A Probabilistic Approach to Update the Lower Bound Fracture Toughness using Surveillance Pressure Tube Data

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Abstract

The fitness for service assessment of pressure tubes requires demonstrating that there is sufficient margin against the rupture of the pressure tube. The CSA-Standard N285.8 specifies a lower bound fracture toughness (K_c,) for zirconium alloy that would provide adequate protection against fracture. A probabilistic approach to establish the lower bound of K_c is desirable, since it can account for variability associated with K_c a population of pressure tubes. The paper presents a probabilistic interpretation of lower bound K_c, which encompasses both aleatory and epistemic uncertainties. The paper proposes a new method to update the lower bound K_c, as new data become available from the testing of surveillance pressure tubes removed from any reactor. The main advantage of the proposed approach is that it provides a practical, risk-informed basis for fracture toughness assessment of the pressure tube.

1. Introduction

1.1 Background

The fracture toughness (K_c) of zirconium alloy is an important material property that provides protection against fracture of pressure tubes. It plays a key role in assuring the leak-before break in the event of through wall cracking of a pressure tube. The fracture toughness exhibits considerable variability in a population of pressure tubes due to changes in microstructure, texture, chemical impurities and the extent of irradiation. The variability in K_c is evident from fracture toughness data obtained through burst testing of samples taken from surveillance pressure tubes removed from various CANDU reactors over past several years [1].

In a deterministic assessment method, so long as fracture toughness values obtained from a surveillance pressure tube exceed a specified lower bound, the assessment is considered successful. The CSA Standard N285.8 [2] specifies deterministic the lower bound K_c as a function of the temperature:

$$K_c = \begin{cases} 27 + 0.30T & (T \le 150°\text{C}) \\ 72 & (T > 150°\text{C}) \end{cases} \text{ MPa}\sqrt{\text{m}} \quad (1)$$

A deterministic approach is somewhat restrictive, as it done not account for variability associated with K_c, which in principle should be modelled as a random variable. Therefore, the industry has been moving towards a probabilistic approach to establish a lower bound K_c. A probabilistic lower bound can be defined as a percentile in the lower tail of the distribution of K_c corresponding to a probability level ranging from 1% to 10%. The percentile level is selected based on industry's consensus about the performance and safety requirements.

1.2 Proposed Definition of the Probabilistic Lower Bound

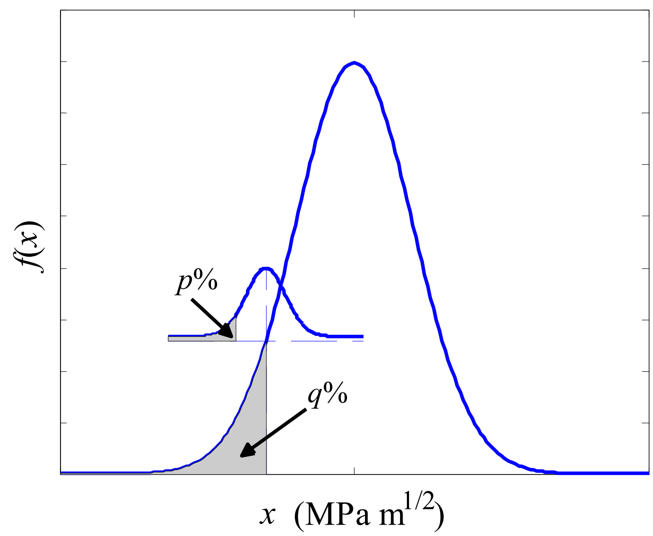


Figure 1: Proposed definition of the probabilistic lower bound of fracture toughness

The estimation of probabilistic lower bound has its own challenges. The reason is that typically a small sample of data is the basis for fitting the distribution function and computing its parameters, which introduces sampling (or epistemic) uncertainty. In other words, a sample estimate of a percentile value is also a random variable, so that lower bound should correspond to a high level of confidence.

In general, a lower bound can be defined as $X_{q|p}$, which is q^{th} percentile of X estimated at $(1\text{-}p)^{th}$ confidence level as shown in Figure 1. The fracture toughness in the population is expected to exceed the lower bound $X_{q|p}$ with probability $(1 - q)$. With reference to a sample estimate of lower bound, this is expected to be true with $(1 - p)$ probability. As a matter of illustration, we propose 5^{th} percentile ($q = 5\%$) of K_c at 95% confidence level ($p = 5\%$).

Because of sampling uncertainty associated with a lower bound estimate, a method is needed to update the confidence associated with it, as new data become available from the testing of surveillance pressure tubes removed from any reactor. Although new data are mostly expected to exceed the lower bound, there is a possibility that a few data points can be lower than the bound. It is reasonable, since a random variable can take any value in its entire range. Thus, a few low values of K_c would not invalidate the lower bound, though it would revise the confidence associated with it. The selected lower bund should be revised, only when the associated confidence level is severely eroded due to new observations,

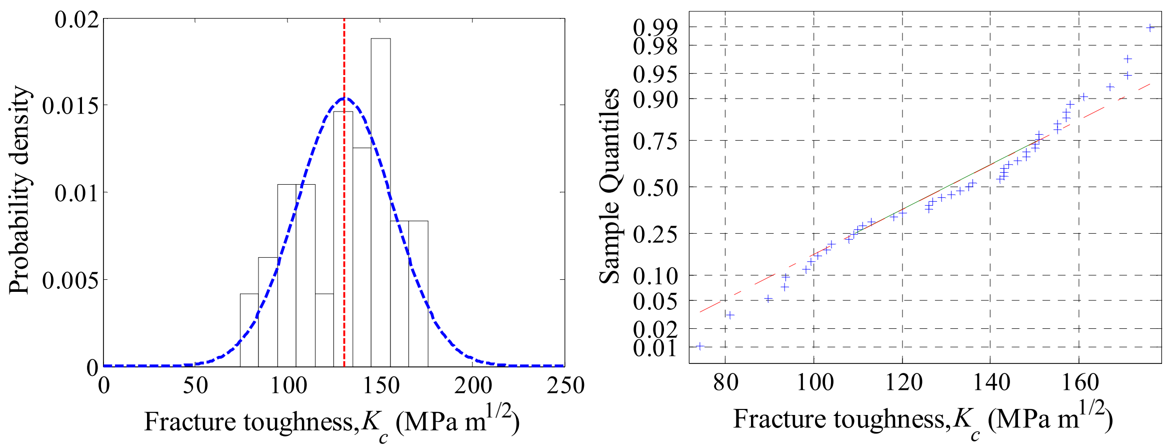
1.3 Research Objectives

The objectives of this papers are to (1) propose definition and estimation of the lower bound, (2) develop a Bayesian method to update the lower bound, and (3) evaluate sensitivity of the lower bound to potential new values of K_c.

The paper is organized as follows. The next Section summaries the proposed probabilistic approach. A case study based on a sample of K_c is presented in Section 3 to illustrate the proposed method. Conclusions of this study are presented in Section 4, and mathematical details of the formulation are given in the Appendix.

2. Probabilistic Model

2.1 Data



(a) Histogram of K_c data

(b) Normal probability paper plot

Figure 2: Illustration of a sample of fracture toughness data

For illustrative purposes, the paper utilizes a sample of 47 fracture toughness (K_c) values obtained from burst testing (at 250°C) of samples taken from irradiated pressure tubes (Pandey and Radford 2008). The sample ranges from 74 to 176 MPa√m with sample mean and sample standard deviation of 131 and 26 MPa√m, respectively (Figure 2a). The sample values are plotted on the Normal probability paper in Figure 2(b), which shows that the normal distribution provides a good fit to the data.

A probabilistic lower bound of K_c is defined in terms of q^{th} percentile of the distribution. Considering the normal distribution model for K_c, the 1%, 2.5% and 5% percentiles are computed as 70.5, 80 and 88.2 MPa√m, respectively. The deterministic lower bound 72 MPa√m specified in CSA N285.8 is 1.16% percentile of the distribution.

2.2 Basic Approach

The fracture toughness is treated as a random variable, *X*, which is normally distributed with the probability density function (PDF) given as

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{1}{2\sigma^2}(x-\mu)^2 \right] \tag{2}$$

A q^{th} percentile of the distribution, which can serve as a lower bound of K_c , is defined as

$$F(x_q) = P[X \le x_q \mid \mu, \sigma] = q \ \text{ or } \ x_q = F^{-1}(q) \tag{3}$$

where $F(x)$ denotes the cumulative distribution of *X*. If the mean (μ) and standard deviation (σ) of K_c were known precisely, the percentile value can be taken as a fixed (non-random) value. However, the crux of the problem is that sample estimates of μ and σ are affected by the sampling or epistemic uncertainty [3]. In other words, μ and σ should also be treated as random variables, such that the percentile value becomes a function of random variables. The distribution of the percentile value would provide a confidence measure.

2.3 Formulation

In the proposed model, the mean and variance of fracture toughness are treated as random variables and a method is developed to update the distribution using new data. The PDF of K_c (Eq. 2) is rewritten in terms of a new parameter called precision (τ), which is defined as the reciprocal of the variance, $\tau = (1/\sigma)^2$. Thus,

$$f(x) = \frac{\sqrt{\tau}}{\sqrt{2\pi}} \exp\left[-\frac{\tau}{2}(x-\mu)^2 \right] \tag{4}$$

Firstly, the precision is modeled as a gamma distributed variable as [4]

$$f(\tau) = \frac{\beta^\alpha}{\Gamma(\alpha)} \tau^{\alpha-1} \exp\left[-\beta\tau \right] \tag{5}$$

Note that α and β are distribution parameters. The PDF of the standard deviation (σ) can be derived from Eq. (5) as

$$f(\sigma) = \left| \frac{d\tau}{d\sigma} \right| f(\tau) = \frac{2\beta^\alpha}{\Gamma(\alpha)} (\sigma)^{-(2\alpha+1)} \exp\left(-\beta/\sigma^2 \right) \tag{6}$$

The expected value and variance of σ are given as

$$\mathrm{E}(\sigma) = \frac{\Gamma(\alpha - 1/2)}{\Gamma(\alpha)} \sqrt{\beta} \ \text{ and } \ \mathrm{VAR}(\sigma) = \frac{\beta}{\alpha - 1} - \left[\mathrm{E}(\sigma) \right]^2 \tag{7}$$

The conditional distribution of mean given the precision is modeled as normally distributed variable [4]:

$$f(\mu|\tau) = \frac{(\tau\lambda)^{1/2}}{\sqrt{2\pi}} \exp\left[-\frac{\tau\lambda}{2}(\mu-\theta)^2\right] \tag{8}$$

Here λ and θ are distribution parameters. The marginal distribution of the mean is obtained as

$$f(\mu) = \int_0^\infty f(\mu|\tau) f(\tau) d\tau = \frac{\sqrt{\lambda}\Gamma[\alpha+\tfrac{1}{2}]}{\sqrt{2\beta\pi}\Gamma(\alpha)}\left[1+\frac{(\mu-\theta)^2}{2\beta/\lambda}\right]^{-(2\alpha+1)/2} \tag{9}$$

Thus, μ follows a *t*-distribution with 2α degrees of freedom. The expectation and variance of μ are given as

$$\mathrm{E}(\mu) = \theta \text{ and } \mathrm{VAR}(\mu) = \frac{\beta}{(\alpha-1)\lambda} \tag{10}$$

The marginal distribution of X can be obtained by integrating the conditional distribution of X, Eq. (3), over the distributions of μ and τ in the following manner [5]:

$$f(x) = \iint_{\mu,\tau} f(x|\mu,\tau) f(\mu|\tau) f(\tau) \mathrm{d}\mu \mathrm{d}\tau \tag{11}$$

This leads to a *t*-distribution for X given as

$$f(x) = \frac{\sqrt{1+1/\lambda}\,\Gamma[\alpha+\tfrac{1}{2}]}{\sqrt{2\beta\pi}\Gamma(\alpha)}\left[1+\frac{(x-\theta)^2}{2\beta/(1+1/\lambda)}\right]^{-(2\alpha+1)/2} \tag{12}$$

The q^{th} percentile, X_q, is computed from mean and standard deviation as

$$X_q = \mu + k_q\sigma \text{ or } X_q = \mu + k_q/\sqrt{\tau} \tag{13}$$

where $k_q = \Phi^{-1}(q)$ is a q^{th} percentile of the standard normal distribution with denoted as $\Phi(\cdot)$. Since the joint distribution of μ and τ, $f(\mu,\tau) = f(\mu|\tau)f(\tau)$, is defined from Eqs. (5) and (8), a trick is to transform this into a new joint distribution in terms of the q^{th} percentile as $f(X_q,\tau)$. The transformation is based on Eq. (13) as $\mu = X_q - k_q/\sqrt{\tau}$, and the final result is obtained as

$$f(x_q,\tau) = \frac{\tau^{\alpha-\frac{1}{2}}}{c}\exp\left\{-\frac{\tau}{2}\left[2\beta+\lambda\left(x_q-\theta-k_q/\sqrt{\tau}\right)^2\right]\right\} \tag{14}$$

where

$$c = \sqrt{\frac{2}{\lambda}}\Gamma\left(\frac{1}{2}\right)\Gamma(\alpha)(\beta)^{-\alpha}$$

The marginal PDF of X_q can be computed by integrating out τ from Eq. (14). This completes the derivation of the distribution of a q^{th} percentile of the fracture toughness. A method based on Bayes' theorem to update these distributions is presented in Appendix A of the paper.

2.4 Illustration

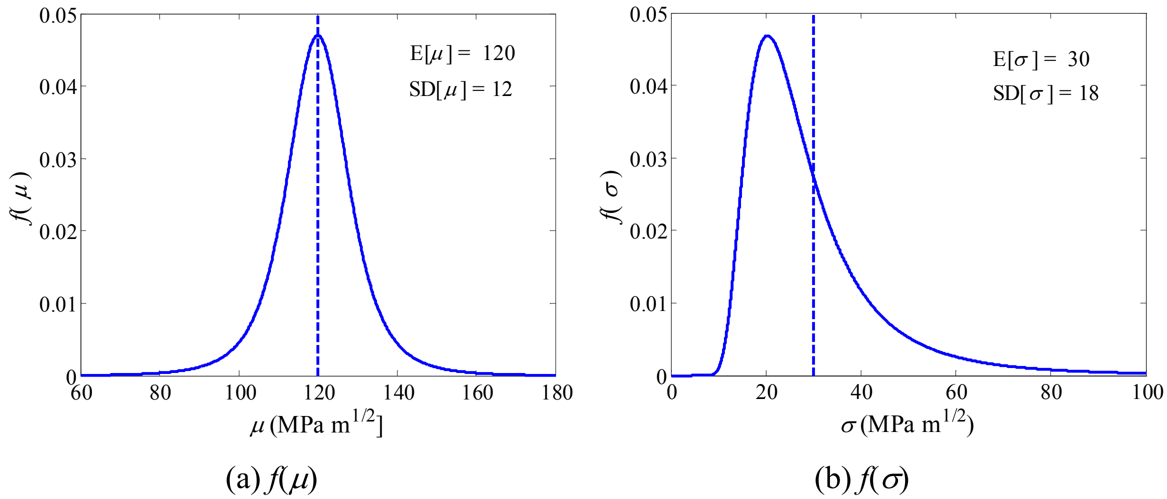


Figure 3: Prior distributions of mean (μ) and standard deviation (σ) of K_c

Formulation given in the previous section is illustrated here using the data described in Section 2.1. Firstly, we consider mean (μ) of the toughness as a random variable (Eq. 9). The average and coefficient of variation (COV) of the mean toughness are taken as E(μ) = 120 MPa√m and COV = 0.1. The standard deviation of K_c is also random (Eq. 6) with an average E(σ) = 30 MPa√m and COV = 0.6. Using this data, four parameters of the distributions of μ and σ are back calculated using Eqs. (7) and (10), and the results are: $\alpha = 1.77$, $\beta = 943.98$, $\theta = 120.0$ and $\lambda = 8.50$. Using these parameters, the prior distributions of μ and σ are plotted in Figure 3.

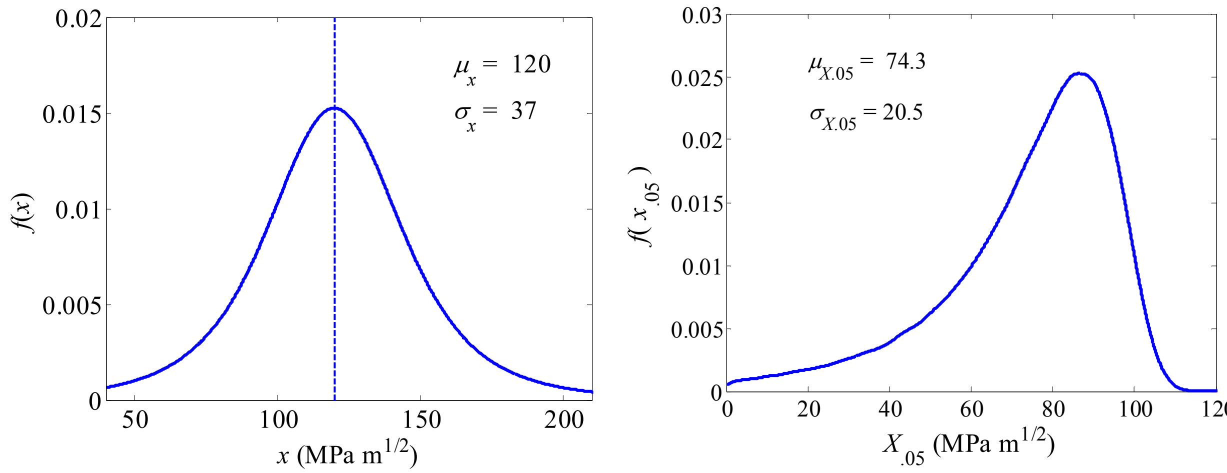


Figure4: Prior distributions of (a) K_c and (b) 5% percentile of K_c

The prior distribution of fracture toughness computed from Eq. (12) is plotted in Figure 4(a). The mean of X is the same as prior mean of 120 MPa√m, but its standard deviation (37 MPa√m) is higher due to uncertainty associated with μ and σ.

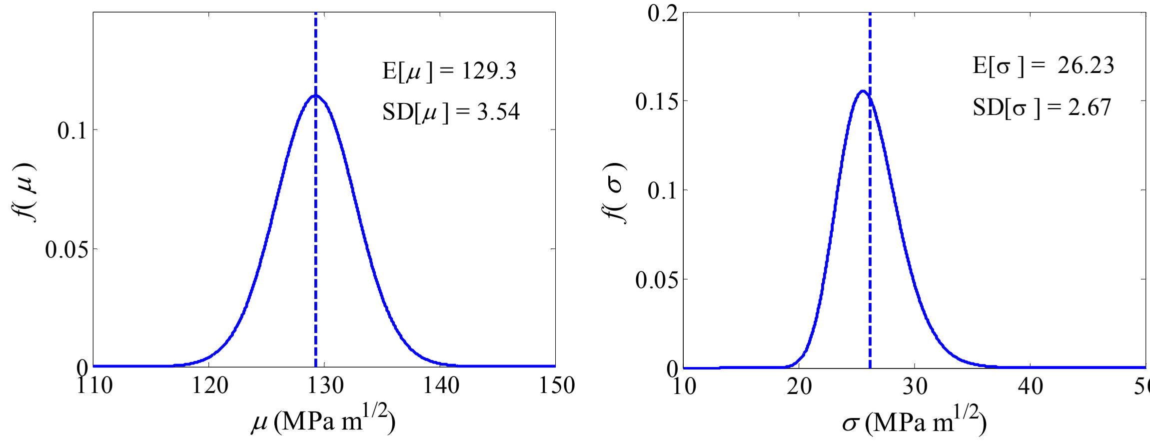
For the sake of illustration, the lower bound toughness is defined as q = 5% percentile of the distribution of X. Figure 4(b) shows the prior distribution of 5% percentile ($X_{.05}$) computed from Eq. (14). It is interesting to see that distribution of $X_{.05}$ is highly skewed with a mean of 74.3 and a large standard deviation of 20.5 MPa√m.

These prior distributions are somewhat tentative starting point of the analysis. They can be calibrated using the available data, as shown in the next section.

3. Case Study

3.1 Updating the Distribution of Fracture Toughness

The prior distributions of μ and σ are updated using a sample of 47 values of fracture toughness (Figure 1). The Bayesian updating method is described in Appendix. The updated parameters of the distributions of μ and σ are obtained as $\alpha' = \alpha + n/2 = 25.27$, $\lambda' = \lambda + n = 55.50$, $\theta' = \frac{1}{\lambda'}\left(\sum_{i=1}^{n} x_i + \lambda\theta\right) = 129.3$, and $\beta' = \beta + \frac{1}{2}\left(\sum_{i=1}^{n} x_i^2 + \lambda\theta^2 - \lambda'\theta'^2\right) = 16869.5$. The updated mean values are E[μ] =129.3 and E[σ] = 26.23 MPa√m, and updated standard deviations are SD[μ] = 3.54 and SD[σ] = 2.67.



(a) $f(\mu)$ (b) $f(\sigma)$

Figure 5: Posterior marginal distributions of (a) μ and (b) σ

Updated distributions of μ and σ are plotted in Figure 5. It is interesting to note that posterior of mean of μ has slightly increased to 129 from its prior value of 120 MPa√m, but its standard deviation (variability) has decreased significantly from 12 to 3.5 MPa√m. The posterior mean of σ has decreased slightly to 26 from 30, but its standard deviation is also reduced drastically to 2.67 from its prior value of 18 MPa√m. In summary, posterior distributions contain much less uncertainty than their prior counterparts.

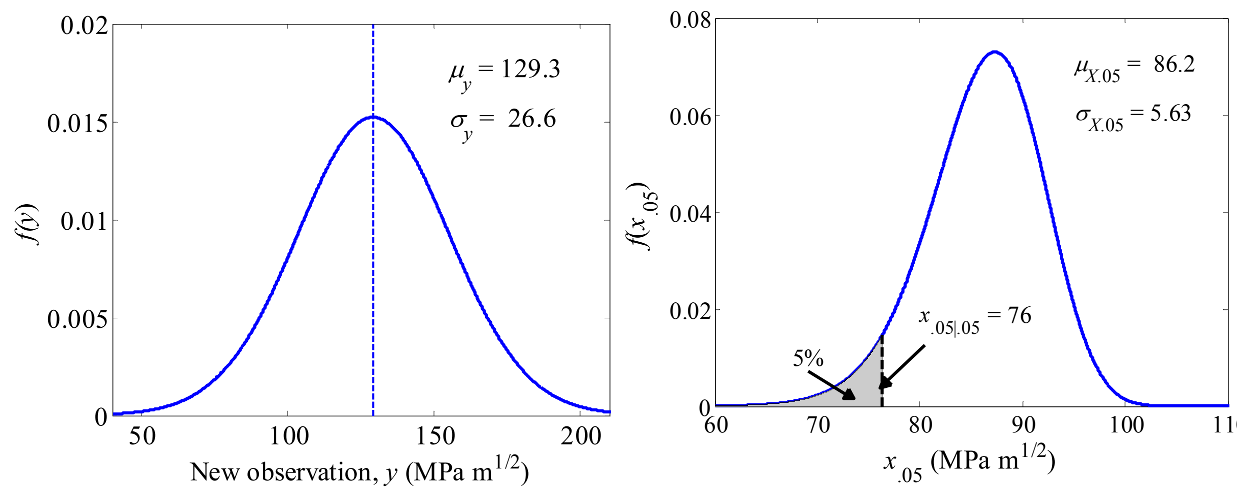


Figure 6: Posterior distributions (a) K_c and (b) 5% percentile of K_c

The posterior distribution of K_c is plotted in Figure 6(a), which also shows that the standard deviation is reduced to 26 MPa√m from 37 MPa√m. The deterministic lower bound value of 72 given in the code is equivalent to 98.7% of the distribution, that is, $\Pr[X_q < 72] = 1.3\%$.

Table 1: Illustration of different values of $X_{q|p}$

Percentile q %	Percentile Values $X_{q\|p}$ (MPa√m)				
	Confidence Level (1- p)%			Mean of X_q	SD of X_q
	2.5%	5%	10%		
2.5%	64	67	70	77.9	6.32
5%	74	76	79	86.2	5.64
10%	85	87	89	95.7	4.92

As a matter of illustration, probability distributions of q = 2.5%, 5% and 10% percentiles of K_c were derived and from these distributions, lower bounds corresponding to probability level of p = 2.5%, 5% and 10% were computed. These results in Table 1 basically show variation of of lower bound with respect to q and p. In this paper, 5% percentile at 5% probability (or 95%) confidence level), $X_{.05|.05}$ = 76 MPa√m, is proposed as an example of the lower bound. The probability distribution of this lower bound K_c is plotted in Figure 6(b).

3.2 Impact of New K_c Data on the Lower Bound

Suppose a of a surveillance pressure tube is removed from a reactor and through the burst testing the fracture toughness of sample at 250°C is measured as y MPa√m. Based on this observation, $(1\text{-}p)^{th}$ confidence level associated with the lower bound ($X_{.05}$ = 76 MPa√m) can be updated.

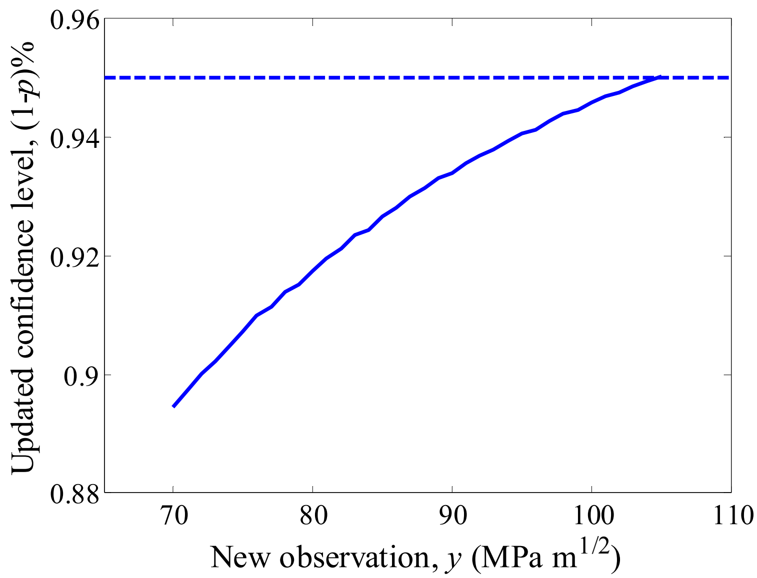


Figure7: Updated confidence level associated with the bound K_c

To illustrate these concepts, it is assumed that a single new value of fracture toughness (y) can vary from 70 to 105 MPa√m. Given one single value of y, the lower bound distribution was updated using the Bayesian method described in the paper. The revised probability (p%) level versus new K_c value is plotted in Figure 7, which shows that p increases slowly when y decreases from 105 to 70 MPa√m. It is interesting that even if a value of y = 70 MPa√m less than the lower bound were observed, the confidence level decreases slightly from 95% to 90%. This small decrease in the confidence level should not challenge the lower bound, and shall be updated as new data arrive in the future.

4. Conclusions

The paper presents a probabilistic approach to establish the lower bound fracture toughness considering both aleatory and epistemic uncertainties. The paper also presents anew Bayesian approach to update the confidence level associated with lower bound, as new data become available from the testing of a surveillance pressure tube. The basic idea is that a new test observation revises the confidence level associated with the lower bound, but it should not change the lower bound until the confidence level is significantly deteriorated.

The paper defines the lower bound fracture toughness as $x_{q|p}$, which is a q^{th} percentile of K_c at a (1- p)% confidence level. Using the available data for K_c measured at 250°C, the lower bound is proposed as $x_{05|.05}$, = 76 MPa√m as an illustration. It is 5th percentile of K_c with a 95% confidence. The impact of new fracture toughness data on the lower bound is further examined. It shows that the confidence level associated with the lower bound decrease slightly from 0.95 to 0.90 as a new value of new K_c varies from 105 to 70 MPa√m.

The proposed probabilistic approach is more versatile for fitness for service assessments than the deterministic method.

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5. References

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6. Appendix: Derivation of Bayesian Updating Method

6.1 General Concept

Bayesian analysis is a process of updating the distribution of a random variable X given new evidence in form of a sample of data, $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$. The probability distribution of X given the parameters ξ (a scalar or a vector quantity) is denoted as $f(x|\xi)$. The distribution parameter ξ is not known a priori and therefore it is treated as a random variable with a distribution, $f(\xi)$, also known as the prior distribution. Given a sample of data, the prior distribution can be updated using Bayes' theorem [6] as

$$f\left(\xi|\mathbf{x}\right) = \kappa f\left(\mathbf{x}\,|\,\xi\right) f\left(\xi\right) \tag{15}$$

where $f(\xi|\mathbf{x})$ is also referred to as posterior distribution. The likelihood of a sample given a parameter value is given by the joint density $f(\mathbf{x}\,|\,\xi)$; and $\kappa = [\int f(\mathbf{x}|\xi)f(\xi)]\mathrm{d}\xi]^{-1}$ is a normalizing constant. The updated distribution of X can be obtained using the posterior distribution of the parameter, $f(\xi|\mathbf{x})$ (Press, 1989):

$$f\left(x|\mathbf{x}\right) = \int_{\xi} f\left(x|\xi\right) f\left(\xi|\mathbf{x}\right) \mathrm{d}\xi \tag{16}$$

6.2 Analysis of the Proposed Model

For the normal-gamma model discussed in Section 2, the likelihood function of a sample of n fracture toughness values $\mathbf{x} = (x_1, x_2, \ldots x_n)^T$ is written as

$$f(\mathbf{x}\,|\,\mu,\tau) = \prod_{i=1}^{n} f\left(x_i|\mu,\tau\right) = \left(\frac{\tau}{2\pi}\right)^{n/2} \exp\left[-\frac{\tau}{2}\sum_{i=1}^{n}(x_i-\mu)^2\right] \tag{17}$$

By substituting the prior densities (Eqs. 5 and 8) and the likelihood function (Eq. 17) in Eq. 15 leads to the joint posterior density distribution of the distribution parameters as

$$f\left(\mu,\tau|\mathbf{x}\right) = \frac{(\beta')^{\alpha'}\sqrt{\lambda'}}{\Gamma\left(\alpha'\right)\sqrt{2\pi}} \tau^{\alpha'-1/2} \exp\left\{-\frac{\tau}{2}\left[2\beta' + \lambda'\left(\mu-\theta'\right)^2\right]\right\} \tag{18}$$

The updated parameters, denoted by prime (′) are obtained as

$$\alpha' = \alpha + n/2,\ \lambda' = \lambda + n,\ \theta' = \frac{1}{\lambda'}\left(\sum_{i=1}^{n} x_i + \lambda\theta\right),\ \text{and}\ \beta' = \beta + \frac{1}{2}\left(\sum_{i=1}^{n} x_i^2 + \lambda\theta^2 - \lambda'\theta'^2\right). \tag{19}$$

Note that updating is done by simply augmenting the sample information, because the prior distributions belong to a conjugate family. From this joint posterior distribution, the marginal posteriors of μ and σ can be derived, which are of the same form as those given in Eqs. (20) and (21):

$$f(\mu) = \frac{\sqrt{\lambda'}\Gamma[\alpha' + \tfrac{1}{2}]}{\sqrt{2\beta'\pi}\Gamma(\alpha')}\left[1 + \frac{(\mu - \theta')^2}{2\beta'/\lambda'}\right]^{-(2\alpha'+1)/2} \tag{20}$$

$$f(\sigma) = \frac{2\beta'}{\Gamma(\alpha')}(\sigma)^{-(2\alpha'+1)}\exp\left(-\beta'/\sigma^2\right) \tag{21}$$

The predictive distribution of X, as given by Eq. (16) again turns out to be the t-distribution with $2\alpha'$ degrees of freedom, mean of θ', and precision of $\sqrt{\alpha'/\beta'}\Big/\sqrt{1+1/\lambda'}$, i.e.

$$\frac{x - \theta'}{\sqrt{\beta'/\alpha'}\sqrt{1+1/\lambda'}} \sim t_{2\alpha'} \tag{22}$$

Finally, the updated distribution of the q^{th} percentile (X_q) can be obtained from Eq. (18) by replacing the distribution parameters by their posterior estimates.