-Graduação em Engenharia de Produção
Porto Alegre – Rio Grande do Sul – Brasil
tencaten@producao.ufrgs.br

Abstract

The reliable determination of materials' mechanical properties is a fundamental factor for their application in engineering, and the estimation of the measurement uncertainty in testing laboratories has a direct impact on the interpretation of the results. Recent literature demonstrates that one of the most widely used methodologies for uncertainty estimation, the Guide to the Expression of Uncertainty in Measurement (GUM), has limitations, especially in cases where the mathematical model has a high degree of non-linearity. Furthermore, it makes approximations for the final probability distribution. In these cases, it is recommended that the measurement uncertainty is determined by the Monte Carlo Method (MCM), which considers the propagation of the distribution rather than the propagation of uncertainties. Thus, given the limitations of the GUM method and the importance of estimating the measurement uncertainty of mechanical tests, this work aims to implement the measurement uncertainty estimation for the plane-strain fracture toughness (K_{IC}) test of metallic materials through the Monte Carlo Method. The results of the work confirm the importance of estimating the measurement uncertainty of fracture toughness tests.

Keywords: Monte Carlo, measurement uncertainty, plane-strain fracture toughness K_{IC}.

1. Introduction

The correct expression of measurement uncertainty by test laboratories is considered to be a fundamental factor, since it has a direct impact on the interpretation of the results (Jornada, 2009), and is required by the ISO / IEC 17025 standard. The Guide to the Expression of Uncertainty in Measurement (GUM) is a document that establishes the criteria for calculation and expression of measurement uncertainty, considering the different influences of each parameter that composes the uncertainty value. For this estimation, it is necessary to describe the effect of each input quantity in relation to the measurand using sensitivity coefficients (partial derivatives of each uncertainty source in relation to the measurand) (JCGM, 2008a). For cases where the description of the mathematical function considering each source of uncertainty is difficult, it is recommended that measurement uncertainty be determined by other mathematical methods, such as the Monte Carlo Method (MCM). Supplement 1 of GUM shows each of the steps for determining measurement uncertainty by this method (JCGM, 2008b).

Fracture toughness tests evaluate the strength of the material in front of a crack. The goal of Fracture Mechanics is to determine if a defect will or not lead a component to catastrophic fracture at normal service tension, also allowing to determine the degree of safety of a cracked component (Anderson, 2005).

In metallurgical testing, it is import to obtain fracture toughness properties because increasingly the oil & gas industries require high performance materials. Therefore, for this application, it is indispensable to know the K_{IC} value of materials (Fabricio *et al.*, 2016).

One of the fields of Fracture Mechanics is the Linear-Elastic Fracture Mechanics (LEFM), used in situations where the fracture still occurs in the linear-elastic regime, presenting a limited amount of plastic deformation at the crack tip (Strohaecker, 2012). The most used parameter to evaluate the fracture toughness of metallic materials in the LEFM is the critical value of the stress intensity factor for the tensile mode of load application (plane-strain fracture toughness K_{IC}), which is an intrinsic property of the material. The K_{IC} can correlate the applied stress on the material with the type and size of the defect.

In order to obtain the K_{IC} value of the material from mechanical testing, a provisional value, named K_Q, is initially calculated as a function which depends on the span (S) between the external loading points on the three-point test specimens, the applied load (P_Q), the specimen thickness (B), the initial crack size (a) and f, a dimensionless function of a/W, where W represents the specimen width. This ratio is given in Equation 1, according to ASTM E399-12e3 standard (ASTM, 2012).

$$K_Q = S \frac{P_Q}{BW^{3/2}} f\left(\frac{a}{W}\right) \qquad \text{Equation 1}$$

The Guide to the Expression of Uncertainty in Measurement (GUM) calculates the measurement uncertainty associated to the measurand (Y) based on the uncertainty propagation approach of the input quantities (X_1, X_2, ..., X_N). Meanwhile, the basic idea of the Monte Carlo Method (MCM) is the propagation of distribution rather than the propagation of uncertainties.

The Monte Carlo Method can be described as a statistical method in which a random number sequence is used to perform a simulation (Gonçalves and Peixoto, 2015) or an artificial sampling method that numerically operates complex systems with independent input quantities (Bruni, 2008).

The steps for performing a Monte Carlo simulation include problem formulation, data collection, identification of the random variables to be simulated and their respective probability distributions, model formulation, model evaluation, and finally, the simulation (Gonçalves and Peixoto, 2015).

Jie (2011) describes the procedure of MCM in the following steps: (a) Select the number of Monte Carlo trials (M) to be made. (b) Generate M vectors, by sampling from the assigned probability density function (PDF) for the input quantities Xi. (c) For each such vector, form the corresponding measurement model of Y, obtaining M model values (output quantities). (d) Sort these M output quantities into strictly increasing order, to provide G. (e) Use G to form an estimate y of Y and the standard uncertainty u(y) associated with y. (f) Use G to form an appropriate coverage interval for Y, for a stipulated coverage probability α.

Literature presents several applications of MCM in the measurement uncertainty estimation. For example, it is used in the field of medicine, for perspiration measurement systems (Chen and Chen, 2016), diffusion tensor imaging (Zhu *et al.*, 2008), and in dimensional X-ray computed tomography (Hiller and Heindl, 2012). It is also used in mechanical and dimensional measurements, such as: gear measurement instruments (Kost *et al.*, 2015), dynamic coordinate measurements (Garcia *et al.*, 2013) and Brinell hardness testing (Leyi *et al.*, 2011). In the field of physics and electricity, applications are found for nonlinear physical laws (Vujisić *et al.*, 2011), for passive electrical circuits (Stanković *et al.*, 2011) and for conducted emission measurement (Kovačević *et al.*, 2011). In the field of chemistry, this method was used for the estimation of plutonium (Heasler *et al.*, 2006), in the determination of Pb content in herbs (Lam *et al.*, 2010) and in the measurement of nitrogen content in liquid fuel (Theodorou *et al.*, 2015). Other applications found are density measurement (Mondéjar *et al.*, 2011), hydrological data (Marton *et al.*, 2014) and digitized data processing (Locci *et al.*, 2002). Thus, this method is applicable in very different areas. MCM implementation in the field of mechanical testing is still limited, especially for Fracture Mechanics testing.

Some typical situations in which the GUM Supplement 1, which uses the Monte Carlo Method, is especially indicated for the uncertainty calculation are (JCGM, 2008b):

- The contributory uncertainties are not of approximately the same magnitude;
- It is difficult or inconvenient to provide the partial derivatives of the model, as needed by the law of propagation of uncertainty;
- The probability density function (PDF) for the output quantity is not a Gaussian distribution or a scaled and shifted t-distribution;
- An estimate of the output quantity and the associated standard uncertainty are approximately of the same magnitude (for example, for measured values close to zero);
- The models are arbitrarily complicated;
- The PDFs for the input quantities are asymmetric.

The Monte Carlo simulation is

easy to deploy and returns complete information about the probability distribution. However, it has some limitations: the simulation time can be long in some cases of greater complexity, the selection of PDFs for the input data can be difficult because of the inaccuracy of the data or a little understanding of the process. The accuracy of the numerical simulation depends on the quality of the random number generator (Herrador and González, 2004), but the majority of the commercial software packages are suitable for this application (Locci *et al.*, 2002).

In addition to the Monte Carlo Method being little applied for the calculation of the measurement uncertainty of mechanical tests, no application of the method was identified for the plane-strain fracture toughness K_{IC} test, as evidenced in a literature review in Science Direct and IEEEXplore databases, for works published between 1995 and 2016. Thus, the following research problem was stated: how to estimate the measurement uncertainty of the fracture toughness K_{IC} test through the Monte Carlo method?

Given the limitations of the GUM method, especially its restriction for measurement models with a high degree of non-linearity or complexity (as is the case of the K_{IC} test measurement model), this work has as its main goal to implement the calculation of measurement uncertainty for the plane-strain fracture toughness K_{IC} test through Monte Carlo simulation.

2. Material and method

Three point bend test specimens (SEB) of base material obtained from R350HT high-strength rails were tested, according to EN 13674-1 standard (EN, 2011). The specimens were obtained from three railroad segments, i.e., from three runs, named runs I, II and III, with three samples for each run, totaling nine test specimens.

The specimens were removed from the rail head indicated by EN 13674-1, as shown in Figure 1. The figure also shows a schematic drawing of the test specimen used (EN, 2011). Before being subjected to the pre-crack and test, the samples were cleaned and sanded on the surface to facilitate visualization of the crack. Sanding was carried out through increasing and sequential sandpapers with 80, 120, 220, 320, 400, 600 and 1200 grit.

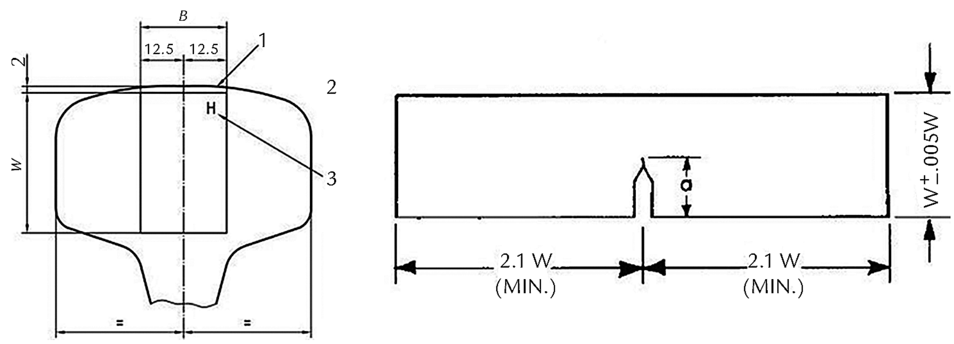

Figure 1
Section of fracture toughness test specimens and scaling (EN, 2011).

Test temperature was set to (-20 ± 1) °C, obtained through dry ice and alcohol and controlled by a thermocouple located in the test specimens. Tests were performed in a universal electromechanical test machine with a capacity of 250 kN. The fatigue pre-cracks were opened with a 200 kN servo-hydraulic test machine. Tests were performed based on standards EN 13674-1 (product standard) and ASTM E399 (test standard).

In order to calculate the measurement uncertainty using the Monte Carlo Method, a spreadsheet considering GUM Supplement 1 was built through Crystal Ball® software, applying the K_{IC} measurement model (Equation 1). According to Herrador and González (2004), Crystal Ball® is a user-friendly and customizable Excel add-in that easily enables Monte-Carlo simulations to be performed. Thus, using Crystal Ball® the value contained in an Excel cell can represent a random variable featured by its expected value (the value of the cell) and its assumed PDF (Normal, Uniform, Triangular, Lognormal, Weibull, Binomial, Poisson, etc.) together with a given dispersion measurement (standard deviation). For each parameter affecting the measurand, an Excel cell is built. The measurand value is computed in another Excel cell by applying the corresponding mathematical operations with the parameters cells. The measurand cell that contains the computed value is chosen as the forecast cell and the simulation is started once the number of trials M (and other features) is selected.

3. Results and discussion

A spreadsheet was implemented on Crystal Ball® software at a 95.45% coverage probability using 1,000,000 iterations for each simulation. From the K_Q measurement model (Equation 1), the uncertainty sources associated to the test were identified. Note that when the calculated K_Q value is valid, $K_Q = K_{IC}$ is assumed.

Input quantities S, B and W in Equation 1 are dimensional, and obtained from digital caliper measurement. The acceptance criterion of equipment calibration, which is considered as a source of uncertainty for these three variables, is ± 0.02 mm, according to normative standards for dimensional measurements. The form factor f(a/W) was considered, for purposes of calculation, as a constant of the material. Thus, any sources of uncertainty associated with this parameter were considered negligible. The input quantity P_Q represents a strength measure obtained from the load cell. For this equipment, the maximum acceptable error is 1% of the measured value, and this value is used as the source of uncertainty for this variable. Thus, the uncertainty sources to be considered in this work can be summarized according to Table 1.

Input quantity	Uncertainty source	Value	PDF
P_Q	Equipment acceptance criterion	$1\%P_Q$	Rectangular
W	Equipment acceptance criterion	0.02 mm	Rectangular
B	Equipment acceptance criterion	0.02 mm	Rectangular
S	Equipment acceptance criterion	0.02 mm	Rectangular
f(a/w)	None (considered constant)	-	-

Table 1
Uncertainty sources for K_{IC} test.

Sometimes, it is difficult to define the probability distribution function (PDF) associated to each uncertainty source. In this work, PDFs were considered as following a rectangular (uniform) distribution, which would be the most severe possible situation.

After the fracture toughness tests, the Monte Carlo simulations were performed on Crystal Ball®. Figure 2 presents the worksheet in the software, including the construction of scenarios within the program, and Figure 3 shows the simulation execution and the obtainment of the probability distribution of the output data.

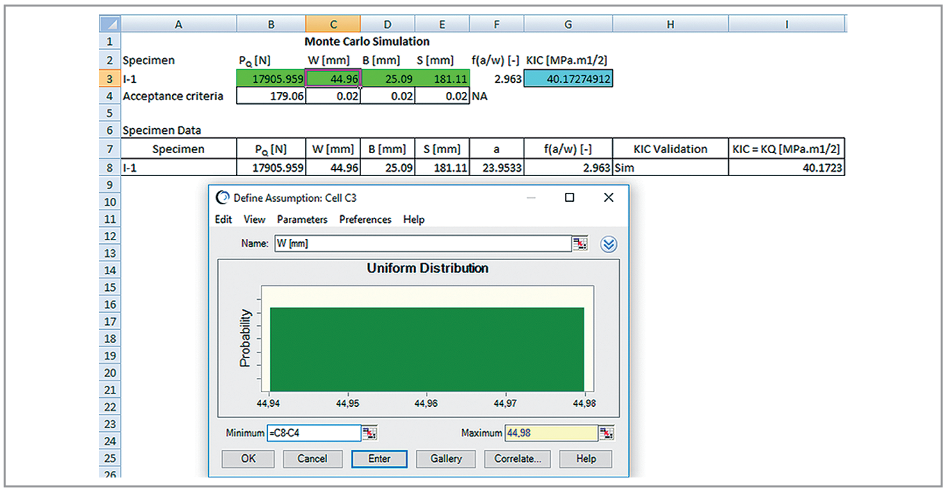

Figure 2
Scenario definition.

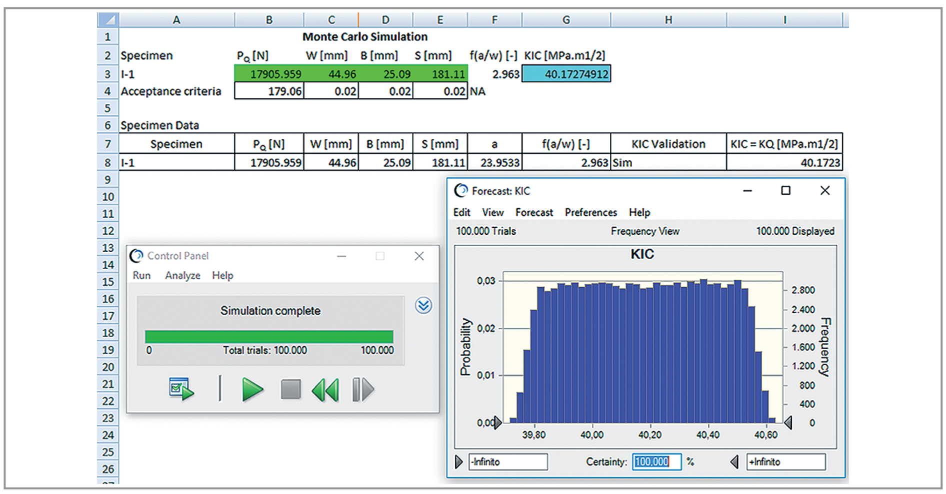

Figure 3
Simulation and output data.

Crystal Ball® allows obtaining the coverage interval through the required percentiles (in this case, 2.275% and 97.725%) for the measurement uncertainty calculation, but also allows obtaining many other statistical values, such as average, standard deviation, among others. From the percentiles obtained, the uncertainty can be calculated according to Equation 2.

$$U = \frac{Percentile_{97.725\%} - Percentile_{2.275\%}}{2} \qquad \text{Equation 2}$$

After applying the spreadsheets for each condition, measurement uncertainty values for the K_{IC} test were obtained. The calculated values for each test specimen and condition are shown in Table 2.

Number	Run	Sample	K_{IC} validation	$K_{IC} = K_Q$ [MPa.m$^{1/2}$]	Measurement uncertainty (U) [MPa.m$^{1/2}$]
1	I	I-1	Yes	40.1723	0.3878
2	I	I-2	Yes	41.8708	0.4046
3	I	I-3	Yes	42.2654	0.4082
4	II	II-1	Yes	33.3541	0.3221
5	II	II-2	Yes	34.0196	0.3286
6	II	II-3	Yes	32.6377	0.3151
7	III	III-1	Yes	33.3782	0.3224
8	III	III-2	Yes	33.1136	0.3199
9	III	III-3	Yes	34.1662	0.3298

Table 2
Plane-strain fracture toughness K_{IC} test results and measurement calculation.

As shown in Table 2, measurement uncertainty values are different among them. However, when the measured values are observed within the same run, the values seem close to each other, with a smaller standard deviation.

It is important to note that the calculated measurement uncertainty values are on the order of 1% of the K_{IC} values. There is no description of maximum/minimum uncertainty values accepted by the fracture toughness test standard, but it specifies an acceptance criterion for the material K_{IC}. For R350HT high-strength rails, the minimum acceptable K_{IC} is 30 MPa.m$^{1/2}$ (EN, 2011). The K_{IC} measured values were above this specification and, furthermore, since the measurement uncertainty values were small, no 'false positives' were generated in the interpretation of this specification. For several mechanical tests, such as Brinell hardness, Rockwell hardness and tension testing, a proportional value of measurement uncertainty at 1% is considerably accepted.

The metallic material studied is used in the manufacture of railway rails, and considering the cost required in replacing these rails, the monitoring of their service conditions is fundamental. When a crack occurs on a rail, it is not immediately replaced, but monitored until the crack reaches a critical size, which would be the maximum acceptable value of 'a' (Equation 1). Thus, when the crack reaches a critical size, the rail must be replaced. Cracks in rails do not necessarily mean the need for replacement, which leads to high costs.

4. Conclusions

This article demonstrated that the adaptation and use of the Monte Carlo Method to calculate the measurement uncertainty for the plane-strain fracture toughness K_{IC} test of metallic materials was efficient and important to overcome limitations of other methods for uncertainty estimation. The importance of MCM is emphasized because it is easy to associate the probability distribution of the different sources of uncertainty considered, and it is applicable for non-linear measurement models, such as K_{IC}.

As for the influence on the fracture, a high K_{IC} value means that a material with a previous defect (a crack) has a greater resistance to brittle fracture. The K_{IC} relates the size (a) and the type (Y) of the defect with the applied stress (σ). The K_{IC} is directly proportional to the form factor (i.e., the defect type) and the applied stress, and is directly proportional to the square root of the defect size, that is, $K = Y(\pi a)^{1/2}$. Thus, for a material with a given 'a' size defect, the larger the K_{IC}, the greater the stress the material supports before breaking. Or, for a material subjected to a given stress 'σ', the larger the K_{IC}, the larger the crack size the material will withstand before breaking.

The comparison of the values obtained by the Monte Carlo method with other mathematical methods used in the measurement uncertainty calculation is relevant. GUM or Kragten methods, for example, could be used for comparison between values.

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