MODELING THE TEMPERATURE DEPENDENCE OF TERTIARY CREEP DAMAGE OF A NI-BASE ALLOY

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ABSTRACT
To capture the mechanical response of Ni-base materials, creep deformation and rupture experiments are typically performed. Long term tests, mimicking service conditions at 10,000 hours or more, are generally avoided due to expense. Phenomenological models such as the classical Kachanov-Rabotnov model can accurately estimate tertiary creep damage over extended histories. Creep deformation and rupture experiments are conducted on IN617 a polycrystalline (PC) Ni-base alloy over a range of temperatures and applied stresses. The continuum damage model is extended to account for temperature dependence. This allows the modeling of creep deformation at temperatures between available creep rupture data and the design of full-scale parts containing temperature distributions. Implementation of the Hayhurst triaxial stress formulation introduces tensile/compressive asymmetry to the model. This allows compressive loading to be considered for compression loaded gas turbine components such as transition pieces. A new dominant deformation approach is provided to predict the dominant creep mode over time. This leads to development of a new methodology for determining the creep stage and strain of parametric stress and temperature simulations over time.

INTRODUCTION
Gas turbines generate power through a compression-combustion process that forces super heated, highly pressurized exhaust gas through various components. High pressure in the compression area coupled with combustion chamber exit temperatures of up to 1350° C create a situation where material design and selection play a major role in the long term reliability of gas turbine parts. Drives to increase gas turbine efficiency require raising turbine firing temperatures which in the end negatively impact component life. Under these conditions high strength materials are needed to provide long life at elevated temperatures.

The traditional method of determining the service life of gas turbine components depends on practical experience, experimental data, along with finite element analysis. The boundary conditions, temperature, stress gradient, environmental conditions, and time dependent variations induce a number of damage mechanisms which cause crack initiation and eventual rupture. Common practice in the gas turbine industry is to conduct high temperature mechanical testing on sample sized specimens over a period of time and use practical experience (from previous design) to extend empirical models to failure time. Creep rupture life is estimated using experience and secondary creep modeling. Unfortunately this method does not include the effects of temperature dependence, strain-softening behavior (tertiary creep modeling), or observations of tensile/compressive asymmetry. Not including these damage mechanisms create both strain history and component life estimates of limited accuracy. Using a tertiary creep damage model improves the ability to predict component life. Creep deformation and rupture experiments are used to determine the constants of the material model. A numerical parametric study is carried out to predict the conditions that are most detrimental to the performance of the material.

TERTIARY CREEP DAMAGE MODEL
A method has been established for modeling tertiary creep at high temperatures. This method is based on the Norton power law for secondary creep, i.e.,

\[ \dot{e}_{ct} = A\sigma^n \]  

where \( A \) and \( n \) are the creep strain coefficient and exponent, respectively, and \( \sigma \) is the von Mises effective stress. The coefficient \( A \) exhibits Arrhenian temperature-dependence, e.g.

\[ A = B \exp \left(-\frac{Q_{cr}}{RT} \right) \]

Here \( Q_{cr} \) is the activation energy for creep deformation, and \( T \) is the temperature measured in Kelvin. The term \( R \) is the universal gas constant. Both \( A \) and its temperature-independent counterpart, \( B \), have units \( \text{MPa}^{-n} \text{hr}^{-1} \). It should be noted that the exponent \( n \) may also exhibit temperature-dependence.

During the transition from secondary to tertiary creep, stresses in the vicinity of voids and microcracks along grain boundaries of polycrystalline materials are amplified. The stress concentration due to local reduction of cross-sectional area is the phenomenological basis of the Kachanov-Rabotnov [1, 2]
damage variable, \( \omega \) that is coupled with the creep strain rate and has a stress-dependent evolution, i.e.,

\[
\dot{\varepsilon}_c = \dot{\varepsilon}_{cp}(-T, \omega, ...) \quad \dot{\omega} = \dot{\omega}(-T, \omega, ...)
\]

A straightforward formulation implies that the damage variable is the net reduction in cross-sectional area due to the presence of defects such as voids and/or cracks, e.g.

\[
\bar{\sigma}_{net} = \frac{A}{\bar{\sigma}_{net}} = \frac{\sigma}{(1 - \frac{A_{eff} - A}{A})} = \bar{\sigma}
\]

An essential feature of damage required for application of continuum damage mechanics concepts is a continuous distribution of damage. Generally, micro-defect interaction (in terms of stress fields, strain fields, driving forces) is relatively weak until impingement or coalescence is imminent. By substituting Equation (4) into (1), the steady-state creep strain is expressed as a modified secondary creep rate

\[
\dot{\varepsilon}_{cr} = A \left( \frac{\bar{\sigma}}{1 - \omega} \right)^n
\]

The isotropic damage variable, \( \omega \), is scalar-valued from 0 for an initial state (e.g. undamaged) to 1 at final state (e.g. completely ruptured). Its evolution was given by Rabotnov [1] as

\[
\dot{\omega} = M \bar{\sigma}^\chi (1 - \omega) \phi
\]

where \( M \) is the creep damage coefficient having units of \( MPa^{-\chi} hr^{-1} \). In an earlier study, Kachanov [2] developed a similar formulation with the exception that the creep damage exponents, \( \chi \) and \( \phi \) were equivalent. Time hardening, tensile/compressive asymmetry, and multi-axial behavior can be accounted for in the model by replacing the effective stress with one which considers multiaxial stress.

\[
\dot{\omega} = M \sigma_r^\chi (1 - \omega) \phi t^m
\]

The exponent \( m \), accounts for time hardening and the units of \( M \) are in \( MPa^{-\chi} hr^{-1} \); however, in most cases \( m \) is defined to be 0 [3, 4]. Here \( \sigma_r \) describes the triaxial stress and is related to the principal stress, \( \sigma_1 \), hydrostatic (Mean) stress, \( \sigma_m \), and the Mises effective stress, \( \bar{\sigma} \). The triaxial stress is given by Hayhurst [5] as

\[
\sigma_r = (\alpha \sigma_1 + 3\beta \sigma_m + (1 - \alpha - \beta) \bar{\sigma})
\]

where \( \alpha \) and \( \beta \) are weighing factors valued between 0 and 1 and are determined from multiaxial creep experiments. This formulation disallows damage under uniaxial compression when \( \alpha + 2\beta \geq 1 \). More recent investigations have extended this damage evolution description to account for anisotropic damage resulting from multiaxial states of stress [6]. In these cases, damage is described by a second-rank tensor.

The formulation given in Equations (5), (7), and (8) can be applied to model the gradual reduction of load carrying capability (e.g. secondary through tertiary creep). Since \( \omega \) characterizes the microstructural evolution of the material and is dependent on stress and temperature, the damage variable is an internal state variable (ISV). Clearly, the coupled evolution equations reduce to secondary creep when \( M = 0 \). This formulation has been used in a variety of studies of turbine and rotor materials. The constants \( A, n, M, \chi, \phi \) are considered material properties. For example, in Waspaloy at 700°C, \( A = 9.23 \times 10^{34} MPa^{-\chi} hr^{-1}, n = 10.65, M = 1.18 \times 10^{25} MPa^{-\chi} hr^{-1}, \chi = 8.13, \) and \( \phi = 13.0 [3] \). For stainless steel at 650°C, \( A = 2.13 \times 10^{13} MPa^{-\chi} hr^{-1}, n = 3.5, M = 9.0 \times 10^{10} MPa^{-\chi} hr^{-1}, \) and \( \chi = \phi = 2.8 [4] \). In these previous studies, isotonic and constant stress conditions were applied. It should be noted that no rule for the temperature dependence of the tertiary creep constant has been established.

Table 1. Nominal chemical composition of IN617

<table>
<thead>
<tr>
<th>IN617</th>
<th>Cr</th>
<th>Co</th>
<th>Ti</th>
<th>Al</th>
<th>Mo</th>
<th>C</th>
<th>B</th>
<th>Fe</th>
<th>Ni</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>22.5</td>
<td>12.5</td>
<td>0.6</td>
<td>1.0</td>
<td>9.6</td>
<td>0.08</td>
<td>0.004</td>
<td>0.98</td>
<td>Bal.</td>
</tr>
</tbody>
</table>

CREEP EXPERIMENTS

Polycrystalline (PC) nickel-chromium-cobalt-molybdenum alloys are a modern class of materials commonly used in gas-turbine components. One such material is wrought Ni-base alloy sheets of IN617. This non-proprietary material has several equivalent monikers (e.g. Inconel-617, INCO-617, Nicrofer® 5520 Co – Alloy 617, Haynes 617). The nominal chemical composition is given in Table 1. The chemical composition of the material allows the alloy to withstand a range of conditions critical to gas turbine components. The combination of various elements produces a strong atomic structure that imparts strength at high temperatures. Although it is suitable below 1000°C, IN617 displays exceptionally high levels of creep-rupture strength, even at temperatures of 980°C (180°F). An inherent feature of the material is it has good corrosion resistance compared to other standard Ni-base alloys such as alloy 556, alloy 230, and alloy Hastelloy-X, etc. [7]. It carries a good combination of resistance to oxidation and carburizing atmospheres which are important for components that undergo long term loading. Thermal shock resistance is another key feature that forwards the uses of Ni-base materials [8]. All these features result in a material which has good resistance to creep deformation. The material also has relatively good weldability allowing field repair another important requirement of gas turbines. One major detractor for this material is that it is susceptible to intense nitridation at elevated temperatures while undergoing thermal cycling. This susceptibility is due to the development of crack defects in the oxide scale which perpetuate the nitridation process, allow surface intrusion of oxides, leading to crack initiation and eventual failure [9]. Additionally, alloy 617 encounters deep internal defects through the development of aluminum nitrides (AIN) which severely hinder the load carrying capability of the material. Despite this condition, alloy 617 is still found to be the best combination of overall material properties. Proper turbine operation has been shown to produce gas turbine transition pieces of alloy 617 which last up to 15,000 total
operating hours [10] way beyond other Ni-base gas turbine components.

Creep deformation and rupture experiments were conducted according to an ASTM standard E-139 [11] at 649, 760, 871, and 982°C on samples incised from wrought slabs of IN617. From this variety of creep deformation and rupture experiments, the subject PC material exhibits primary, secondary, and tertiary creep strain depending on the combination of test temperature and stress, as shown in Figure 1.

Based on these strain histories, the deformation mechanisms can be inferred from investigations that complemented mechanical experimentation with microscopic analysis [12, 13]. Deformation at 649°C at low stresses and short times is mostly due to elastic strain, along with primary and secondary creep. During primary creep, the strain rate, which is initially high, decreases significantly. This transient phenomenon is due to the ease at which dislocations can occur upon initial loading (due to initially present dislocations in untreated workpieces) and the saturation of the dislocation density which inhibits continued creep deformation. Secondary creep arises due to the nucleation of grain boundary (GB) cavities and grain boundary sliding. The deformation mode of tertiary creep was not observed in these cases. At higher temperatures (760°C and above), deformation is dominated by secondary and tertiary creep facilitated by the coalescence of grain boundary voids into microcracks. Sharma and coworkers [14] show that at temperatures above 800°C, dynamic recrystallization is found to occur. This process is a part of the hot deformation process which decreases average grain size as stress increases. This has the effect of rapidly reducing dislocation density in the alloy at higher temperatures and thus reducing primary creep deformation. Notwithstanding, primary creep was still observed, but its contribution to the overall deformation was negligible compared to that of secondary and tertiary creep.

The obtained creep rupture data at 649, 760, 871, and 982°C compares well to a comprehensive study [7] of creep rupture data at temperature between 600 and 1000°C, from previous studies [15-17]. Figure 2 shows stress versus rupture time of both the obtained and study creep rupture data. Generally, rupture time increases with either decreasing applied stress or decreasing temperature. In the obtained creep rupture data, scatter is present. This is due to both alloy and test variability. The comprehensive studies multiple data sources are used to compensate for this natural occurrence and help build a well established trend line. The figure shows that the obtained creep rupture data sits within the bounds of creep rupture data at adjacent temperature from the comprehensive study.

![Figure 1. Stress and temperature combinations of available creep experiments](image1)

![Figure 2. Creep rupture data at various temperatures](image2)
NUMERICAL METHODOLOGY

The constitutive model described in Equations (5), (7), and (8) has been implemented in a general purpose finite element analysis (FEA) software in order to determine the constants for the constitutive model used in the secondary-tertiary creep formulation. Both equations were written into a FORTRAN subroutine in the form of a user-programmable feature (UPF) in ANSYS. The subroutine is incorporated with an implicit integration algorithm. This backward Euler integration algorithm is more accurate over long time periods than other practical numerical integration methods. This allows larger time steps to be taken that reduce numerical solve time. Since the viscoplastic/creep behavior of materials is significant at extended histories, the backward Euler method is the desired method for integration of creep constitutive equations [18].

This implementation allows for the update of the internal state variable, ω. Initially, ω = 0.0 and during loading, ω increases. To prevent the singularity that is caused by rupture (e.g. ω = 1.0), the damage is restricted to a maximum of 0.90. Comparison of creep rupture data to numerical simulations shows that rupture occurs as low as ω = 0.42; therefore, damage cannot be used as a suitable measure of rupture time. To prevent an excessive model solve time and large deformation errors, a simulation was terminated once total strain reached 100%. If needed, this model can be applied with time-independent and time-dependent plasticity models in a straightforward manner.

The UPF has been used to simulate the stress/temperature loading conditions of a series of uniaxial creep and rupture experiments. A single, solid, three-dimensional, 8-noded element was used, and the appropriate initial and boundary conditions were applied to numerically simulate the uniaxial creep deformation curves shown in Figure 1. The loads and temperatures applied numerically simulated those of the obtained creep rupture experiments. Histories of creep deformation, ε_c(t) and damage, ω(t) were recorded to a data file and subsequently compared with experiments.

A goal of the project was to provide a uniaxial creep deformation formulation that was capable of matching the material response up to 5% of the total strain determined from experiments.

The secondary creep constants (e.g. A and n) were evaluated directly from the available creep deformation and rupture data for IN617 at each temperature. Based on these constants and Equation (3), B and Q_ω were approximated as 2.95×10³ MPa⁻ⁿhr⁻¹ and 5.42×10⁵ J/mol, respectively. The tertiary creep constants (e.g. M, χ, and φ) were determined for each temperature by iterative trial and error. Both χ and φ were taken to be equivalent, and α and β were set to 0 to produce a triaxial stress equivalent to uniaxially applied stress. Coupling Norton’s law for secondary creep with the Kachanov-Rabotnov formulation for tertiary creep allows the finite element model to display a strain history that is in close proximity to experimental results. The strain histories simulated with the Norton-Rabotnov formulation correlate well with the analogous experimentally-obtained ε(t). An example of the simulated creep deformation response is shown in Figure 3. Tertiary creep constants were optimized for every combination of temperature and stress. In most cases the trajectory of each of the correlated creep curves matched the corresponding experimental curve.

![Figure 3. Comparison of experimental and numerically simulated creep deformation of IN617 at 871°C (1600°F).](image)

TEMPERATURE DEPENDENCE

All of the creep curves exhibiting creep softening could be generated by varying M, χ, and φ. The creep damage rate coefficient, M, displays temperature dependence; however, the damage rate exponents χ and φ exhibit temperature independence. The constants at each temperature are plotted in Figure 4. Based on the experiments, the temperature dependence for each of the constants is mathematically represented. The elastic modulus of IN617 was written as a third order polynomial, e.g.

\[
E(T) = E_0 T^3 + E_2 T^2 + E_1 T + E_0
\]

with T measured in degrees Celsius. In a similar manner, regression analyses were performed to model the temperature dependence of the secondary creep and creep damage constants. The secondary creep coefficient was determined using the Arrhenius relation Equation (2) as a function of temperature, where B and Q_c are independent of temperature. In Equation (2), T is measured in Kelvin. The secondary creep exponent was related by a polynomial function, e.g.

\[
n(T) = (n_3 T^3 + n_2 T^2 + n_1 T + n_0) + n_{min}
\]

where T is measured in degrees Celsius. The McCauley brackets and n_{min} term are used in this case so that the minimum value of n is 5. This was implemented to insure numerical convergence of the UPF at low temperatures. The creep damage coefficient is expressed as a 2-parameter exponential power law function, e.g.
where $T$ is measured in degrees Celsius. Here $M_1$ and $M_2$ are constants. The fit of Equations (9) through (11) is compared with optimized constants for each temperature in Figure 4. The square of the Pearson product-moment correlation coefficient, $R^2$, indicates that each of the relations model the temperature dependence of the elastic-creep properties of IN617 with an accuracy greater than or equal to 0.90. The temperature dependence of the constants was coded into the Fortran Subroutine so that predictions of creep deformation could be made through a range of temperatures.

Using these new constants, the tensile/compressive creep deformation response at 815.5°C and various stresses is demonstrated in Figure 6. The graph shows an overall reduction in the creep strain rate with respect to decreasing applied stress levels. This is attributed to the modified tri-axial stress facilitating a smaller effective stress to the damage rate Equation (7) and as a result producing a lower creep strain rate. Based on the constants $\alpha$ and $\beta$, the triaxial stress in uniaxial tension is twice that during compression.

Using the tertiary creep model, Figure 6 shows a factor of 4.7 difference in the time to 5% total strain between tension and compression at 100 MPa. At 10% total strain, this factor is increased to 5.5. The $\chi$ and $\phi$ constant have great significance due to the time dependence of damage and strain and the extensive amount of time required to reach rupture at lower stress levels. As the stress applied is increased the dissolution of grain structure which produces voids, crack propagation, and leads to rupture. Capturing the compressive behavior can be just as important as accurately modeling the tensile behavior especially for materials used in transition pieces. Transition pieces undergo a myriad of stresses and high temperatures which can cause creep induced buckling [19]. An accurate estimate of service intervals could allow the preemptive patched repair maintenance of transition pieces which has been seen to extend the life of these components up to 8,000 hours [10]. The weight constants $\alpha$ and $\beta$ in Equation (8) modify triaxial stress and allow compression to occur when $\alpha + 2\beta < 1$. Figure 5 shows several yield surfaces that result from modifying these values. Hayhurst [20] showed that material constants of $\alpha=0$ and $\beta=0.25$ produce a comparable offset yield surface for Ni-base alloys which increases a materials ability to withstand compressive loads. The constitutive model was modified to use these new constants. This produces a triaxial stress which is three-fourths Von Mises stress and one-fourth hydrostatic stress. All other constants associated with Equations (5) and (7) were left unchanged. It should be noted that the $\alpha$ and $\beta$ constants chosen reproduce the general shape of the yield surface and were not optimized for the IN617 alloy due to compressive experimental creep data not being available.

TENSILE/COMPRESSIVE ASYMMETRY

There is a difference in the resulting mechanical response of a body undergoing compressive versus tensile loading. This is due to the tendency for tensile loads to enhance the tensile behavior especially for materials used in transition pieces. Transition pieces undergo a myriad of stresses and high temperatures which can cause creep induced buckling [19]. An accurate estimate of service intervals could allow the preemptive patched repair maintenance of transition pieces which has been seen to extend the life of these components up to 8,000 hours [10]. The weight constants $\alpha$ and $\beta$ in Equation (8) modify triaxial stress and allow compression to occur when $\alpha + 2\beta < 1$. Figure 5 shows several yield surfaces that result from modifying these values. Hayhurst [20] showed that material constants of $\alpha=0$ and $\beta=0.25$ produce a comparable offset yield surface for Ni-base alloys which increases a materials ability to withstand compressive loads. The constitutive model was modified to use these new constants. This produces a triaxial stress which is three-fourths Von Mises stress and one-fourth hydrostatic stress. All other constants associated with Equations (5) and (7) were left unchanged. It should be noted that the $\alpha$ and $\beta$ constants chosen reproduce the general shape of the yield surface and were not optimized for the IN617 alloy due to compressive experimental creep data not being available.

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tensile/compressive asymmetry is reduced as seen through the reduction of the 5% and 10% factors. This is caused by the reduction in time before rupture occurs. Less time allowed for less alteration of the damage and strain rate equations before rupture.

**DOMAIN DEFORMATION MODELING**

One of the key goals of this research was to demonstrate the relationship between the elastic, secondary creep, and tertiary creep stages at varies stress and temperatures over extended histories with tensile/compressive relations. Using the established thermal dependence temperature boundaries 649 to 982°C at 8.325°C intervals and stress from -500 to 500 MPa at 25 MPa intervals, 41² simulations were created. These simulations were carried in increasing magnitudes of hours from 1 to 100,000 hours. To prevent excessive model solve time and large deformation errors, a simulation was terminated once creep strain reached 100% of the un-deformed length.

The dominant deformation mechanism was determined by creating dominance contours. The ratio of a partitioned strain over total strain for each stage was found. The partition with the largest ratio was considered dominant. Simulations were conducted in both elastic and secondary creep (e.g. M=0), and tertiary creep. The following equations were used to determine the curves of dominance transition.

\[
\varepsilon_{\text{total}} = \varepsilon_{\text{elastic}} + \varepsilon_{\text{secondary}} + \varepsilon_{\text{tertiary}}
\]

\[
\text{Mechanism} = \max \left\{ \frac{\varepsilon_{\text{elastic}}}{\varepsilon_{\text{total}}}, \frac{\varepsilon_{\text{secondary}}}{\varepsilon_{\text{total}}}, \frac{\varepsilon_{\text{tertiary}}}{\varepsilon_{\text{total}}} \right\}
\]  

With the help of these equations, Figure 7 shows that over time tertiary creep becomes dominant. To plot the creep dominance lines for the complete set of simulations, the lowest stress for each temperature at which a dominance shift occurred was found at time intervals of \(10^0, 10^1, \ldots, 10^5\) hrs. Figure 8 shows the creep stage dominance of the complete simulation set at these intervals. The region below the white line signifies simulations were the elastic stage is dominant. The region between the white and black line represents secondary creep stage dominances, and anything above the black line produces tertiary creep stage dominances. The figure shows that at extended histories creep strain becomes dominantly tertiary following expected experimentally reproducible trends. Notice that at 1,000+ hours secondary creep dominance begins to disappear. This is signified by the tertiary dominance line passing the secondary dominance line. This is a result of mechanical load, time, and temperature producing a situation where the secondary creep stage is no longer viable in any of the simulations. The compressive/tensile relationship is demonstrated in this graph using the established \(\alpha\) and \(\beta\) constants. It shows that for compressive loads the disappearance of secondary creep dominance and the growth of the tertiary regime were delayed. This is expected due to the reduction in both the damage and creep strain rates.
Figure 8. Total strain deformation maps from creep simulations.
CONCLUSIONS

The materials used in gas turbine components fail by a number of physical mechanisms and combinations thereof. The focus of this investigation was modeling the creep deformation of materials used to fabricate turbine parts that exhibit strain softening at high temperatures. Creep cavitation, void coalescence along and within the boundaries of grains leads to area-reduction transverse to the applied loading axis. This leads to gradual loss of stress-carrying ability. The Kachanov-Rabotnov-type creep damage formulation was used to account for this behavior found in creep deformation and rupture experiments carried out on the three distinct Ni-base materials.

To account for temperature dependence, phenomenological models were developed for several mechanical properties. The damage formulation was modified and directly implemented into the constitutive model routine [e.g. ABAQUS User-defined Material (UMAT)] so that predictions of creep deformation could be made through a range of temperatures. The correlated curves show excellent agreement with trends from creep deformation experiments. Utilizing the Hayhurst triaxial stress formulation, the model was shown to replicate the tensile/compressive asymmetry expected of Ni-Base Superalloys. The creep stage dominance over an extensive range of mechanical load, temperature, and time configurations was determined using a new dominant deformation mechanism formulation. The difference between tensile and compressive dominance was also determined. Later studies will involve the development of a material constant optimization routine and an anisotropic temperature dependent Tertiary creep model based on similar theories.

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