The Simulation of a Unified Viscoelastic Model at Elevated Temperature

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Abstract. In this paper, a Chaboche unified constitutive model has been used to describe the cyclic plasticity and viscoplasticity of Nimonic alloy 75. A non-linear optimization algorithm has been applied in numerically simulation of this alloy at elevated temperature. Optimization algorithm has facilitated a step-by-step method to obtain the initial material parameters, while a non-linear least-square approach were used to obtain the optimized material parameters. Uniaxial experiments were carried to obtain the full cyclic stress-strain and stress relaxation data at 600°C. Satisfactory results have been obtained for the simulation of the transient and steady state cyclic stress-strain and stress relaxation behavior of dwell cyclic test.

Introduction

Characterization of material deformation behavior at elevated temperature plays an important role in the design of components such as the hot sections of modern jet engines and power plants. Understanding and simulating of plastic and viscoplastic deformation behavior is an essential part of the prediction of fatigue life of such hot components. Consequently, a unified theory of plasticity and viscoplasticity may be necessary to model the inelastic deformation behavior.

Over past decades, a number of constitutive models describing elastic-plastic deformation for the elevated temperature have been proposed [1-6]. Within these models, a group of state variables is introduced to represent the internal structural changes such as cyclic hardening/softening, relaxation and creep. Ideally, a good unified model should be physically based, able to cover important ranges of loading/temperature conditions and should contain the least number of state variables and associated material parameters. The material parameters in the unified equations must be determined from a suitable set of experiments representing a range of monotonic, cyclic, relaxation and creep tests. The quality of the parameters obtained critically depends on the quality of the experimental data and the estimation procedures.

The minimization algorithm used in this project is the gradient-based Levenberg-Marquardt method [7-8] based entirely on first order partial derivatives. This method begins using a steepest descent method, when the solution is far from the minimum, but gradually becomes an inverse-Hessian method near the minimum. The current parameter estimates are used with a very small step factor, which corresponds to a large perturbation of the model. The process is repeated automatically until the same set of parameter estimates is returned from each restart. Nonetheless, such a procedure is a deterministic one and does not guarantee that a global minimum will be found or that it is reasonable.

Nimonic alloy 75 is an 80/20 nickel-chromium alloy with controlled additions of titanium and carbon. For its good mechanical properties and oxidation resistance at high temperatures, first introduced in the 1940s for turbine blades in the prototype whittle jet engines, it is now mostly used for sheet applications calling for oxidation and scaling resistance coupled with medium strength at high operating temperature. It’s still used in gas turbine engineering and in nuclear engineering and also for industrial thermal proceeding, components of industrial furnaces, heat-treatment equipment and fixtures.
This paper presents some of our most recent work on the modeling of rate-dependent behavior of this special material alloy including stress relaxation and cycling tests using a Chaboche unified constitutive model. A gradient-driven non-linear optimization algorithm has been applied for the parameter optimization and simulation of Nimonic alloy 75 at elevated temperature. The numerical results were compared with the experimental data.

**Experimental Description**

The experimental results were obtained in a Nimonic Alloy 75. Smooth specimens with a diameter of 16 mm and gauge length of 30 mm were used for the experiments. An MTS809 servo-hydraulic testing machine was used with the computer controlled loading spectra programmed as required. An electric resistance furnace was used with the temperature controlled at 600±2°C. An extensometer (25±2.5/-2.5mm) was used to monitor the strain. All tests were carried out under strain control at a constant strain rate of \( \text{d}\varepsilon/\text{dt} = 0.005\%/\text{s} \).

A baseline cyclic test and a dwell cyclic test were carried out to obtain the full cyclic stress-strain. A strain ratio \( R_\varepsilon = -1 \) and the strain range of 2% were used for both of the two tests. In the dwell test the strain was held constant at selected strain levels ±1.0% for 100 seconds. The stress relaxation was recorded during the test.

**Non-linear Optimization Algorithm**

A Fortran program, based on the Levenberg-Marguardt algorithm has been written and used to simulate the non-linear equations of Chaboche model. The program integrates the non-linear equations using the Runge-Kutta method with variable step-size control, and computes the minimization of least squares, finally it optimizes material parameters in the Chaboche model using the Gauss-Newton method. The program also provides a number of statistical measures including the asymptotic correlation matrix and confidence interval of the optimized parameters.

As the types of experiment are different, the error variance is not homogeneous, therefore a weighted least squares estimation is more appropriate than a standard least square optimization [9]. The object function is given by

\[
F(X, \theta) = \frac{1}{2} \sum_{i=1}^{ME} \sum_{j=1}^{MP} W_{ij} [y_{ij}^\text{ex} - y_{ij}^\text{th}(X, \theta)]^2
\]

where \( y_{ij}^\text{th}(X, \theta) \) represents the model dependent-variable response prediction, \( y_{ij}^\text{ex}(X, \theta) \) represents the experimental data, \( X \) represents the independent variable, \( \theta \) is the set of parameters of the material, \( ME \) is the number of test data sets, and \( MP \) is the number of data points in the ith test data set. A weight factor \( W_{ij} \) was introduced to ensure the equal contribution from each type of the experimental data, irrespective of the number of the data points in each experiment. In this case, the weighting function is either the normalizing stress or strain (depending upon which is the dependent variable).

The optimized program identifies, firstly, a local minimum, then gradually finds a smaller local minima and finally approaches the global minimum. But sometimes, the global minimum cannot be found in the search space, because a boundary is reached. To overcome this, it is necessary to adjust the penalty function and the Tikhonov regularization function, and to enlarge experimental data set, until a reasonable global minimum is found [9].

**Estimation of Parameters**

The identification of the material parameters begins with a step-by-step procedure to obtain an initial set of parameters. These initial parameters are then used to obtain the optimized parameters in a simultaneous procedure [9]. The proximity of the initial parameters to the optimized values is critical.
as the optimiser is a first order non-linear least square minimization Eq.1, where the minimum in the difference between the numerical and the experimental results is sought.

The initial parameters estimated were used as inputs in a simultaneous identification procedure [9] to obtain an optimum set of parameters. The essence of this method is to seek a global minimum in the difference between the numerical and the experimental observables such as stress or strain. In this work, the difference between the values of stress/strain from the numerical analyses and the experiments were represented in an objective function Eq.1.

The parameters were grouped based on their physical meanings and optimized using sensitive input data. Kinematic hardening parameters were optimized first, utilizing the cyclic data primarily. A gradient-based Levenberg-Marquardt algorithm was used to obtain the optimum set of the material parameters. Global optimization was carried out after the successful “staggered” optimization of the groups of the parameters. Penalty functions were introduced at each stage to ensure that the solutions are within the realistic physical and thermodynamic boundaries. Once all the parameters were optimized, a perturbation was made and the optimization process was repeated until the optimized parameters were returned [9]. The initial and the optimized parameters are presented in Table 1.

**Comparison of the Numerical Solution and the Experimental Results**

The simulated results using the initial and optimized material parameters are compared with those obtained experimentally. Figure 1 presents the evolution of stress amplitude as a function of the number of cycle for a simple cyclic test (NM009), where the strain range was 2% and the saturation was achieved at approximately 35\textsuperscript{th} cycles. The transient behavior between the first cycle and the saturation seems to be well described by the simulation using the optimized parameters.

A dwell cyclic test (NM012) at strain hold levels $\pm 1.0\%$ was also depicted using the simulation in Figure 2, where horizontal axis indicates the duration time of relaxation test. In this figure, the simulated results using the initial and optimized parameters are compared with the experimental results. Again, the results from the optimized parameters seem to be closer to the experimental results at the strain hold period.

<table>
<thead>
<tr>
<th>Table 1. Materials parameters estimated.</th>
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<tr>
<td>Initial parameters</td>
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<tr>
<td>( b ) (MPa)</td>
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<td>( Q ) (MPa)</td>
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<tr>
<td>( a_1 ) (MPa)</td>
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<td>( a_3 ) (MPa)</td>
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<td>( C_3 )</td>
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<td>( Z ) (MPaS(^{1/n}))</td>
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<td>( n )</td>
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<tr>
<td>( K ) (MPa)</td>
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<td>( \Phi_0 ) (MPa)</td>
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<td>( b_1 )</td>
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**Closure Remarks**

Based on representative experimental data obtained from carefully controlled experiments, the initial and the optimized parameters were obtained for a Nimonic Alloy 75. The simulation using the optimized parameters offers much improved results compared with our early results [9] on advanced nickel-based superalloys. Given the fact that virtually the same optimization procedure has been followed in all the work presented, the significance of the quality of the experimental data cannot be over-emphasized. In particular, the viscous behavior captured during the stress relaxation in the dwell test seems to be critical in the determination of the parameters \( Z \) and \( n \). Since the optimizer was based
on a gradient approach that seeks the “deepest descent”, the closeness of the initial parameters to the optimized parameters is important to ensure fast and reliable convergence.

Figure 1. The evolution of stress amplitude as a function of the number of cycle.

Figure 2. Stress relaxation: comparison of the experimental and simulated results (21st cycle of the dwell test).

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Appendix I: The Chaboche unified model adopted in this work

Yield Surface

\[ f = J(\dot{\sigma} - \dot{\chi}) - R - k \leq 0 \]
\[ J(\dot{\sigma} - \dot{\chi}) = \sqrt{3/2}(\ddot{\sigma}' - \ddot{\chi}') : (\dot{\sigma}' - \dot{\chi}') = \sqrt{3/2}|\ddot{\sigma}' - \ddot{\chi}'| \]

(A1)

Kinematic Hardening

\[ \dot{\chi} = \sum_{i=1}^{n} \dot{\chi}_i \]
\[ \dot{\chi}_i = C_i (a_i \dot{\varepsilon}_p - \dot{\chi}_i \Phi \dot{\rho}) \]
\[ \Phi = \Phi_\infty + (1 - \Phi_\infty) e^{-\alpha \rho} \]

(A2)

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Isotropic Hardening  \[ \dot{R} = b(Q - R)\dot{p} \quad (A3) \]

Flow Rule  \[ \dot{\varepsilon}_p^e = \frac{3}{2} \left( \frac{J(\hat{\sigma} - \bar{x}) - R - k}{Z} \right)^{\nu} \frac{\hat{\sigma} - \bar{x}}{J(\hat{\sigma} - \bar{x})} \]
\[ \langle x \rangle = xH(x) \quad H(x) = \begin{cases} 1, & x \geq 0 \\ 0, & x < 0 \end{cases} \]

Accumulated Plastic Strain  \[ \dot{p} = \sqrt{\frac{2}{3}\dot{\varepsilon}_p^e : \dot{\varepsilon}_p} \quad (A5) \]

Parameters to be identified: E, Z, n, k, b, Q, a1, C1, a2, C2, a3, C3, \( \Phi_\infty \), b1.

References


