# PROBABILISTIC MODELLING FOR THE QUANTIFICATION OF UNCERTAINTY IN FRACTURE DATA

P. L. Windle* and R. Moskovic†

A probabilistic model is described which consists of two distinct phases. An initial stage in which expert opinion identifies, on the basis of the prevailing understanding of the mechanisms, a model which can be used as an exploratory tool for data analysis and an explanatory tool for prediction. In the second phase a statistical method of data analysis, based on the model, is presented which produces probability estimates by adopting a Bayesian approach using a Markov Chain Monte Carlo sampling algorithm. The methodology is illustrated in an analysis of the effect of irradiation on a Charpy impact energy dataset.

## INTRODUCTION

The use of the probabilistic approach in support of structural integrity analysis is becoming a necessary feature in the safety assessment of structures. Current procedures adopted for the analysis of fracture data are unsatisfactory in the context of providing the inputs required for a probabilistic analysis since they usually produce an estimate of best-fit model parameters together with their standard errors and, sometimes, claim to have obtained a probability estimate for a particular material property value. The former information is not much use either in propagating uncertainty in a multi-parameter model or when underlying populations are not approximately symmetric and the latter is a misleading claim since the probability estimate is, in reality, conditional on the choice of parameter values used (ie the best-estimates). The provision of probability estimates requires the development of analytical methodologies which give predictions of probability distributions, as opposed to just confidence limits. This paper presents an approach to the analysis of fracture data which addresses the needs of the probabilistic assessment.

* Royal Naval College, Greenwich, London SE10 9NN
† Magnox Electric, BTC, Berkeley, Gloucestershire, GL13 9PB

The method is described in the next section and its use is illustrated in an application to the analysis of the effect of neutron irradiation on the Charpy impact properties of reactor pressure vessel steels.

## METHODOLOGY

For this method of analysis, it is postulated that the parameters characterising the fit between the data and an appropriate model are actually drawn from populations of possible values. A strategy is then adopted which derives information on these populations by interrogating the data using Bayes theorem. Bayes theorem, see Naylor and Smith (1), indicates that information concerning the probability distribution of a parameter subsequent to further data can be obtained from:

posterior probability distribution $\alpha$ Likelihood x prior distribution.

Likelihood is numerically the same as the joint probability of the obtaining the measured data given the model but it is viewed primarily as a function of the parameters conditional on the observations. The prior distribution is our knowledge of the parameter probability distributions before the further data became available which could be based on expert opinion and/or previous datasets.

The strategy is as follows:

(i) Formulate a model with components which have the mathematical form appropriate to describe the data, the physical processes linking these data and a probability distribution describing the spread. The full set of model parameters constitute a parameter vector $\mathbf{\Theta}$.

(ii) Using the probability distribution, write an expression for the probability associated with each observation , $C_i$, and hence for the joint probability, which is just the product of the individual probabilities, for all the data. This joint probability is equivalent to the Likelihood function for $\mathbf{\Theta}$, $\mathbf{L(\Theta;C_i)}$.

(iii) Use the procedure of Maximum Likelihood Estimation to obtain best estimates of the parameter values together with the covariance matrix for the sampling distribution of these estimates which can be shown to be a Multi-variate Normal (MVN). This set of model parameter values, $\mathbf{\Theta_0}$, and the associated Likelihood $\mathbf{L(\Theta_0;C_i)}$ act as a starting point for a Monte Carlo Markov Chain sampling procedure based on the Metropolis-Hastings algorithm developed by Metropolis et al. (2) and by Hastings (3).

(iv) From the MVN centred at $\mathbf{\Theta_0}$ randomly select a new parameter vector, $\mathbf{\Theta_1}$, and calculate $\mathbf{L(\Theta_1;C_i)}$. Then, on assuming a Uniform prior distribution, the posterior distribution is proportional to the Likelihood and the ratio of the values of the posterior distribution at $\mathbf{\Theta_0}$ and $\mathbf{\Theta_1}$ is the ratio of the Likelihoods.

(v) If this ratio is greater than a random number selected in the range 0 to 1 then accept $\Theta_1$ otherwise retain $\Theta_0$. Each accepted vector, which will be either the new value or the initial value, is the starting point for a repeat of step (iv).

(vi) The accepted $\Theta$s are samples from the posterior distributions of the model parameters from which probability estimates can be made.

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.

## APPLICATION

### Model Formulation

From Oldfield (4), it is known that the Charpy impact energy curve is sigmoidal. The effects of irradiation are a shift to higher temperatures, a tilt of the curve, a change of shape of the curve and a reduction in the upper shelf Charpy energy. These characteristics can be modelled by the Burr distribution function:

$$F(T_i) = [1 + \exp(-(T_i - T_0)/\xi)]^{-\nu} \tag{1}$$

with $T_i$ the test temperature, and $T_0$ is an offset parameter which locates the curve on the temperature axis.

The measured Charpy values are given by:

$$C_i = C_u\, F(T_i) + \text{random error} \tag{2}$$

In the absence of a theory-based error structure and to facilitate the illustration, the random error term is assumed to be Normally distributed with variance $\sigma^2$ but, to model the data variability which is a minimum on the upper and lower shelves and a maximum in the transition region, the variance is assumed to have a dependence on the test temperature of the following form:

$$\sigma = \sigma_1 + F(T_i)[1-F(T_i)]^{2 \cdot \sigma_2} \tag{3}$$

Neutron irradiation dose is included in the model through its effect on the parameter $T_0$ in a form which reflects an understanding of the physical processes of the mechanisms of irradiation damage as discussed by English et al. (5) ie:

$$T_0 = \gamma_0 + \gamma_1\sqrt{\text{dose}} \tag{4}$$

The full parameter vector is, therefore, $\Theta(\gamma_0, \gamma_1, C_u, \xi, \nu, \sigma)$ and the

Likelihood function has the form:

$$\prod_{i=1}^{n}\left(\frac{1}{\sqrt{2\pi\sigma^2}}\right)\ \exp\left(-\frac{C_i-C}{2\sigma^2}\right) \tag{5}$$

Using this together with the model described the sampling procedure produces the probability distribution for each of these parameters in the parameter vector.

Results and Predictions

The results of the sampling procedure is a set of estimates of the parameter vector from which the frequency distribution for each parameter can be marginalised to produce probability estimates. An example of the posterior density function thus provided is shown for the model parameter $\gamma_0$ in Figure 1; similar results are obtained for the other parameters. This set of parameter vector estimates is also used in conjunction with Equations (1) to (4) to generate a population of predicted Charpy energy values at any dose and test temperature of choice; an exampl of this is given in Figure 2. These populations then provide the basis for deriving predicted Charpy curves at 50%, 5%, and 95% probability levels for comparison with the measured data as shown in Figure 3.

It is also possible to obtain probability estimates for values of derived quantities. An important factor in the prediction of the effect of irradiation is a value for the shift in the location of the Charpy curve to higher temperatures as a result of a certain level of irradiation dose. One such estimator of this effect is the shift in the temperature at which a Charpy energy of 40J is reached ie $\Delta T_{40J}$ . Using the inverted form of model:

$$T_{40J} = T_0 - \xi \ln\left[\left(\frac{C_u}{40}\right)^{\frac{1}{v}} - 1\right] \tag{6}$$

and the model parameter samples, populations of $\Delta T_{40J}$ can be generated at any dose, as shown in Figure 4, from which a dose damage relationship for shift in $\Delta T_{40J}$ temperature as a function of $\sqrt{}$dose may be derived.

## CONCLUDING COMMENTS

A statistical methodology has been described which uses recent developments in the application of numerical methods within a Bayesian framework. An application to the analysis of the effect of irradiation on fracture properties has shown that the following can be attained:

1. a statistically rigorous quantification of all the uncertainties in the predictions

2. the provision of probability estimates for use in Probabilistic Risk Assesments.

## SYMBOLS USED

$C$ = predicted mean Charpy impact energy (J)
$C_i$ = measured Charpy impact energy
$C_u$ = upper shelf Charpy impact energy
$F(T_i)$ = Burr Distribution function
$T_i$ = test temperature
$T_0$ = offset parameter
$\xi$ = scale parameter
$\nu$ = shape parameter
$\gamma_0,\gamma_1$ = model parameters related to irradiation damage mechanisms
$\sigma,\sigma_1,\sigma_2$ = model parameters related to variance
$\boldsymbol{\Theta}_0,\boldsymbol{\Theta}_1,\ldots$ = parameter vector samples
$\mathbf{L}(\boldsymbol{\Theta}_0;\mathbf{C}_i)$ = Likelihood function evaluated at $\boldsymbol{\Theta}_0$

## REFERENCES

(1) Naylor J. C. and Smith A. F. M., Applied Statistics, Vol. 31, No. 3, 1982, pp. 214-225.

(2) Metropolis N., Rosenbluth A. W., Rosenbluth M. N., Teller A. H. and Teller E., Journal of Chemical Physics, Vol. 21, pp.1087-1091.

(3) Hastings W. K., Biometrika, Vol. 57, 1970, pp. 97-109.

(4) Oldfield W., JTEVA, Vol. 1, No. 6, 1979, pp. 326-333.

(5) English C. A., Fudge A. J., McElroy R. J., Phythian W. J., Buswell J. T., Bolton C. J. and Jones R. B., Int. J. Pressure Vessel and Piping, Vol.54, No. 49, 1993.

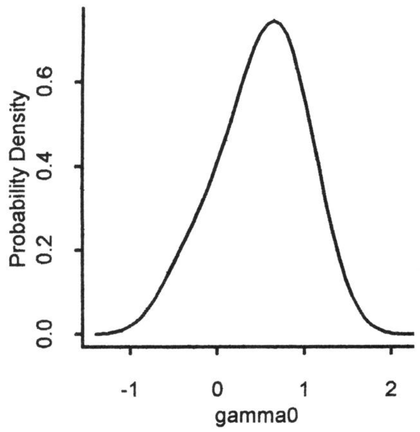


Figure 1 $\gamma_0$ Probability Distribution

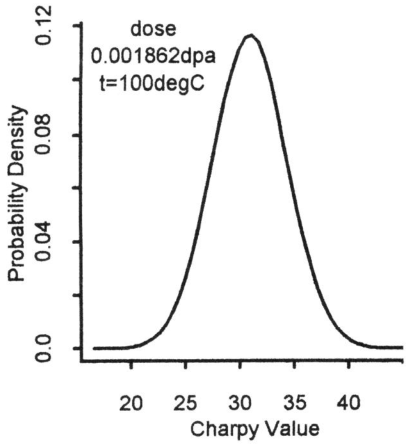


Figure 2 Charpy Values Probability Distribution

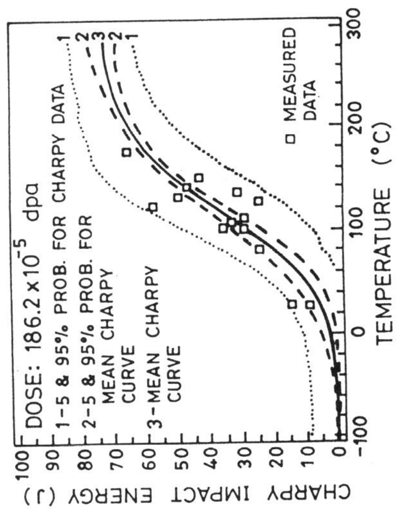


Figure 3 Predicted Charpy Curves and Observed Data

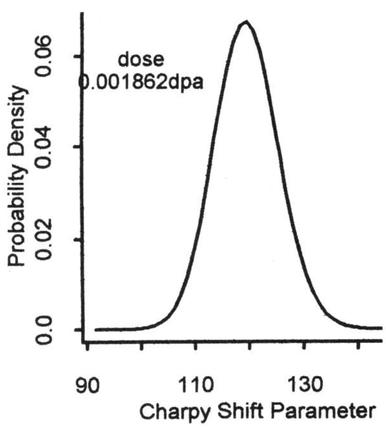


Figure 4 $\Delta T_{40J}$ Probability Distribution