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A frailty model for the analysis and prediction of creep and creep fracture: with application to high temperature plant life assessment using 1Cr–1Mo–0.25V

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Abstract This paper develops a modification of the shared frailty model that allows for the distribution of the response and the random effects to be determined by the data (from within the exponential family of distributions). A simulated maximum likelihood and a computationally simpler simulated linear least squares approach to estimating this model are also presented. These generalizations are important for modelling high-temperature deformation because they allow life time predictions to be made with levels of confidence attached to them, for the real world situation where repeated experimental observations are not normally distributed and not independent of each other. An application to a commonly used material in power generation revealed that ignoring these characteristics lead to an underestimate of the minimum safe life when operating at 773 K and stresses above 235 MPa.

Introduction

With many power plants within the UK approaching the end of their working lives, the accurate determination of a components safe life has again become an important topic. The published literate on failure analysis seems to have evolved in two main directions with little or no link up between them. This is especially true when looking at materials operating at elevated temperatures. On the one hand, there is a vast statistical literature on lifetime data analysis which reflects the fact that data on failure times tend to have a strong stochastic component—(see Nelson [1] for an excellent introduction and overview of this literature). However, the deterministic components of these statistical models are quite basic and often fail to resemble the models obtained through detailed scientific and engineering analysis of failure mechanisms—(Rabotnow [2]), Ion et al. [3] and Evans [4] are classic papers on deformation mechanisms at high temperatures). This paper can be seen as an attempt to bridge the gap between these two branches of study.

More recently Wilshire and Battenbough [5], in their reappraisal of copper, have provided new insights into the failure mechanisms governing high-temperature deformation. From this analysis, they derived a new parametric procedure for predicting the life of components operating at high temperatures which can be summarised in the equation

$$\left(\frac{\tau}{\tau_{\mathrm{TS}}}\right) = \exp\left\{-k_1\left[t_{\mathrm{f}}\exp\left(\frac{-Q_c^*}{RT}\right)\right]^{u_1}\right\} \tag{1a}$$

where t_{F} is the time to failure for a component operating at a stress τ and temperature T. R is the universal gas constant (= 8.314 J mol^{-1} K^{-1}), Q_C^* is the activation energy for self diffusion, τ_{TS} is the tensile strength of the material at temperature T and u_1 and k_1 are unknown constants. Wilshire [5] has never suggested any particular physical mechanism that could lead to Eq. 1a, except to emphasis the requirement that the functional form chosen must have the property that the failure time tends to infinity as τ/τ_{TS} tends to 0 and that the failure time tends to zero as τ/τ_{TS} tends to 1. Equation 1a has exactly this property, although there are many other functional forms that also have this property. As the failure time is the dependent variable, Eq. 1a can also be expressed in, perhaps, a less familiar form

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$$t_f = \exp\left[a_0 + a_1 \ln\{-\ln(\tau/\tau_{TS})\} + Q_c^*/RT\right] \quad (1b)$$

where $a_0 = -\ln(k_1)/u_1$ and $a_1 = 1/u_1$. In fact, the values for a_0 and a_1 are expected, from theories on the movement of dislocations, to be different above and below the yield stress. The model given by Eq. 1a has been successfully applied to a wide range of steel alloys (see Wilshire and Scharning [6–8]).

This model is markedly different in nature to the original parametric models which typically had a form similar to that proposed by Larson and Miller [9]

$$t_F = b_0 \exp\left(Q_c^*/RT + b_1\tau/T\right) \quad (1c)$$

where b_0 and b_1 are further unknown parameters.

Whilst this new methodology appears to be successful over a wide range of materials, none of the applications to date have been able to produce predictions with levels of confidence because emphasis has been placed on the deterministic component of high temperature deformation. Thus, on a second front Evans [10, 11] has developed a framework for incorporating a stochastic component into Eq. 1b that has enabled confidence limits to be derived. Whilst this study provided a suitable framework for modelling failure times that do not follow a normal distribution, the study was only a partial solution to the problem, because it did not fully take into account the nature of the existing data sets used to find values for the unknown parameters in Eq. 1b.

In particular, the databases available for estimating the models described above are very hierarchical in nature, with test specimens being cut from different batches (more generally referred to as units) of the same material. Consequently, observed material properties, such as failure times, within these databases will not be independent. Whilst estimation remains consistent in the presence of dependent test results, it will be less efficient than it could be. The test results, on average, will therefore tend to differ more from the true values than is appropriate and confidence intervals will therefore be under estimated. The size of this underestimation has never been quantified because all of the published literature involving the application of Eq. 1b to component life assessment at high temperatures has ignored this fundamental issue.

The aim of this paper is to provide a suitable statistical framework for Eq. 1b that will allow predictions to be made with confidence given the hierarchical nature of these data bases and given the long-tailed nature of the distributions for this data (Sect. Statistical models). A suitable estimation procedure for this framework is given in the Appendix to this paper (and the paper can be read without the need to reference this Appendix). This is followed, in Sect. "Application to component lifting at high temperatures", by a detailed application to one important material used in power generation, namely, 1Cr–1Mo–0.25V steel. The paper ends with a conclusion section that draws out the main findings from this research and suggests areas for future research.

Statistical models

Accelerated testing

A common approach to lifting materials that operate within harsh environments is to test specimens at condition in excess of their normal operating conditions, so inducing failures over relatively short time spans. The trick is then to develop a model capable of explaining this short-term data and then using it to extrapolate to the operating conditions, and in this way obtain an estimate of the safe working life for a material. In lifetime data analysis, there is a considerable body of work on model specification for analysing data of this nature.

A broad class of regression models for lifetime data

In log-location-scale models, the distribution for the time to failure (t_F) is explicitly stated. Specifically, log-location-scale regression models take the distribution for y (= $\log(t_F)$), given a vector of test conditions $\mathbf{x}$ (which, for example, could contain stresses and temperatures), to be of the form

$$S(y|\mathbf{x}) = S_0\left(\frac{y - \mu(\mathbf{x};\boldsymbol{\beta})}{\sigma}\right) = S_0(z) \quad (2a)$$

where $\mathbf{x}$ is a vector of test conditions, $S(y|\mathbf{x})$ is the survivor function of y at the test conditions given by $\mathbf{x}$ and $S_0(z)$ is a baseline survivor function, i.e. $S_0(z)$ is independent of $\mathbf{x}$. $\mu(\mathbf{x};\boldsymbol{\beta})$ is a function containing all the test conditions and a series of parameters (where p parameters are contained in the vector $\boldsymbol{\beta}$) whose values are unknown and σ is a further unknown parameter. The survivor function for y shows how the probability of surviving a length of time, measured in natural logarithmic units, varies with time. Another way to express this type of model is as

$$y = \mu(\mathbf{x};\boldsymbol{\beta}) + \boldsymbol{\sigma} z \quad (2b)$$

where z is a random variable with survivor function $S_0(z)$. The survivor function for t_F is then given by

$$S(t|\mathbf{x}) = S_0^*\left(\frac{t}{\phi(\mathbf{x})}\right)^{\delta} \quad (3)$$

where $\phi(\mathbf{x}) = \exp(\mu(\mathbf{x};\boldsymbol{\beta}))$, $\delta = b^{-1}$ and $S_0^*(t) = S_0(y)$. The general applicability of such a model stems from the fact

that as the test conditions change the shape of the distribution for t_F remains the same (i.e. it is the same distribution at all test conditions). The failure time distribution simply shifts with changing test conditions.

A major advantage of these log-location-scale regression models for making Eq. 1b stochastic is that it is of a form similar to many parametric models of high-temperature deformation derived from studying the failure mechanisms themselves. Theories of high temperature deformation are expressed in terms of how material properties, such as failure times and rates of deformation, vary with the test conditions. For example, in comparing Eq. 1c with Eq. 2b it is clear that

$$\mu(\mathbf{x};\boldsymbol{\beta}) = \ln(b_0) + b_1\frac{\tau}{T} + Q_c^*/RT \tag{4}$$

A proposed stochastic framework

However, for Eq. 2b to be suitable for modelling high-temperature deformation a number of generalisations are required. First, Eq. 2a should be replaced by

$$S(g(t;\alpha)|\mathbf{x}) = S_0\left(\frac{g(t;\alpha) - \mu(\mathbf{x};\boldsymbol{\beta})}{\sigma}\right) = S_0(z) \tag{5a}$$

where $g(t;\alpha)$ is a transformation of time to failure that depends on the value for the parameter α. The log-location-scale model is given by the special case $g(t,1) = \log(t)$, when, as suggested by Lawless [12],

$$g(t;\alpha) = (t^\alpha - 1)/\alpha. \tag{5b}$$

This generalisation will be referred to as a location-scale model. For the Wilshire model give by Eq. 1b, $\alpha = 1$ and

$$\mu(\mathbf{x};\boldsymbol{\beta}) = a_0 + a_1\ln\{-\ln(\tau/\tau_{TS})\} + Q_c^*\frac{1}{RT} \tag{5c}$$

where the a's are the parameters within $\boldsymbol{\beta}$ that are unknown in value and $\mathbf{x}$ is made of different transformed stress and temperature combinations, namely, $\ln(-\ln(\tau/\tau_{TS}))$ and $1/RT$.

Second, the distribution for z must be made explicit. As the existing knowledge on deformation mechanisms at high temperatures offers little in the way of identifying how the time to failure will be distributed, it is important to have a very general specification for the distribution of z. Only then is it possible to see which distribution, contained as a special case within this general specification, is actually supported by the data. One such general distribution, suggested by Bartlett and Kendall's [13], is the log gamma distribution. More recently, this distribution has been modified by Prentice [14] because in its original form the distribution had no limits. In this modification, the random variable z is taken to have the probability density function (PDF) given by

$$f(z) = \frac{\lambda^{k-0.5}}{\Gamma(\lambda)}\exp\left(\sqrt{\lambda}(z-c) - \lambda\exp\left[(z-c)\Big/\sqrt{\lambda}\right]\right) \tag{6a}$$

with

$$c = \sqrt{\lambda}\{\psi(\lambda) - \ln(\lambda)\} \tag{6b}$$

where $\psi(\lambda)$ and $\psi'(\lambda)$ are the di gamma and tri gamma functions, respectively. Abromowitz and Stegan [15] showed that these functions can be approximated by

$$\begin{aligned}\psi(\lambda) &= \ln(\lambda) - \frac{1}{2\lambda} - \frac{1}{12\lambda^2} + \frac{1}{120\lambda^4} - \frac{1}{252\lambda^6};\\ \psi'(\lambda) &= \frac{1}{\lambda} + \frac{1}{2\lambda^2} + \frac{1}{6\lambda^3} - \frac{1}{30\lambda^5} + \frac{1}{42\lambda^7}\end{aligned} \tag{6c}$$

where $\Gamma(\lambda)$ is the gamma function. Prentice has shown that when the parameter $\lambda = 1$, z has an extreme value distributions. However, when $\lambda = \infty$, z has a normal distributions. Further, when $\lambda = 1$ and $\sigma = 1$ z has an exponential distribution. The gamma distribution is also a special case. Hence, the specification given by Eq. 6a allows for many of the distributions contained within the exponential family of distributions. Within this generalisation, the mean and variance for z are given by

$$E[z] = 0 \quad \text{and} \quad \mathrm{Var}[z] = \sigma^2\lambda\psi'(\lambda) \tag{6d}$$

As λ tends to infinity, $\lambda\,\psi'(\lambda)$ tends to unity and $\psi(\lambda)$ tends to $\ln(\lambda)$. Consequently, z then follows a normal distribution whose mean is zero and whose variance is equal to σ.

Third, the location-scale model needs to be amended so that it can cope with hierarchical data sets. A common approach to the specification of such a model is through random effects. It is important to realise that such models have a very wide sphere of applicability and are, therefore, known by different names in the academic literature. In the social sciences they are known as multilevel models (see Goldstien [16] for a review), in the statistical and econometrics literature as random effect models (see for example Laird and Ware [17] and Lindstrom and Bates [18] and Maddalla et al. [19]) and in the lifetime data analysis literature as shared frailty models (see Hougaard [20] for an excellent review).

Expressed as a location-scale model, the shared frailty model takes the form

$$g(t;\alpha_{ij}) = \mu(\mathbf{x};\boldsymbol{\beta}_j) + \sigma z_{ij} \tag{7a}$$

where the subscript ij on the response refers to the transformed failure time of the ith test specimen contained within the jth unit or batch of material. The vector of parameters, $\boldsymbol{\beta}_j$, in $\mu(\mathbf{x};\boldsymbol{\beta}_j)$ vary randomly between the units so that

$$\boldsymbol{\beta}_j = \boldsymbol{\beta} + \mathbf{u}_j \tag{7b}$$

where $\mathbf{u}_j$ now follows a joint distribution with a mean vector of zero and a covariance matrix given by $\mathbf{D}$, with the

z_{ij} being independent of the $\mathbf{u}_j$. The final step is then to specify a joint distribution for $\mathbf{u}_j$. To keep consistency with the specification given to z_{ij}, this will be taken to be the joint version of the log gamma distribution given in Eq. 6a. That is

$$f(v_{kj}) = \frac{\lambda^{k-0.5}}{\Gamma(\lambda)} \exp\left(\sqrt{\lambda}(v_{kj} - c) - \lambda \exp\left[\left(v_{kj} - c\right)\Big/\sqrt{\lambda}\right]\right) \tag{8a}$$

where v_{kj} is the standardised value for u_{kj}, i.e.

$$\begin{aligned} v_{kj} &= \frac{u_{kj}}{\sigma_k^*} && \text{if } k = 0 \\ v_{kj} &= \frac{u_{kj}}{\sigma_k^*} - \frac{\sigma^*_{(k-r)k}}{\sigma_k^*} \sum_{r=1}^{k} v_{(k-r)j} && \text{otherwise} \end{aligned} \tag{8b}$$

and $\sigma^*_{(k-r)k}$ and σ_k^* are further parameters whose values are unknown. The relationship between the random vector $\mathbf{u}_j$ and its standardised equivalent, $\mathbf{v}_j$, is therefore given by $\mathbf{u}_j = \mathbf{\Lambda}\mathbf{v}_j$, where $\mathbf{\Lambda}$ is a lower triangular matrix made up of the above σ_k^* and $\sigma^*_{(k-r)k}$ parameters

$$\mathbf{\Lambda} = \begin{bmatrix} \sigma_0^* & 0 & 0 & \cdots & 0 \\ \sigma_{01}^* & \sigma_1^* & 0 & \cdots & 0 \\ \sigma_{02}^* & \sigma_{12}^* & \sigma_2^* & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \sigma_{0p}^* & \sigma_{1p}^* & \sigma_{2p}^* & \cdots & \sigma_p^* \end{bmatrix} \tag{8c}$$

The full variance–covariance matrix for $\mathbf{u}_j$ is then found by letting $\mathbf{\Lambda}\mathbf{\Lambda}' = \mathbf{\Omega}$, so that the variance–covariance matrix for any value of λ is given by

$$\mathbf{D} = \Omega(\lambda\psi'(\lambda)) = \begin{bmatrix} \sigma_0^2 & & & & \\ \sigma_{01} & \sigma_1^2 & & & \\ \sigma_{02} & \sigma_{12} & \sigma_2^2 & & \\ \vdots & \vdots & \vdots & \ddots & \\ \sigma_{0p} & \sigma_{1p} & \sigma_{2p} & \cdots & \sigma_p^2 \end{bmatrix} (\lambda\psi'(\lambda)) \tag{8d}$$

When λ is infinity, $\lambda\ \psi'(\lambda) = 1$, and so then $\mathbf{\Omega}$ is the variance–covariance matrix for $\mathbf{u}_j$, where the terms off the diagonal are the covariance's and the terms on the diagonal are the variances. More generally, i.e. for any other value for λ, $\mathbf{D}$ will be the variance–covariance matrix.

Application to component lifting at high temperatures

The experimental data

In this paper, the above shared frailty model is applied to a steel alloy typically used in power generation, namely, 1Cr–1Mo–0.25V. The databases available for estimating models of this nature are very hierarchical in nature, with test specimens being cut from different batches of the same material. These batches differ slightly in the types of heat treatment and chemical compositions (but all the compositions are within the specification defining this steel alloy) and the batch to batch variation is a very large component of the total variability present in the recorded times to failure. Figure 1 shows the structure of the data base for 1Cr–1Mo–0.25V steel. This data base was obtained and published by the National Institute for Materials Science, Japan (NIMS, [21]) in their data sheet No. 9B. Details of heat treatment and chemical compositions can be found in [21]. In Fig. 1, only the first and last few results are shown for each batch, and the data base is sorted by batch then by temperature and finally by stress to give an impression of the nature of this data base. Notice that there are $m = 9$ batches, and the number of specimens in each batch is variable. In total, some 243 specimens were tested over eight different temperatures and over a wide range of different stresses with the resulting failure times varying from just a few hours through to over 100,000 h.

The Wilshire–Scharning parametric model as a frailty model

To the best of our knowledge, the clustering structure that is clearly present in high-temperature deformation data bases, of which [21] is typical, has never been taken into account during the growing number of applications of Eqs. 1a, b. Consequently, all the estimated models in the literature are subject to the biases and inefficiencies briefly described in the introduction section, and this is further elaborated on within the Appendix to this paper. The parametric model given by Eq. 1b can be expressed as a shared frailty model in the following way

$$g(t;1)_{ij} = \ln(t_F)_{ij} = y_{ij} \tag{9a}$$

and

$$\mu(\mathbf{x};\boldsymbol{\beta}_j) = \beta_{0j} + \beta_{1j}x_{1ij} + \beta_{2j}x_{2ij} + \beta_{3j}x_{3ij} \tag{9b}$$

where

$$x_{1ij} = \max[0, \ln(-\ln(\tau/[\tau_{TS}])_{ij} - \tau_0];$$
$$x_2^T = \max[0, \tau_0 - \ln(-\ln(\tau/[\tau_{TS}])_{ij}]; \quad x_{3ij} = \left[\frac{1000}{RT_{ij}}\right]$$

and where $(t_F)_{ij}$ is the time at which specimen i cut from batch j fails, $(\tau/\tau_{TS})_{ij}$ is the normalised stress of the ijth specimen, R is the universal gas constant (8.314 J mol^{-1} K^{-1}), T_{ij} the temperature to which the ijth specimen is subjected to and and τ_0 is the yield stress. The max function allows $\mu(\mathbf{x};\boldsymbol{\beta}_j)$ to

Specimen, i	Batch, j	Stress, MPa	Temperature, K	Failure Time, h	
1	1	373	723	15484.7	$n_1 = 44$
2	1	412	723	3533.5	
43	1	47	948	1095.4	
44	1	98	948	136.2	
45	2	235	773	90473.9	$n_2 = 23$
46	2	265	773	21244	
66	2	98	923	448.8	
67	2	137	923	141.3	
68	3	265	773	49698.1	$n_3 = 25$
69	3	294	773	20397.4	
91	3	98	923	539.9	
92	3	137	923	127.4	
93	4	235	773	112223	$n_4 = 24$
94	4	265	773	47021.8	
115	4	98	923	702.3	
116	4	137	923	166.9	
117	5	235	773	152460.8	$n_5 = 23$
118	5	265	773	44440.8	
137	5	69	923	1950.7	
138	5	98	923	659.8	
139	5	137	923	174	
140	6	235	773	107663	$n_6 = 26$
141	6	265	773	97032	
164	6	98	923	696.2	
165	6	137	923	139.4	
166	7	235	773	107711	$n_7 = 24$
167	7	265	773	73217.8	
188	7	98	923	916	
189	7	137	923	233.2	
190	8	235	773	152237.8	$n_8 = 23$
191	8	265	773	42620.4	
211	8	98	923	784.3	
212	8	137	923	186.8	
213	9	235	773	112392	$n_9 = 22$
214	9	265	773	59986.5	
233	9	98	923	813.5	
234	9	137	923	198.1	

Fig. 1 The NIMS creep data base for lCr–lMo–0.25V steel

be different above and below the yield stress. Thus, when $\ln(-\ln(\tau/\tau_{TS}))_{ij} > t_0$, Eq. (9b) becomes

$$\mu(\mathbf{x};\boldsymbol{\beta}_j) = (\beta_{0j} - \beta_{1j}\tau_0) + \beta_{1j}\ln(-\ln(\tau/[\tau_{TS}])_{ij} + \beta_{3j}x_{3ij}$$

and when $\ln(-\ln(\tau/\tau_{TS}))_{ij} < t_0$, Eq. (9b) becomes

$$\mu(\mathbf{x};\boldsymbol{\beta}_j) = (\beta_{0j} + \beta_{2j}\tau_0) - \beta_{2j}\ln(-\ln(\tau/[\tau_{TS}])_{ij} + \beta_{3j}x_{3ij}$$

Bringing all this together gives

$$y_{ij} = (\beta_0 + u_{0j}) + (\beta_1 + u_{1j})x_{1ij} + (\beta_2 + u_{2j})x_{2ij} + (\beta_3 + u_{3j})x_{3ij} + \sigma z_{ij} \quad (9c)$$

where β_3 is an estimate of the activation energy for self diffusion, and z_{ij} follows the distribution given by Eq. 6a and the standardised values for the u_{kj} come from Eq. 8a–d.

Estimation of the Wilshire–Scharning parametric model

To demonstrate the predictive accuracy of this model, the data base described above was split into two parts. Equation 9c was then estimated from all those results where time to failure is 5,000 h or less. The estimated model is then used to predict the failure times in the remaining part of the data set. The Appendix to this paper shows the detail behind this estimation exercise, and it essentially involves using simulation and non linear optimisation algorithms to maximise Eq. 17 of the Appendix at a given value for λ. The parameters of Eq. 9c were estimated in this way using various values of λ, and Table 1 summarises the log likelihood values (as given by Eq. 17) associated with each of these λ values. It can be seen from this table that the mean log likelihood is maximised when $\lambda = 100$. Further, a 90% confidence interval for λ suggests that λ values below 3 are not supported by the data. The log normal distribution for t_F and the random effects, whilst not being rejected by the data, is not the most supported distribution at the 10% significance level. This suggests that it is best to use the generalised log gamma distribution (with $\lambda = 100$) to model the time to failure and the random effects, although any λ values between 3 and 200 are probably equally well supported by the data given the simulated nature of the log likelihood estimates.

Table 1 Variations of the mean log likelihood, given by Eq. 17, with λ

λ	Mean log likelihood, $\ln(L\|\mathbf{x};\mathbf{u}_j)$	χ_1
∞	−15.1506	2.25
1000	−14.9889	1.92
400	−14.9006	1.75
200	−14.4988	0.94
100	−14.0271	0
12	−14.5558	1.06
10	−14.0547	0.06
7	−14.4177	0.78
4	−13.3405	0.09
3	−14.4477	0.84
2	−15.3343	2.61#
1	−16.6308	5.21#
0.5	−19.8632	11.67#

χ_1 is twice the difference between the shown mean log likelihood and −14.0271. As such it follows a chi square distribution with one degree of freedom. Number of iterations $R = 150$

Statistically significant at the 10% level

Table 2 shows the simulated maximum likelihood (SML) estimates of the parameters in Eq. 9c for three different values of λ, including the λ value associated with the log normal distribution. All the parameters appear to be statistically significant at the 10% significance level. There is little difference between the parameter estimates associated with the log normal and generalised gamma distributions, but the estimates assuming a Weibull distribution are a little smaller. The estimate for the activation energy over all batches is around 252 kJ mol^{-1} (This is lower than the assumed value of 300 kJ mol^{-1} used by Whilshire and

Table 2 Simulated maximum likelihood estimates of the parameters in Eq. 9c

Parameters	Log normal distribution ($\lambda = \infty$)	Extreme value distribution ($\lambda = 1$)	General gamma distribution with ($\lambda = 100$)
β_0	$-28.6674^{\#}$ (0.2951)	$-27.7858^{\#}$ (0.4296)	$-28.6176^{\#}$ (0.3197)
β_1	$4.1109^{\#}$ (0.0346)	$4.0224^{\#}$ (0.0609)	$4.1051^{\#}$ (0.0396)
β_2	$-7.9821^{\#}$ (0.1126)	$-7.6166^{\#}$ (0.1442)	$-7.9613^{\#}$ (0.1199)
β_3	$252.6631^{\#}$ (2.1433)	$247.1061^{\#}$ (3.0364)	$252.3733^{\#}$ (2.3007)
σ	$0.2753^{\#}$ (0.0078)	$0.2433^{\#}$ (0.0098)	$0.2724^{\#}$ (0.0083)

Standard errors shown in parenthesis, Estimates obtained using $\tau_0 = -0.25$. Number of iterations $R = 150$

$^{\#}$ Parameters statistically significant at the 10% level

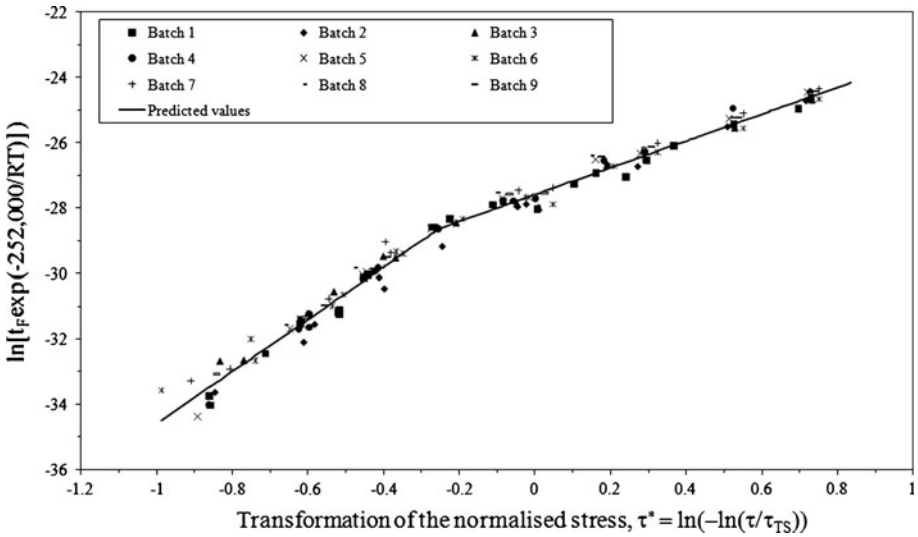

Fig. 2 Dependence of $\ln(t_F \exp(-Q_C/RT))$ on $\ln[-\ln(t/t_{TS})]$ for lCr–lMo–0.25V at 723–948 K with $Q_c = 252$ kJ mo1^{-1} and with $t_F < 5{,}000$ h

Scharning [7]) and may be explained by the fact that it is estimated from only part of the data set, i.e. from all those results where time to failure are 5,000 h or less).

In this estimated model, the low τ/τ_{TS} region is defined as any value for $\tau_0 < -0.25$ and high τ/τ_{TS} is defined any value for $\tau_0 > -0.25$. A unit change in x_1 brings forth a 4.11 unit change in log failure times in the low regions, but a 7.96 unit change in the high region. ($\tau_0 = -0.25$ approximately corresponds to the average yield stress of this material over the range of experimental temperatures). The 'kinked' nature of this model is more clearly seen in Fig. 2 where the $\ln(t_F) \; -252x_{3ij}$ is plotted against $\ln(-\ln(\tau/\tau_{TS}))$ to remove the effect of temperature. As can be seen from this figure, the model of Eq. 9c, with the parameter values shown in the last column of Table 2, predicts the shown failure times very well.

Table 3a to 3c shows the estimated variance covariance matrix, **D**, for the $\mathbf{u}_j$ in the shared frailty model for the three different λ values shown in Table 2. The variance for β_{2j} is an order of magnitude larger than the variance for β_{1j}, and this is shown in Fig. 2 as increased batch to batch variation when $\tau_0 < -0.25$. The largest batch to batch variation is for the estimated activation energy. As might be expected, the elements of **D** when $\lambda = \infty$ and when $\lambda = 100$ are very similar in size, but when $\lambda = 1$, the estimates for the elements of **D** become much larger.

Creep life prediction using the Wilshire–Scharning parametric model

In Fig. 3, Eq. 9c together with the values shown in the last column of Tables 2 and 3c are used to obtain predicted failure times at a temperature of 773 K. These were obtained using the simulation approach described in Sect. "Confidence intervals" of the Appendix. It is important to remember that the values shown in these tables were estimated from date up to 5,000 h only. Thus, the predictions beyond this time are in fact extrapolations rather than interpolations. The thicker lines shown in this figure are the predicted median times to failure and the 0.5 and 99.5% from the simulated distributions of times to failure derived at the shown stresses. Taken together, these predictions are a reasonable description of the experimental data—even out to over 100,000 h worth of failure times.

Table 3 Simulated maximum likelihood estimate of the variance–covariance matrix **D**

	$\sigma_0^2\{\lambda\psi'(\lambda)\}$	$\sigma_1^2\{\lambda\psi'(\lambda)\}$	$\sigma_2^2\{\lambda\psi'(\lambda)\}$	$\sigma_3^2\{\lambda\psi'(\lambda)\}$
(a) *When* $\lambda = \infty$ *(Log normal distribution for* t_F*)*				
$\sigma_0^2\{\lambda\psi'(\lambda)\}$	0.9843 (1.2030)	–	–	–
$\sigma_1^2\{\lambda\psi'(\lambda)\}$	−0.0968 (0.1500)	0.0282 (0.0275)	–	–
$\sigma_2^2\{\lambda\psi'(\lambda)\}$	0.1750 (0.3834)	0.0193 (0.0448)	0.2133 (0.1701)	–
$\sigma_3^2\{\lambda\psi'(\lambda)\}$	−6.9532 (8.5124)	0.6087 (1.0366)	−1.4564 (2.5410)	49.6120 (60.4525)
(b) *When* $\lambda = 1$ *(Weibull distribution for* t_F*)*				
$\sigma_0^2\{\lambda\psi'(\lambda)\}$	1.8729 (2.3881)	–	–	–
$\sigma_1^2\{\lambda\psi'(\lambda)\}$	−0.1786 (0.2552)	0.0339 (0.0364)	–	–
$\sigma_2^2\{\lambda\psi'(\lambda)\}$	0.3331 (0.6324)	0.0053 (0.0713)	0.3021 (0.2340)	–
$\sigma_3^2\{\lambda\psi'(\lambda)\}$	−13.2345 (16.9210)	1.1980 (1.7780)	−2.5957 (4.5282)	94.0251 (120.1191)
(c) *When* $\lambda = 100$ *(Generalised gamma distribution for* t_F*)*				
$\sigma_0^2\{\lambda\psi'(\lambda)\}$	1.3197 (2.1952)	–	–	–
$\sigma_1^2\{\lambda\psi'(\lambda)\}$	−0.1161 (0.2398)	0.0258 (0.0310)	–	–
$\sigma_2^2\{\lambda\psi'(\lambda)\}$	0.2459 (0.5369)	0.0136 (0.0583)	0.2531 (0.2050)	–
$\sigma_3^2\{\lambda\psi'(\lambda)\}$	−9.3747 (15.5391)	0.7608 (1.6831)	−1.9771 (3.8532)	67.0667 (110.1050)

Standard errors shown in parenthesis

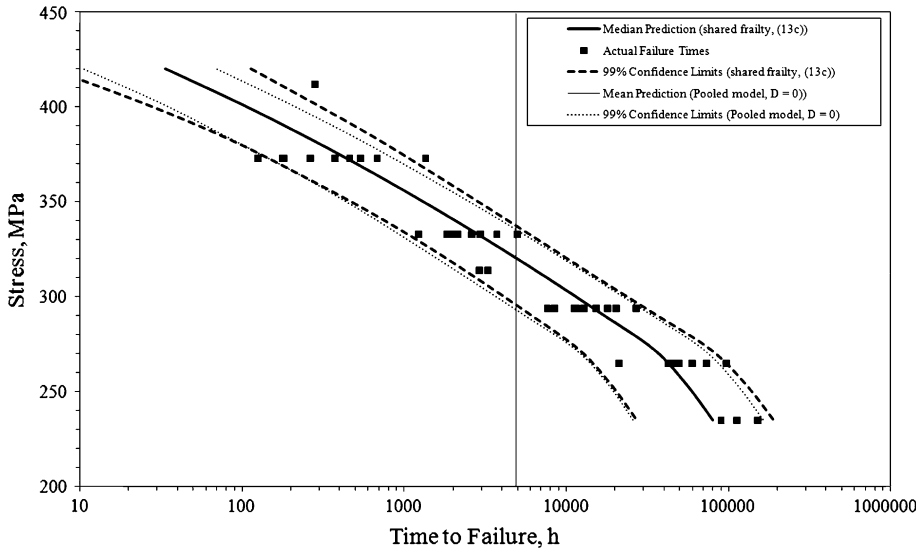

Fig. 3 Variations in times to failure with stress, together with predicted values and confidence limits, at 773 K

Figure 3 also compares the predictions obtained from the shared frailty model with the so called pooled model obtained by setting $\mathbf{D} = 0$. This of course corresponds to the classical or traditional application of the Wilshire model (as published, for example, in [7]). The predictions from this model are given by the thinner lines. Whilst the median prediction from this pooled model is almost identical to that from the shared frailty model, the simulated percentiles do not correctly identify the magnitude of the scatter present in the experimental data—especially for the upper end of the distribution and at higher stresses. Interestingly, ignoring the lack of independence in test results (using the pooled model) has had no measurable effect on the estimate made for the safe life of the material at operating conditions (i.e. low stresses) as seen by the equivalence of the 0.5% confidence limit at such stresses. However, at higher stresses, the pooled model seriously under estimates this safe life. This may not be true for other materials.

Conclusions

A modification to the shared frailty model has been presented that allows for the distribution of the response and the random effects to be determined by the data (from within the exponential family of distributions). A SML and a computationally simpler simulated linear least squares

(SLLS) approach (when $\mu(\mathbf{x};\boldsymbol{\beta})$ is linear) to estimating this model has also been presented. These generalizations are important for modelling high-temperature deformation because they allow a reformulization of the recently proposed Wilshire–Schering methodology that allows life time predictions to be made with levels of confidence attached for engineering components operating at high temperatures. When applied to 1Cr–1Mo–0.25V steel, it was found that failure times were distributed as a generalized gamma distribution (with $\lambda = 100$)—as were the random effects. The mean activation energy was estimated at around 252 kJ mol^{-1}—which is close to the reported values of the activation energy for lattice self diffusion in the 1Cr–1Mo–0.25V alloy steel matrixes. However, there was substantial batch to batch variation in these estimated activation energies.

It was shown that ignoring these random effects resulted in predictions that were not such a good description of the experimental data. Only when random effects were included did the resulting confidence limits reflect the actual variability present in the experimental data—especially at the higher stresses and at the top tail of the distribution. Interestingly, it was shown that ignoring the lack of independence in test results (i.e. using the pooled model) had no measurable effect on the estimate made for the safe life of the material at operating conditions. However, this may not be the case when this method is applied to other steel alloys used for high-temperature power generation.

Areas for future study include the extension of the above model to three or more levels so that results for different products (bar plate and tubes) and from different laboratories for the same material can be analysed using a single model.

Appendix

Estimation

Heteroscedasticity

Estimation of the shared frailty model is not straightforward. For example, consider the simplest specification where $\mu(\mathbf{x};\boldsymbol{\beta}_j)$ is linear in $\mathbf{x}$ and where there are p test condition variables. Then Eq. 7a can be written as

$$g(t,\alpha)_{ij} = \beta_0 + \beta_k \sum_{k=1}^{p} x_{kij}^{\mathrm{T}} + w_{ij} \tag{10}$$

where

$$w_{ij} = z_{ij} + u_{0j} + \sum_{k=1}^{p} u_{kj} x_{kij} \tag{11}$$

The random error term (w_{ij}) in Eq. 10 is clearly a function of the covariates and its variance, Var[w_{ij}], is given by (assuming that the u_{kj} and z_{ij} are independent of each other)

$$\mathrm{Var}[w_{ij}] = \mathrm{Var}[z_{ij}] + \mathrm{Var}[u_{0j}] + \sum_{k=1}^{p} \mathrm{Var}[u_{kj}] x_{kij}^2 \tag{12}$$

and so also varies with the covariates. This heteroscedasticity has important implications for parameter estimation. It means that if the linear least squares formula is used to estimate the β parameters in Eq. 10, by minimising Σw_{ij}^2, the resulting estimates will be unbiased but inefficient (have higher variances than if Var[w_{ij}] were constant). Further, the estimates made of the standard errors of these parameters will be biased, so invalidating any standard tests of statistical significance or any constructed confidence limits. Hence some other estimation procedure is required.

Simulated maximum likelihood

It follows from Eqs. 6a, 8a that the log likelihood for the n_j observations in batch or unit j is the sum of the logs of the densities

$$\ln(L_j|\mathbf{x};\boldsymbol{\beta}_j) = \sum_{i=1}^{n_j} \left\{ \begin{array}{c} (\lambda - 0.5)\ln(\lambda) - \ln\Gamma(\lambda) - \ln(\sigma) + \sqrt{\lambda}\left[\frac{g(t;\alpha)_{ij} - \mu(\mathbf{x};\boldsymbol{\beta}_j)}{\sigma}\right] \\ -\lambda \exp\left[\frac{g(t;\alpha)_{ij} - \mu(\mathbf{x};\boldsymbol{\beta}_j)}{\sigma\sqrt{\lambda}}\right] \end{array} \right\} \tag{13}$$

The log likelihood for the full sample, when there are m units in all, is then

$$\ln(L) = \sum_{j=1}^{m} \ln(L_j|\mathbf{x};\boldsymbol{\beta}_j) \tag{14}$$

Inserting the expression $\boldsymbol{\beta}_j = \boldsymbol{\beta} + \mathbf{u}_j$ into Eqs. 13, 14 yields

$$\ln(L|\mathbf{x};\mathbf{u}_j) = \sum_{j=1}^{m} \sum_{i=1}^{n_j} \left\{ \begin{array}{c} (\lambda - 0.5)\ln(\lambda) - \ln\Gamma(\lambda) - \ln(\sigma) + \sqrt{\lambda}\left[\frac{g(t;\alpha)_{ij} - \mu(\mathbf{x};\boldsymbol{\beta}+u_j)}{\sigma}\right] \\ -\lambda \exp\left[\frac{g(t;\alpha)_{ij} - \mu(\mathbf{x};\boldsymbol{\beta}+u_j)}{\sigma\sqrt{\lambda}}\right] \end{array} \right\} \tag{15}$$

In principle this log likelihood could be maximised with respect to $\boldsymbol{\beta}$ and σ. However, there are two problems with this approach. First, the covariance matrix for $\mathbf{u}_j$ is not present and so cannot be estimated. This is easily solved by making use of the expression $u_j = \Lambda v_j$ allowing Eq. 15 to be written as

$$\ln(L|\mathbf{x};\mathbf{u}_j) = \sum_{j=1}^{m}\sum_{i=1}^{n_j}\left\{\begin{array}{r}(\lambda-0.5)\ln(\lambda)-\ln\Gamma(\lambda)-\ln(\sigma)+\sqrt{\lambda}\left[\frac{g(t;\alpha)_{ij}-\mu(\mathbf{x};\boldsymbol{\beta}+\Lambda\mathbf{v}_j)}{\sigma}\right]\\ -\lambda\exp\left[\frac{g(t;\alpha)_{ij}-\mu(\mathbf{x};\boldsymbol{\beta}+\Lambda\mathbf{v}_j)}{\sigma\sqrt{\lambda}}\right]\end{array}\right\} \tag{16}$$

The second problem is that in Eq. 16 the $\mathbf{v}_j$ are unobserved and so the log likelihood cannot be computed. The solution requires $\mathbf{v}_j$ to be integrated out of the above conditional likelihood, but such integrals typically do not have an analytical solution. However, integrals of this nature can be adequately evaluated by simulation methods. More formally, estimates for $\boldsymbol{\beta}$, σ and $\boldsymbol{\Lambda}$ are obtained by maximising the simulated log likelihood given by

$$\ln(L|\mathbf{x};\mathbf{u}_j) = \sum_{j=1}^{m}\sum_{i=1}^{n_j}\left\{\begin{array}{r}(\lambda-0.5)\ln(\lambda)-\ln\Gamma(\lambda)-\ln(\sigma)+\sqrt{\lambda}\left[\frac{g(t;\alpha)_{ij}-\mu(\mathbf{x};\boldsymbol{\beta}+\Lambda\mathbf{v}_j)}{\sigma}\right]\\ -\lambda\exp\left[\frac{g(t;\alpha)_{ij}-\mu(\mathbf{x};\boldsymbol{\beta}+\Lambda\mathbf{v}_j)}{\sigma\sqrt{\lambda}}\right]\end{array}\right\} \tag{17}$$

where v_j contains p random draws from the distribution given by Eq. 8a. This maximisation procedure is then repeated R times yielding R values for $\boldsymbol{\beta}$, σ and $\boldsymbol{\Lambda}$. The average of these R values can be taken as the SML estimates for these parameters, and the standard deviation in these R values as an estimate of their standard errors. This estimation procedure can be repeated using different values for λ, and the value for λ that maximises the average log likelihood over all R iterations is chosen as the correct value for λ.

This is quite a straightforward procedure in practice because obtaining random draws from Eq. 8a is easily implemented within popular and commercially available software packages such as Microsoft Excel [22] or more specialised Econometric software such as Regression Analysis of Time Series [23] or RATS for short. Subtracting from this random draw the natural log of λ, multiplying by the square root of λ and then subtracting c then gives a random draw from the PDF given by Eq. 8a, i.e. a random value for v_{kj}. This last transformation is required for the log gamma distribution to be non degenerate as λ tends to infinity and for its mean to be zero. Even without specialised software like RATS, obtaining random values for v_{kj} is straightforward. All that is required is an ability to draw random numbers from a standard normal distribution because the value of a variable drawn from a chi square distribution with λ degrees of freedom is equal to half the value of a variable drawn from the one parameter gamma distribution with $\lambda/2$ degrees of freedom (see Johnson and Kotz [24] for more details).

Simulated linear least squares

If $\mu(\mathbf{x};\boldsymbol{\beta})$ is linear in $\mathbf{x}$, as in Eq. 10, a much simpler estimation procedure presents itself—that of SLLSs. Equations 10, 11 can be written as

$$\begin{aligned} g(t;\alpha)_{ij} = {} & \beta_0 + \beta_k\sum_{k=1}^{p}\mathrm{x}_{kij}^{\mathrm{T}} + \sigma_0^*v_{0j} + \sigma_k^*\sum_{k=1}^{p}(\mathrm{v}_{kj}\mathrm{x}_{kij}^{\mathrm{T}}) + \sigma_{0k}^*\sum_{k=1}^{p}(v_{0j}x_{kij}^{\mathrm{T}}) \\ & + \sigma_{1k}^*\sum_{k=2}^{p}(v_{1j}x_{kij}^{\mathrm{T}}) + \sigma_{2k}^*\sum_{k=3}^{p}(v_{2j}x_{kij}^{\mathrm{T}}) + \ldots\ldots + \sigma_{(p-1)p}^*v_{(p-1)j}x_{pij} + \sigma z_{ij} \end{aligned} \tag{18}$$

As z_{ij} is by assumption homoscedastic, the linear least squares formula could be applied to Eq. 18 to obtain estimates for β_0, all the β_k,s and all the elements of $\mathbf{\Lambda}$, using the simulated values for v_{0j} and v_{kj}. This procedure is then repeated R times yielding R values for all these parameters. The average of these R values can be taken as the SLLSs estimates for these parameters. This procedure avoids the need for non linear maximisation algorithms which in its self is a considerable simplification, but may yield inefficient estimates (especially for σ). When $\mu(\mathbf{x};\boldsymbol{\beta})$ is non linear in $\mathbf{x}$, non linear least squares can be used but then there is no computational advantage over SML.

Notice also that σ in Eq. 18 can then be estimated as

$$\frac{1}{\lambda\psi'(\lambda)\left(\sum_{j=1}^{m} n_j m - C\right)} \sum_{i=1}^{n}\sum_{j=1}^{m} z_{ij}^2 \tag{19}$$

where C is the number parameters to estimate in Eq. 18.

Confidence intervals

A simulation approach can also be used to obtain confidence limits for the frailty model of Eq. 7a. This approach requires first simulating values for $\mathbf{u}_j$, using $\mathbf{u}_j = \tilde{\mathbf{\Lambda}}\mathbf{v}_j$, where the tilde refers to the SML estimate of $\mathbf{\Lambda}$ and the $\mathbf{v}_j$ are simulated in the way described above**.** Then $\boldsymbol{\beta}$ is simulated using

$$\boldsymbol{\beta} = \tilde{\beta} + \{\tilde{\Lambda}/m\}\mathbf{v}_j \tag{20}$$

where for large m, $\mathbf{\Lambda\Lambda}' = \mathbf{D}$, otherwise $\lambda\ \psi'(\lambda)[\mathbf{\Lambda\Lambda}'] = \mathbf{D}$. The tilde refers to the SML value for $\boldsymbol{\beta}$. These simulate values for $\boldsymbol{\beta}$ and $\mathbf{u}_j$ are then inserted into Eq. 7b to simulate a value for $\mu(\mathbf{x};\boldsymbol{\beta}_j)$.

Then simulated values for z_{ij} are drawn from Eq. 6a to obtain $\tilde{\sigma}z_{ij}$ where the tilde represents the SML estimate for σ. Substituting the simulated values for $\mu(\mathbf{x};\boldsymbol{\beta}_j)$and $\tilde{\sigma}z_{ij}$ into Eq. 7a gives a simulated value for $g(t;\alpha)_{ij}$. Repeating this a large number of times yield an empirical distribution for $g(t;\alpha)_{ij}$ and, therefore, t_F at a particular value for $\mathbf{x}$. From this, any percentile of the empirical distribution can be obtained to represent confidence limits around the simulated median prediction. Repeating this for other values of the covariates completes the calculation of predictions with confidence limits for t_F.

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