THE ESTIMATION OF PROBABILITY VALUES FOR FRACTURE TOUGHNESS AFTER NEUTRON IRRADIATION

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ABSTRACT

The prediction of Fracture Toughness in the Ductile to Brittle transition region for irradiated material is a multi-stage process involving the estimation of start-of-life Fracture Toughness and Charpy Impact energy curve shift due to irradiation. The estimation of the uncertainty in Fracture Toughness after irradiation requires a framework for combining the uncertainties at each stage. This can only be achieved by determining probabilities from the analysis of the data at each stage. A three step strategy for obtaining these probabilities is described together with a procedure for combining them.

KEYWORDS

Fracture Toughness, Ductile to Brittle transition, neutron irradiation, Charpy Impact energy, probability model, Likelihood, Bayesian method, Monte Carlo Markov Chains.

INTRODUCTION

The assessment of the safety, against catastrophic failure, of reactor pressure vessels which experience neutron irradiation induced material property changes is usually based on an estimate of the start-of-life (SOL) fracture toughness in the ductile-to-brittle transition region and a dose dependent shift parameter to give end-of-life (EOL) values at a particular dose level. In many instances the effect of neutron irradiation dose on the properties of reactor steels has been monitored through Charpy impact energy measurements over a range of temperatures which encompass the ductile-to-brittle transition.

In order to provide an input to a deterministically argued safety case, both the SOL fracture toughness and the Charpy data are usually analysed to give best-estimate values and confidence limits. EOL best-estimate and limit predictions are then determined by a combination of the SOL and temperature shift from which only very pessimistic predictions of unquantifiable uncertainty can be made, although more precisely defined confidence limits are often claimed. This methodology does not provide the probability estimates for the EOL properties which are required for a Probabilistic Safety Assessment (PSA) and which would also better serve a deterministic argument.

The purposes of this paper are to describe a strategy which would provide EOL fracture toughness probability curves on the basis of SOL plus shift estimate; to identify the elements which are already in place and, by comparison, emphasize the inadequacy of the present procedure. The paper is structured firstly to describe the main stages in the methodology for producing predictions of the EOL curves at various probability levels and, secondly, to explain how data at each stage may be analysed to provide probability estimates which are the only quantities providing the mechanism for a rational combination of uncertainties.

METHODOLOGY FOR PREDICTION

The main features of the analytic process for developing fracture toughness predictions are shown in Fig. 1. The process and the attendant statistical needs can be summarised as follows:

i. measure and analyse SOL toughness data to provide a best-estimate curve fit and uncertainty estimates,

ii. show by experiment that it is reasonable to link a point on the SOL curve with a secondary property - in this case the Charpy Impact energy,

iii. measure Charpy data for a range of neutron doses and analyse the results at each dose to derive a Charpy curve and hence the T_{40J} value,

iv. obtain best-estimate ΔT_{40J} and uncertainty estimates,

v. analyse ΔT_{40J} in terms of dose to obtain a best-estimate fit and uncertainty estimates limits,

vi. apply this shift estimator to the SOL curve and generate the best-estimate and uncertainty limits for toughness curve at the appropriate dose (so-called end-of-life, EOL).

This is evidently a multi-stage process with each stage usually requiring an analysis of the data in terms of models which are described by more than one parameter. A key question here is whether the analytic approach and techniques used do provide a mechanism for linking uncertainties in multi-parameter, multi-stage processes. It should be noted that if the populations from which the data are sampled are non-symmetric then the usual route for representing uncertainty in terms of standard errors and confidence limits is inappropriate. This applies to an even greater degree where a combination of such quantities in a multi-stage, multi-parameter is used. These problems can only be overcome by making the objective of the analysis to be one of providing probability estimates at every stage eg at stage iv, the outcome should be a probability distribution for ΔT_{40J}. A general strategy to achieve this is described in the next section and its application is discussed in subsequent sections.

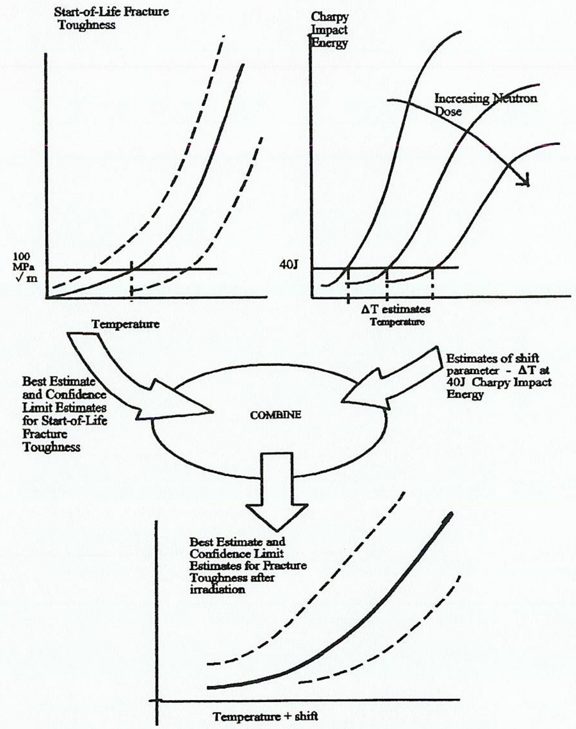

Fig. 1: Predicting Fracture Toughness after Irradiation

GENERAL ANALYTIC STRATEGY

A general strategy for the analysis of material property databases to produce probability distributions is provided by:

i. define probability model
ii. use method of Maximum Likelihood Estimation to determine best-estimates of model parameters and their precision
iii. derive parameter probability distributions using Bayesian concept and a suitable sampling algorithm

A clarification of each of these steps will now be given..

The Probability Model

For a complete probability model, the form of the distribution and the relationships linking the population characterising parameters, such as the mean and variance for a Normal distribution or the shape and scale for a Weibull, with the independent variables would be obtained from theoretical and/or experimental studies of the physical processes. Such a model is shown schematically in Fig. 2 ; the material property measurement is the dependent variable and temperature is the independent variable.

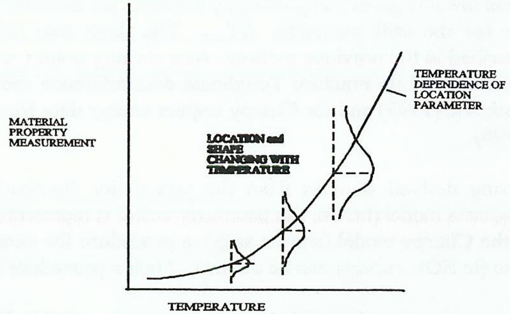

Fig.2: Schematic Probability Model

Note that these probability models are structured to include any understanding, or prior beliefs, about the physical mechanisms which underpin the data and often involve several fitting parameters, the values of which are determined in the data analysis. Having identified a probability model of this nature, the most appropriate tool for analysis uses the Likelihood Theory.

Maximum Likelihood Estimation

The likelihood function is algebraically the same as the joint probability density function (ie the probability of obtaining the set of experimental observations conditional on the value of the parameter vector) which can be defined for the measured material property values on the basis of the model and a parameter vector. It indicates the likelihood, given the data, of specified values of the unknown parameters, or parameter vector $\underline{\theta}$ (say), and it is represented in this paper by $l(\underline{\theta};data)$. Note that there is a shift of emphasis from a consideration of the experimental observations as being the unknown random quantity values to the model parameters being these unknowns with the set of observations fixed.

By varying the values for the model parameters a likelihood surface is constructed from which best-estimate values for the model parameters are identified at the maximum value of the likelihood. The precision in these values is determined from the shape of likelihood surface in the form of standard errors and, hence, confidence limits. It should be noted that such an analysis procedure can only indicate the range of possible values for the best-estimate position at the stated level of confidence and nothing more. The development of probability distributions uses the output of the Likelihood analysis in the procedure described in the next section.

Bayesian Probability Estimation

In the Likelihood theory approach, it is considered that there is only one 'true' value for each model parameter which is then estimated together with its precision. A Bayesian approach views the situation slightly differently but uses the same model formulation. In this, the set of parameters (or parameter vector $\underline{\theta}$) is the value of a random quantity, $\underline{\Theta}$, since the analysis of datasets from similar experiments is likely to produce a different set of values for the parameters ie a different parameter vector $\underline{\theta}$. The parameter vector $\underline{\theta}$ is a possible set of values which lie within the sample space $\underline{\Theta}$, it is one of a population of possible parameter vectors for which a probability estimate can be derived from the data analysis. Equivalently, the observations are considered to have been made on a family of curves each curve being uniquely defined by one set of model parameter values.

The purpose of the procedure is to identify these underlying populations of parameter values by generating samples from them using a Monte Carlo Markov Chain (MCMC) algorithm which is guided by the form of the Likelihood surface, refer to Smith and Roberts (1993) and Hastings (1970). This strategy is illustrated in a simplified form in Figs. 3 and 4.

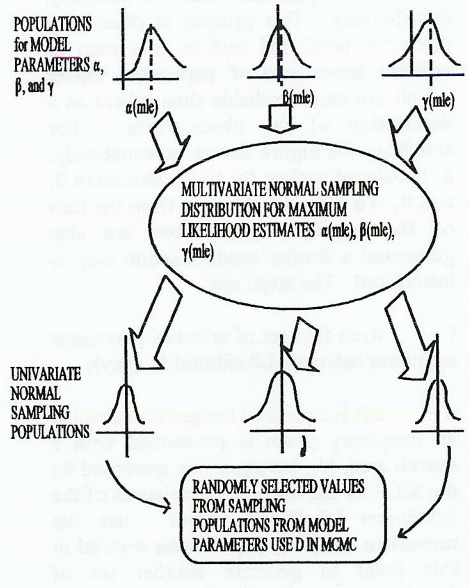

Fig. 3: Procedure to Identify MLE Sampling Distributions for MCMC Algorithm

Figure 3 illustrates diagrammatically the population of values for three parameters (unknown). Maximum Likelihood estimation provides a value from these distributions at, or near, the most probable value together with an indication of the precision with which this value is defined. This is the so-called 'standard error' which represents the width of the sampling distribution of Maximum Likelihood estimates. For a multi-parameter model, the sampling distribution is a multi-variate Normal which can be deconvoluted to separate Univariate Normal sampling distributions for the Maximum Likelihood estimate for each model parameter. These distributions are the starting points for the MCMC routine.

Figure 4 shows the method of generating parameter values which are drawn from the underlying populations (not the sampling distribution). This process is effectively using the likelihood surface as a map to indicate those sets of parameter values which are more probable than others as a description of the observations. For simplicity the Figure shows, schematically, a likelihood surface for two parameters θ_1 and θ_2. To ensure that values from the tails of the parameter populations are also generated a further randomisation step is introduced. The steps are:

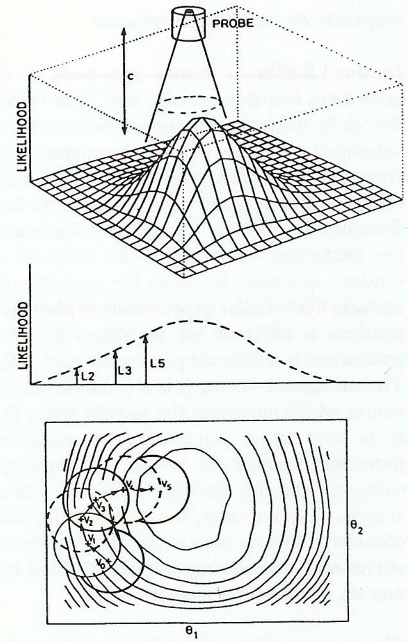

Fig. 4: Process for Generating Samples from Parameter Populations

i. from first set of selected parameter estimates calculate Likelihood L_1 (say);

ii. this is a point on the surface at which an imaginary probe is positioned with a search area, V_1, having a size governed by the MLE for the variance/covariances of the Maximum Likelihood values - use the univariate sampling populations centred at this point to generate another set of parameters;

iii. from second set calculate Likelihood and hence ratio of second to first, L_2/L_1;

iv. compare this ratio with random number chosen in range 0 to 1 and if the ratio is greater then accept second set of parameter values otherwise continue with first set;

v. having determined a second acceptable set, reposition the 'probe' at this location and generate a further set of parameter values from the search area, V_2, which give L_3 for the acceptance/rejection step;

vi. repetition of process generates values from the model parameter probability distributions - the secondary randomisation step described in iv. ensures that values from tails of the distributions are also accepted.

Essentially, this sampling algorithm is determining those values of the parameters which produce a fit between the model and the likelihood surface. Those values which give the better fits will be accepted more frequently than those which do not and hence the appropriate posterior probability density for each is identified. By this process any dataset can be analysed to produce a sample of parameter values generated from initially unidentified probability distributions.

PROBABILITY ESTIMATES FOR END-OF-LIFE TOUGHNESS

A strategy for the derivation of probability estimates for the toughness of irradiated pressure vessel metal requires that probability estimates are available for the start-of-life fracture toughness and for the shift parameter ΔT_{40J}. The three step procedure for obtaining these has been described in the previous section. As a starting point (ie the choice of a probability model) for the Start-of-Life Fracture Toughness data reference should be made to the Wallin (1991) and Moskovic (1993) and for Charpy Impact energy data from irradiated specimens refer to Windle (1996).

Having derived samples from the probability distributions for the parameters of the SOL toughness model (herein, this parameter vector is represented by $\underline{\theta}$) and from those for parameters of the Charpy model (shown as $\underline{\phi}$), a procedure for generating K_{IC} curves at a certain neutron dose (ie EOL curves) can be defined. Such a procedure is as follows:

i. take one value of the parameter vector, call this $\underline{\theta}^1$, for the SOL model from the sample, choose a temperature T_i and calculate K^1(SOL);using the model calculate the temperature, T_{100} (SOL), at which the shift reference point on the SOL curve (ie K_{IC}=100 MPa√m) is reached;

ii. using all the Charpy model parameter vectors, $\underline{\phi}$, together with a 40J Charpy Energy and an appropriate irradiation dose, generate the distribution for ΔT_{40J} and add this to T_i to produce the distribution of temperatures at which K^1(SOL) would be an EOL value;

iii. repeat i and ii for different $\underline{\theta}$ and collect together all the K values at the same temperatures;

iv. repeat steps i to iii for a range of T_i and hence generate populations of K_{IC}(EOL) for each T_i;

v. derive the required probability curves as those connecting the appropriate K_{IC}(EOL) distribution percentiles at each T_i, for example the 5% and 95% points.

CONCLUDING REMARKS

It is an essential requirement for the production of safety assessments for nuclear reactor pressure vessels, of both the deterministic and probabilistic type, that an estimate of the uncertainty in the Fracture Toughness in the Ductile to Brittle transition region, after irradiation, is available. This estimate can only be derived from a combination of the uncertainties obtained from the analysis of start-of-life Fracture Toughness and the analysis of a material property, in this case Charpy Impact energy, which changes with irradiation. Any strategy which attempts to combine uncertainties in the form of confidence limits or standard errors cannot provide a quantifiable estimate of the uncertainty or 'confidence' at the end of a multi-stage procedure. The only route is through the determination of real probabilities at each analytic stage.

A three step procedure to produce probability estimates which has general applicability to any material property database is:

i. define a probability model which incorporates any prior understanding of the physical processes or, if this is not possible, which is empirical;
ii. use the Likelihood theory approach to analyse the data on the basis of the probability model and, hence, obtain Maximum Likelihood Estimates of the model parameters and their standard errors;
iii. use the Bayesian approach and a Monte Carlo Markov Chain sampling algorithm to provide estimates of true probabilities.

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