Numerical Analysis of Creep Brittle Rupture by the Finite Element Method

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SUMMARY

In this work an implicit algorithm is proposed for the numerical analysis of creep brittle rupture problems by the finite element method. This kind of structural failure, typical in components operating at high temperatures for long periods of time, is modelled using either a three dimensional generalization of the Kachanov-Rabotnov equations due to Leckie and Hayhurst or the Monkman-Grant fracture criterion together with the Linear Life Fraction Rule.

The finite element equations are derived by the displacement method and isoparametric elements are used for the spatial discretization. Geometric nonlinear effects (large displacements) are accounted for by an updated Lagrangian formulation. Attention is also focussed on the solution of the highly stiff differential equations that govern damage growth.

Finally the numerical results of a three-dimensional analysis of a pressurized thin cylinder containing oxidised pits in its external wall are discussed.
1. Introduction

The requirements of safety and reliability of structural components operating at high temperature and under severe loading conditions have stimulated increased interest in the study of creep damage and rupture of metals. Current metallurgical investigations indicate that the creep damage of polycrystalline metals occurs by the nucleation and growth of grain boundary defects. The effect of their growth is to cause a progressive weakening of the material and an increase in the creep rate over a significant fraction of the structure lifetime.

The procedures formerly adopted to estimate the rupture time consisted in determining the elastic or steady state stress distribution and to use the corresponding maximum principal stress component together with uniaxial rupture data, such as those given in ASME Code Case N47-12. These approaches have been proved to be deficient on two accounts by ignoring firstly, the influence of multiaxial stress states upon the rupture time and, secondly, the above mentioned softening effect exhibited by metals over the tertiary creep range. This latter effect is a very beneficial one allowing stresses to be transferred from a highly to a less damaged zone, thus increasing the service life of the structure.

In order to overcome these deficiencies Kachanov [1] and Rabotnov [2] introduced the concept of damage into the constitutive relationships in the form of a scalar quantity. The Kachanov-Rabotnov equations, which in their original one dimensional form can be shown to obey the Linear Life Fraction Rule due to Robinson [3], were generalized to multiaxial stress states by Leckie and Hayhurst [4]. Their generalization assumes isotropy of damage or incorporates anisotropy of damage only with respect to the principal stress coordinates fixed in the material.

In the high temperature design of pressure vessels, it is usual practice to assume that the geometry remains unchanged during the life of the component. In certain cases, this standard procedure leads to a considerable error in life prediction [5], which indicates that, at least for selected applications, geometric nonlinear effects should not be disregarded in rupture calculations.

In this work an implicit time marching scheme is proposed for the numerical analysis of creep damage and rupture of metals. To model this kind of structural failure the three dimensional constitutive equations of Leckie and Hayhurst [4] are used. An alternative model based on the Nonkman-Grant fracture criterion [6] and the Linear Life Fraction Rule is also employed. Geometric nonlinear effects (large displacements and deformation dependent loading) are accounted for by an updated Lagrangian formulation. In order to keep the drifting errors within an acceptable tolerance, facilities are provided for automatically reanalysing a particular time step with a reduced time increment length whenever accuracy criterions, based on stress and damage variations, are violated. No iterative equilibrium corrections are performed because, as noted by Argyris et al. [7], in path dependent problems it is impossible to compute the correct residual loads without integration of the prior history and, consequently, there is no possibility of returning to the true solution path without reanalysing the process with smaller time increment lengths.

2. Constitutive equations and rupture criteria

2.1 Generalized Kachanov and Rabotnov equations

The constitutive equations proposed by Leckie and Hayhurst to evaluate the creep strain rate and the damage rate in multiaxial stress states can be respectively written in the
following form
\[ \frac{\Delta e_{ij}}{\Delta t} = \gamma \left( \frac{\sigma}{1-w} \right)^N \frac{\Delta F}{\sigma_{eq}^{ij}} \] (1)

and
\[ \frac{\Delta w}{\Delta t} = A \frac{\sigma_{eq}}{(1-w)^\phi} \] (2)

where \( e_{ij} \) is the tensor of infinitesimal strains, \( \sigma_{ij} \) the Cauchy stress tensor, \( \sigma \) the Von Mises, Tresca, or the maximum principal stress, \( F \) a potential function, \( \gamma, N, \chi, A \) and \( \phi \) temperature dependent material properties and \( \sigma_{eq} \) a scalar quantity that takes account of the rupture characteristics of the material under multiaxial stress states. In a general form
\[ \sigma_{eq} = \sigma_{ij}^q + 2^{\frac{3}{2}} \tau_{ij}^a \max + \tau_{ij}^a \] (3)

where \( \sigma_1 \) is the maximum principal tensile stress, \( \tau_{\max} \) the maximum shear stress, \( J_1 \) the first stress invariant, \( \sigma_{eff} \) the effective stress and \( \sigma_{i}(i=J,4) \) scalar quantities such that \( \Sigma \sigma_i = 0 \). To predict the growths of strain and damage for variable stress histories Leckie and Hayhurst [3] introduced the concept of constant damage contours and suggested a testing procedure for their determination. In the initial undamaged state \( w = 0 \) and rupture is deemed to have occurred when \( w \) reaches a critical value, usually taken as 1.

2.2 - Monkman-Grant fracture criterion and the Linear Life Fraction Rule

In 1956 Monkman and Grant [6] found that an empirical relationship exists between rupture life and minimum (secondary) creep rate for a large number of alloys. This empirical relationship can be written for one-dimensional problems in the form
\[ \varepsilon_{cs} \tau_r = k \] (4)

where \( \varepsilon_{cs} \) is the secondary creep strain rate under a constant stress \( \sigma \), \( (\varepsilon_{cs} = \gamma \sigma^N) \), \( \tau_r \) is the rupture time under this same stress, \( k \) is a material property and a superposed dot indicates time differentiation. The Monkman-Grant criterion is applied in three-dimensional problems by replacing \( \varepsilon_{cs} \) in eq.(4) by an appropriate equivalent strain rate \( (\varepsilon_{cs})_{eq} \) such as, for instance, the effective strain rate \( \varepsilon_{eq} = (\frac{2}{3} \varepsilon_{ij} \varepsilon_{ij})^{\frac{1}{2}} \) or the maximum principal strain rate. In this way the influence of multiaxial stress states upon the rupture time is accounted for. The creep strain rate for this case is also given by eq.(1) but with \( w \) now obtained with the help of the Linear Life Fraction Rule as

\[ w(t) = \sum_{i=1}^{n-1} \frac{\Delta t_i}{\tau_r} \] (5)

where \( \Delta t_i \) is the time under a particular stress and \( \tau_{ri} \), as before, is the rupture time associated with this stress.

2.3 - Non-homogeneity of void growth and its influence on the creep deformation

Material damage in metals under constant uniform stress advances uniformly in the material until a certain critical stage is reached when cavities start to coalesce and grow rapidly. It has been recently argued [8] that such local features of damage growth should not affect equally fracture and deformation processes since the former is a local phenomenon and the latter a global one. It has been argued, furthermore, that the creep rate is less sensitive to the damage state than the rate of damage growth.

Following [8] the non-homogeneity of damage growth and its influence on creep deformation is taken into account in this work by redefining eq.(1) as
\[
\frac{\Delta e_{ij}}{\Delta t} = \gamma_f (1 - CS)^N \frac{\partial F}{\partial \sigma_{ij}}
\]

(6)

where \( c (0 < c < 1) \). Strictly speaking, \( c \) depends on the stress and temperature but, in the absence of more precise experimental values, an average value over the stress and temperature ranges of interest is adopted.

The introduction of the \( c \) factor is additionally convenient when using the Monkman-Grant criterion because, in its original form, this criterion does not consider the influence of damage on the creep rate. Although this influence can now be justified, expression [5] is rather arbitrarily defined and, therefore, the \( c \) factor permits the extent of this influence to be easily controlled.

3. Finite Element Formulation

In this study the incremental finite element equilibrium equations are derived by an updated Lagrangian formulation based on the displacement method. Eight and twenty noded isoparametric elements are used for the spatial discretization. Assuming the standard procedures for assembling the structure matrices, attention is restricted to the derivation of the matrices corresponding to a single element (vectorial notation is used hereafter).

3.1 - Equilibrium Equations

The equilibrium equations to be satisfied at any instant \( t_n \) are

\[
\sum_{v} \int_{V} \sigma_{n}^{T} \delta v = R_{n}
\]

(7)

where \( R_{n} (=R_{n}^{L} + R_{n}^{NL}) \) is the kinematic large displacement matrix relating the strains and the displacements, \( \sigma_{n} \) the Cauchy stresses and \( R_{n} \) the vector of equivalent nodal loads. The \( R_{n}^{L} \) and \( R_{n}^{NL} \) matrices correspond to the linear and nonlinear terms of the general quadratic relationship between strains and displacements as used in updated Lagrangian formulation [9]. In incremental form eq. (7) is rewritten as

\[
\sum_{v} \int_{V} \sigma_{n}^{T} \delta v + \delta K_{n} \delta u_{n} = \delta R_{n}
\]

(8)

where \( K_{n} \) is the geometrical stiffness matrix dependent on the stress level [9], \( \delta u_{n} \) the displacement increments and \( \delta R_{n} \) the change of the external loads during the time increment \( \Delta t_{n} \).

The stress increments are obtained from the elastic strain increment as

\[
\delta \sigma_{n} = \mathcal{D} (\delta \epsilon_{n} - \delta e_{n}^{C}) = \mathcal{D} \left( \epsilon_{n}^C \Delta \epsilon_{n} - \Delta e_{n}^C \right)
\]

(9)

where \( \mathcal{D} \) is the matrix of elastic constants, \( \delta e_{n} \) the total strain increments (it is implicitly assumed that the total strains are the sum of its elastic and creep components) and \( \Delta e_{n}^C \) the creep strain increments.

The creep strain increments are defined using an implicit scheme as

\[
\delta e_{n}^C = \left\{ (1 - \theta) \epsilon_{n}^{C1} + \theta \epsilon_{n+1}^{C1} \right\} \Delta t_{n}
\]

(10)

where \( \theta, 0 \leq \theta \leq 1 \), defines several scheme strategies such as, for instance, Euler forward or explicit (\( \theta=0 \)), Crank-Nicolson (\( \theta=1/2 \)), Galerkin (\( \theta=\frac{1}{3} \)) and Euler backward or fully implicit (\( \theta=1 \).

To determine \( \epsilon_{n+1}^C \) in eq.(10) it is convenient first to rewrite the constitutive eq.(1) as

\[
\dot{\epsilon} = \gamma \frac{\partial F}{\partial \epsilon} = \gamma \dot{\sigma}
\]
where
\[ \gamma = \gamma(w) = \gamma_f / (1 - cw)^N \]  \hspace{1cm} (12)
and
\[ \phi = \phi(q) = (\sigma)^N \]  \hspace{1cm} (13)

The creep strain rate at time station \( t_{n+1} \) is now obtained by using a limited Taylor series expansion as
\[ \dot{e}^C_{n+1} = \dot{e}^C_n + (\frac{\partial \dot{e}^C}{\partial \sigma})_n \Delta \sigma_n + (\frac{\partial \dot{e}^C}{\partial \gamma})_n \Delta \gamma_n \] \hspace{1cm} (14)

Substituting eq.(11) into eq.(10) yields
\[ \Delta \dot{e}^C_n = \dot{e}^C_n + \dot{e}^C_n \Delta \sigma_n + \dot{e}^C_n \Delta \gamma_n \] \hspace{1cm} (15)

where
\[ \dot{e}^C_n = \dot{e}^C_n(q, \gamma) = \dot{\theta} \Delta t_n \left( \frac{\partial \dot{e}^C}{\partial \gamma} \right)_n \Delta \gamma_n \] \hspace{1cm} (16)

and
\[ \dot{e}^C_n = \dot{e}^C_n(q) = \dot{\theta} \Delta t_n \left( \frac{\partial \dot{e}^C}{\partial \gamma} \right)_n \Delta \gamma_n \] \hspace{1cm} (17)

The gradient matrix \( H_2 \) and the gradient vector \( \dot{H}_2 \) are obtained from eq.(11) as
\[ H_2 = \gamma \left( \frac{\partial \dot{e}^C}{\partial \sigma} + \frac{\partial \dot{e}^C}{\partial \gamma} \right) \] \hspace{1cm} (18)

Specific expressions for the flow vector \( \dot{\gamma} \) and gradient of \( \phi \) can be found in [10].

The introduction of eq.(15) in eq.(9) leads to the following expression for the stress increments
\[ \Delta \ddot{\sigma}_n = \Delta \dot{\sigma}_n + \dot{\sigma}^P_n \Delta \tau_n - \dot{e}^C_n \Delta \gamma_n \] \hspace{1cm} (19)

where \( \dot{\sigma}^P_n \) is a symmetric matrix given by
\[ \dot{\sigma}^P_n = (\dot{\sigma}^P + \dot{\sigma}^P_n)^{-1} \] \hspace{1cm} (20)

Substituting eq.(19) into the incremental equilibrium equation (8) gives the increment of displacements \( \Delta d_n \) as
\[ \Delta d_n = (K^T_n)^{-1} \left\{ \int_{V}^T \dot{\sigma}^P_n \Delta \tau_n + \dot{e}^C_n \Delta \gamma_n + \Delta \ddot{\sigma}_n \right\} \] \hspace{1cm} (21)

where the tangential matrix \( (K^T)_n \) is written as
\[ (K^T)_n = \int_{V}^T \dot{\sigma}^P_n \Delta \tau_n + \dot{e}^C_n \Delta \gamma_n \] \hspace{1cm} (22)

The increment of the function required in eq.(21) is obtained from eq.(12) as
\[ \Delta \gamma_n = cN_f \Delta \gamma_n^{D} / (1 - cw_n)^{N+1} = cN_f \Delta \gamma_n^{D} / (1 -cw_n)^{N+1} \] \hspace{1cm} (23)

where it should be noted that the increment of damage \( \Delta \gamma_n^{D} \) has been predicted using the constitutive eq.(2) and an Euler forward scheme.

Once the displacement increments have been evaluated the stress increments are found from eq.(19) and, subsequently, the creep strain increments from eq.(15). With all the increments known the displacements, stresses, creep strains and damage states are updated to their final values at time \( t_{n+1} \) corresponding to the end of the time interval \( \Delta t_n \).
The predicted values of damage increments are corrected considering the new values of stress and damage as,

$$\Delta \omega_n^C = \frac{1}{2} (\dot{\omega}_n + \dot{\omega}_{n+1}) \Delta t_n - \omega_n$$  \hspace{1cm} (24)$$

and provided that accuracy criteria based on stress and damage variations are not violated the values obtained at $t_{n+1}$ are accepted. Otherwise the current timestep length is reduced and the timestep analysis repeated. The accuracy conditions to be satisfied are:

a) $\frac{\| \Delta \omega_n \|}{\| \omega_n \|} \leq \Omega_1$  \hspace{1cm} (25)$$

b) $\frac{\| \Delta \omega_n^C - \Delta \omega_n^P \|}{\| \Delta \omega_n^P \|} \leq \Omega_2$, whenever $\omega_n > 0.1$  \hspace{1cm} (26)$$

where $\| \|$ denotes the Euclidean norm, $\| \|$ the absolute value and $\Omega_1$ and $\Omega_2$ the accuracy tolerances.

Rupture of a particular point in the structure is deemed to have occurred when the damage state variable reaches a critical value taken as 0.99. The remaining stress existing at this point at the instant it is declared ruptured is automatically released and transmitted to adjacent non ruptured elements. The analysis proceeds until a sufficiently large damaged zone develops characterizing the global failure of the structure.

3.2 - Damage Rate Equations

The differential equations governing the damage rate in the Kachanov-Rabotnov based model are highly nonlinear with respect to the stress and damage variables. This characteristic leads to a type of equation system that is referred to as stiff in mathematical terms. In the present work these equations are solved, as mentioned in section 3.1, by a predictor-corrector scheme with an automatic time step length control. Prior to solving these equations, however, a change of variables is performed with the objective of diminishing the degree of nonlinearity of the initial equations. The new variable is defined as

$$z = (1-w) (1+\phi)$$  \hspace{1cm} (27)$$

and its introduction into eqs. (2) and (12) yields

$$\dot{z} = -A(1+\phi) \sigma_{eq}^2$$  \hspace{1cm} (28)$$

and

$$\gamma = \chi_f / \left\{ 1 - c + cz^{1/(1+\phi)} \right\}^N$$  \hspace{1cm} (29)$$

Equation (28) shows that the rate of the new variable $z$ is a function of the stress state only, whereas the rate of the initial variable $w$ is a function of the stress and damage variables. This fact underlines the main advantage of the $z$ variable approach, which is best illustrated in the particular case of constant stress histories. For such situations, $z$ becomes a linear function for its whole domain of definition ($1 \geq z \geq 10^{-2(1+\phi)}$) and its increment $\Delta \omega_n^C$ during any time step can be obtained in an exact manner by the simplest Euler scheme. The $w$ curve, on the other hand, still exhibits a strong nonlinearity (due to the damage influence on the damage rate equation) and therefore a precise evaluation of its increment $\Delta \omega_n$ will require more elaborate integration schemes, smaller time step lengths or rather cumbersome analytical expressions. For variable stress histories the change of variable proposed can be justified following a similar line of argument. Thus, the
Increment of the $Y$ function is obtained from eq. (29) as

$$\Delta Y_n = -cNY_n^{t}n_n^{t} \left\{ (1+\varepsilon)z^0/(1+\varepsilon) \left( 1-c+cz^{1/(1+\varepsilon)} \right)^{N+1} \right\}$$

(30)

4. Numerical Applications

Some numerical applications involving the Kachanov-Rabotnov based model have been reported by the authors elsewhere [11]. Here an application considering the Monkman-Grant based model is presented. It consists of an internally pressurized tube containing oxidized pits in its walls. This study was motivated by oxidisation problems sometimes observed in thin tubes used in nuclear components. The tube has a circular section (internal radius, 15.31mm; thickness, 0.381mm), is made of austenitic steel and is treated as infinitely long (plane strain conditions assumed in the axial direction). The pits were assumed to be hemispherical in shape, uniform in size (diameters, 0.300mm) and uniformly distributed on the outer surface as indicated in fig.1. The material obeys the maximum principal stress deformation and the maximum principal strain rate rupture criteria, and its properties are, $E = 1.4294$ N/mm$^2$, $\nu = 0.3$, $\gamma_f = 1.9199 \times 10^{-15}$ (N/mm$^2$)$^{-5}$/sec, $N = 5.0$, $k = 0.1$ and $c = 0.5$. The initial applied pressure was 1.5N. The finite element mesh consisted of 40 twenty noded isoparametric elements (total of 939 degrees of freedom) and is illustrated in fig.1.

Geometrical effects were accounted for and the applied pressure diminished as the tube expanded. The Crank-Nicolson integration strategy ($\theta = 1/2$) was employed. The tube ruptured at 3.0 hrs. while the same specimen without pits failed at 5.5 hrs. For the second specimen advantage was taken of the axisymmetry of the problem and 10 eight-noded isoparametric elements were used (total of 104 degrees of freedom). It is interesting to note that in the tube without pits the crack front moved outward while in the presence of the pits it moved inward. Damage distribution contours are shown in fig.2 for selected cross-sections.

5. Concluding Remarks

In this work an implicit algorithm has been developed to study creep damage and brittle rupture of metals by the finite element method. Numerical experience to date indicates that qualitative results, both in term of strain and damage distributions can be obtained, but that estimation of time to rupture is more difficult.

This follows as a consequence of the highly nonlinear stress dependence of the damage rate equations, when even a small error in the evaluation of the stress field during the whole lifetime of a component can lead to a large deviation in its life prediction, that can be either conservative or underconservative. Therefore, in design situations where damage distribution and lifetime of components are of prime importance, such as in nuclear applications, an accurate evaluation of the stress field history should be an overriding factor.

(a) - Preliminary result obtained with a coarse mesh of 452 degrees of freedom.
Complete results using the refined mesh were not available at time of printing but will be presented at the Conference.
REFERENCES


Figure 1 - Finite element mesh and pits distribution (arbitrary scale)
(Mesh further subdivided in two in the z direction; $h = 0.400$ mm.)

Figure 2 - Damage growth pattern at selected cross sections (arbitrary scale)

$0.10 > w > 0.04$