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An Improved Unified Viscoplastic Constitutive Model for Strain-Rate Sensitivity in High Temperature Fatigue

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Keywords: Constitutive model; Hyperbolic sine; Cyclic viscoplasticity; P91 steel; Thermo-mechanical fatigue, Strain-rate sensitivity.

Abstract

An improved unified cyclic viscoplastic material model for high temperature fatigue of P91 steel is presented. The primary enhancement over existing models is in relation to strain-rate independence of parameters, for accurate interpolation and extrapolation across a range of strain-rates and stress regimes, as relevant to flexible operation of high temperature power generation plant. The model combines a hyperbolic sine constitutive equation with anisothermal cyclic evolution of isotropic and kinematic hardening variables. The material model is developed from a thermodynamic framework and is implemented in multi-axial form within a user material subroutine. The user material subroutine is calibrated and validated for P91 steel across a range of cyclic (isothermal fatigue and thermo-mechanical fatigue) and non-cyclic high temperature loading conditions. A novel method for identification of the cyclic viscoplastic material parameters is presented here for the first time.

1 Introduction

Fossil-fuel based power generation is currently in transition from 'base-load' to intermittent mode or 'load-following' operation to accommodate the rapid rise in renewable energy. As a result of the ever changing demands of the power generation industry, fossil-fuel based power plants need to operate with increased flexibility. This requirement for more flexible use of plant results in cyclic thermal gradients, which lead to increased thermo-mechanical fatigue (TMF) of plant components and a potentially significant reduction in component life. Next generation power plant are also faced with the requirement to improve overall plant efficiency and reduce CO2 emissions. An ultra-supercritical (USC) cycle may be employed to achieve substantial improvements in plant efficiency, with increases of 37 % to 47 % (based on the higher heating value) observed for coal-fired fossil-fuel based power generation [1]. However, the use of a USC cycle comes with the additional challenges of increased steam pressure (e.g. 16 MPa to 27 MPa, [2]) and temperature (e.g. 500 °C to 600 °C). Coupled with increased TMF, this results in a considerable rise in the loads experienced by plant components. A number of crack types, in particular Type IV cracks, have been observed in plant components operating in a subcritical cycle and moderately flexible loading compared to future conditions [3]. Thus, the requirement exists for an advanced material modelling capability and the development of

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efficient and effective computational methods, which are capable of accurately predicting failure of next generation plant components.

A number of candidate materials have been identified for use with next generation plant. The current study focuses on ‘as new’ P91 steel, a 9Cr martensitic steel, with a typical chemical composition as illustrated in Table 1. P91 is used in plant header and piping systems due to its high creep strength [4-6] and increased resistance to thermal fatigue, compared with other materials used in the power generation industry [6]. This high creep strength is attributed to the mechanical properties and the complex microstructure of high Cr martensitic steels. The microstructure of such materials consists of prior austenite grains which, in turn, contain packets, blocks and laths (sub-grains) in a hierarchical format [6, 7]. It is the coarsening of these sub-grains, coupled with the inclusion of precipitates dispersed along the sub-grain boundaries, that contributes to the high creep strength of P91 steel [8-10]. The choice of P91 steel also allows for (i) increased resistance against the effects of corrosion and oxidation [6, 11] when compared with materials of a lower Cr content, (ii) a reduced value of coefficient of thermal expansion [11, 12] and (iii) reduced pipe thickness, hence reducing the capital cost of commissioning plant. Although P91 steel has a high creep strength (e.g. 95 MPa at 560 °C, [6]), an extensive assessment of the performance and analysis of fitness for use of such candidate materials under the complex loading conditions of next generation plant is required, in particular, to account for the effects of increased TMF.

At the macroscopic level, the pivotal first step in the creation of an advanced materials capability entails the development of a cyclic viscoplastic material model. A key requirement for this material model is the ability to predict the complex constitutive behaviour of candidate materials across a broad range of strain-rates and stress regimes. Also, due to the extreme temperature variations observed at an ever increasing frequency in modern plant [13], the material model must be able to accurately simulate the behaviour of candidate materials across a range of realistic temperatures and heating/cooling rates.

At present, a number of material models exist for predicting the constitutive behaviour of candidate materials. The hyperbolic sine model of Dunne and co-workers [14, 15] and the Hayhurst hyperbolic sine model [16-19] have been used effectively to capture monotonic constitutive behaviour over a wide range of strain-rates. For 9Cr steels, the Arrhenius type power law model [20], the hyperbolic sine material model of Pétry et al. [21] and the Garofalo hyperbolic sine model of Samantaray et al. [22-24] have been applied under monotonic loading conditions. However, only a few viscoplastic material models have been applied under cyclic loading and TMF conditions. The Garofalo-type MATMOD material model has been successfully applied to aluminium [25-28], but requires more than twenty material parameters from a wide range of experiments to calibrate the model [29]. The Chaboche unified power law model has been applied extensively in the literature to a wide range of materials [30-35]. The phenomenological-based Chaboche unified model has the advantage of only requiring information from isothermal fatigue and stress relaxation experiments to calibrate the required material parameters. This is attractive in reducing experimental time and from an economical viewpoint. For high Cr martensitic steels such as P91, only the Chaboche unified model, e.g. [36, 37], and the two-layer viscoplasticity model [13], both based on a Norton power law flow rule, have been applied under cyclic loading conditions. Such models are based on a constant strain-rate sensitivity and are therefore limited to a narrow range of strain-rates [38]. At the component level, the observed strain-rates are much lower than can be realistically achieved in TMF experiments [13, 39] due to the excessive test time such rates would require. To accurately model plant components subjected to modern and next generation TMF conditions, an improved material model is required to capture the creep and cyclic plasticity effects, as well as strain-rate sensitivity and anisothermal effects. This
The material model must be able to simulate both rate-dependent and rate-independent effects. As the loading conditions within a typical fossil-fuel based plant range from room temperature to temperatures above 600 °C, the high temperature loading results in high temperature creep behaviour. Coupled with this creep is the necessity to simulate cyclic loading conditions. Thus, it is essential to model the rate-independent effects associated with TMF and the flexible use of modern plant. Martensitic steels undergo considerable cyclic softening due to coarsening of the microstructure [5, 8, 40], in particular, due to the annihilation of sub-grain boundaries and an increase in sub-grain size [9, 41]. At the continuum level, isotropic hardening is included to account for the cyclic softening effect and contraction of the elastic domain in 3D stress space. The Bauschinger effect, which accounts for the translation of the centre of the elastic domain in 3D stress space, is also observed in isothermal fatigue experiments [36, 37, 42] and is accounted for here through the use of an Armstrong-Frederick type kinematic hardening evolution model. Thus, to include the interaction of both the viscous and cyclic aspects of isothermal fatigue and TMF observed in 9Cr steels under the conditions mentioned above, a unified approach is required [30, 31, 34, 36, 37, 43-46].

The material model is developed within a strict thermodynamic framework [18, 33, 38, 47-50], based on both the observable state variables for strain and temperature and careful choice of internal variables to model the effects of isotropic and kinematic hardening. Consideration is given to typical anisothermal loading conditions observed in modern plant [13] and variations of the material parameters with temperature [35, 43, 51].

The material model is implemented in both uniaxial and multi-axial form. The uniaxial implementation is a standalone computer program. The multi-axial model is implemented in the commercial finite element (FE) code Abaqus, through the use of a UMAT user material subroutine and using an implicit integration scheme to evaluate the increment in plastic strain. Comparisons are made with a range of uniaxial experimental test data available in the literature, including stress relaxation tests [36, 37, 52], creep data [53-59], isothermal monotonic and cyclic testing [36, 37, 42] and TMF tests [37] in the 400 °C to 600 °C temperature range. Currently, there is little or no multi-axial test data for P91 available in the literature.

1.1 Benefits of the Hyperbolic Sine Material Model

9Cr martensitic steels exhibit a linear stress strain-rate relationship at low stress regimes and strain-rates, and an exponential relationship at higher stresses [57, 58], as illustrated by the measured data of Figure 1. As is evident in Figure 1, modern and next generation power plants are subjected to a broad range of stress regimes and strain-rates [13]. Thus, it is clear that a single power law exponent is not sufficient to model the complete stress regime a typical power plant component experiences. However, the use of a hyperbolic sine material model overcomes this drawback and allows for reliable interpolation and extrapolation beyond a limited range of experimental data [38]. This approach also enables the more accurate modelling of the key mechanisms of deformation, i.e. the dominant creep process. Figure 2 depicts a generic deformation-mechanism map for a typical steel, which illustrates the range of different creep processes that a candidate material endures with varying stress and temperature. At low stress regimes, deformation is controlled by diffusion based creep and dislocation creep dominates as the stress increases [60-63]. This conforms well with the work of Shrestha et al. [64], who concluded that P91 steel exhibits diffusion based Nabarro-Herring creep,
with an exponent of unity at low stress regimes and displays power law creep, with an exponent of up to eleven for the higher stress regimes. As illustrated in Figure 3, the hyperbolic sine model permits a smooth transition from one phenomena to another, enabling the hyperbolic sine material model to capture the full strain-rate regime observed in modern plant.

2 Material Model

The Chaboche unified model [30, 31] is modified to allow variable strain-rate sensitivity for application to a wide range of strain-rates with a high degree of accuracy. This is achieved by replacing the power law function by a hyperbolic sine function in the constitutive equation as follows:

\[ \dot{\rho} = \alpha \sinh(\beta f) \] (1)

where \( \alpha \) and \( \beta \) are temperature dependent cyclic viscoplastic material parameters and the function \( f \) (see below) defines the elastic domain if \( f \leq 0 \) and evaluates the viscous stress or overstress, \( \sigma_v \), if \( f > 0 \). The viscous stress accounts for deviations beyond the elastic domain within 3D stress space (see Figure 4). This viscous stress represents the current equipotential surface and \( f \) is defined as [33]:

\[ f = J_2(\sigma - \chi) - R - k \] (2)

where \( \sigma \) is the stress tensor, \( \chi \) accounts for kinematic hardening, \( R \) defines isotropic hardening (see Figure 5), \( k \) is temperature dependent initial yield stress and \( J_2(\sigma - \chi) \) corresponds to the von Mises equivalent stress. This combination of equations (1) and (2) is a new formulation, although conceptually a relatively simple extension of the Chaboche unified model.

2.1 Thermodynamic Framework

The thermodynamic framework is predominately based on the well established framework for the power law model of Lemaitre and Chaboche [33]. The thermodynamic framework satisfies both the first and second laws of thermodynamics and the thermodynamic variables related to the hardening terms are obtained through careful choice of internal variables. Based upon the criterion required to model the constitutive behaviour of high Cr steels, the specific free energy is of the form:

\[ \Psi = \Psi_{el}(\varepsilon^{el}, T) + \Psi_{pl}(\alpha_i, r, T) \] (3)

where \( \Psi_{el} \) represents the elastic specific free energy, \( \varepsilon^{el} \) is the elastic strain tensor, \( \Psi_{pl} \) is the inelastic specific free energy, \( \alpha_i \) represents the kinematic hardening variables, where \( i = 1, 2, r \) corresponds to an isotropic hardening variable and \( T \) is temperature. The free energy is defined as [48]:

\[ \rho \Psi = \rho \Psi_{el} + \frac{1}{3} \sum_{i=1}^{2} C_i \alpha_i : \alpha + h(p) \] (4)

In equation (4), \( \rho \) is the mass density, \( C_i \) is a temperature dependent kinematic hardening material parameter and \( h(p) \) is an isotropic hardening function. Thus, the thermodynamic variables associated with the hardening terms are derived from equation (4) and are defined as:

\[ R = \frac{d h(p)}{dp} \] (5)
\[ \chi_i = \frac{2}{3} C_i \alpha_i \]  

(6)

To relate the hardening thermodynamic variables to a set of complementary laws, a dissipation potential is required. A Legendre-Fenchel transformation is used to obtain the flux variables as a function of the dual variables, to allow the required complementary laws to be calculated through the evaluation of the increment in effective plastic strain. The flux and dual variables are highlighted in Table 2 and for the current material model, the dual form of the dissipation potential is:

\[ \Omega = \Omega(\sigma, \chi, R; T, \alpha, \gamma) \]  

(7)

In this model, it is assumed that the viscoplastic flow is volume preserving and the third invariant is neglected. The dissipation potential is chosen in such a manner that the evolution laws for isotropic and kinematic hardening, outlined in Section 2.2, are preserved and the dissipation potential, \( \Omega \), is defined as [33]:

\[ \Omega = \Omega \left( J_2(\sigma - \chi) - R - k + \frac{1}{2} \gamma_i(p) \frac{1}{C_i} J_2(\chi_i) - \frac{2}{9} C_i \gamma_i(p) \frac{1}{C_i} (\alpha_i); T, \gamma \right) \]  

(8)

where \( \gamma_i \) is a temperature dependent kinematic hardening material parameter. Thus, the complementary laws may be obtained by differentiating equation (7) with respect to the dual variables, resulting in the following set of equations [33, 44]:

\[ \varepsilon^{pl} = \frac{\partial \Omega(f)}{\partial \sigma} = \frac{\partial \Omega}{\partial f} = \frac{\partial \Omega}{\partial f} n \]  

(9)

\[ \dot{\alpha}_i = - \frac{\partial \Omega(f)}{\partial \chi_i} = \varepsilon^{pl} - \frac{3}{2} \gamma_i(p) \chi_i \hat{\gamma} \]  

(10)

\[ \hat{\gamma} = - \frac{\partial \Omega(f)}{\partial R} \]  

(11)

where \( n \) is the tensor normal. The framework outlined here is described in more detail in Appendix A.

2.2 Model Development

Within the constitutive model, it is assumed that the material is isotropic and only small strain deformations occur, such that classical additive decomposition of the increment in strain, \( \Delta \varepsilon \), results in:

\[ \Delta \varepsilon = \Delta \varepsilon^{el} + \Delta \varepsilon^{pl} + \Delta \varepsilon^{th} \]  

(12)

where \( \Delta \varepsilon^{pl} \) is the incremental change in plastic strain tensor and \( \Delta \varepsilon^{th} \) corresponds to the incremental change of the thermal strain tensor. The increment in stress, \( \Delta \sigma \), is evaluated using the multi-axial form of Hooke's law, which is defined with respect to the elastic strain as:

\[ \Delta \sigma = 2\mu (\Delta \varepsilon - \Delta \varepsilon^{th}) + \lambda \text{Tr}(\Delta \varepsilon - \Delta \varepsilon^{th}) I - 2\mu \Delta \varepsilon^{pl} \]  

(13)

where \( I \) is the identity matrix and \( \mu \) and \( \lambda \) are Lamé's constants. The first two terms on the right hand side correspond to the elastic predictor and the final term corresponds to a plastic correction term. The increment in plastic strain is determined using the flow rule described in equation (9). For the material
model considered here, the dissipation potential is obtained retrospectively such that it satisfies the hyperbolic sine constitutive model defined in equation (1), as follows:

\[ \Omega(f) = \frac{\alpha}{\beta} \cosh(\beta f) \, \text{sgn}(f) \]  

(14)

As \( \alpha \) and \( \beta \) are positive values, the \( \text{sgn}(f) \) function ensures that the dissipation potential gives the correct behaviour, i.e.:

\[ \text{sgn}(f) = \begin{cases} 
-1 & \text{if } f < 0 \\
0 & \text{if } f = 0 \\
1 & \text{if } f > 0 
\end{cases} \]

The flow rule describing the plastic strain-rate is then defined as:

\[ \dot{\varepsilon}^{\text{pl}} = \dot{\rho} n \]  

(15)

and the tensor normal, \( n \), is defined as [15, 43]:

\[ n = \frac{3}{2} \left( \frac{s - x}{j_2(s - \chi)} \right) = \frac{3}{2} \left( \frac{s^{\text{tr}} - x}{j_2(s^{\text{tr}} - \chi)} \right) \]  

(16)

where \( s, x, s^{\text{tr}}, \) and \( \sigma^{\text{tr}} \) are the deviatoric stress, the kinematic hardening deviator (which is deviatoric by nature, i.e. \( x = \chi \)), the deviatoric trial stress, and the trial stress respectively. The evolution of the isotropic hardening variable, \( R \), is defined as [35]:

\[ \dot{R} = b(Q - R) \dot{\rho} + \left( \frac{1}{b} \frac{\partial b}{\partial T} + \frac{1}{Q} \frac{\partial Q}{\partial T} \right) R \dot{T} \]  

(17)

where \( b \) and \( Q \) are temperature dependent material parameters and the final term is a temperature rate term. The centre of the elastic domain in 3D stress space is defined by the back stress tensor:

\[ \chi = \sum_{i=1}^{2} \chi_i \]  

(18)

In equation (18), \( \chi_i \) represents the kinematic hardening produced during the initial stages of strain hardening and \( \chi_2 \) accounts for the kinematic hardening due to the latter stages of strain hardening. The evolution of the back stress components is described by the Armstrong-Frederick kinematic hardening model [33], with the inclusion of a temperature rate term [43]:

\[ \dot{\chi}_i = \frac{2}{3} \dot{C}_i \dot{\varepsilon}^{\text{pl}} - \gamma_i \chi_i \dot{\rho} + \frac{1}{\dot{C}_i} \frac{\partial \dot{C}_i}{\partial T} \chi_i \dot{T} \]  

(19)

The three terms in equation (19) correspond to (i) a linear kinematic hardening term, (ii) a recall term to account for the fading memory effect of the deformation path and (iii) a temperature rate term respectively. There is no temperature rate term associated with the recall term as it is time and rate independent [33].

### 2.3 UMAT Implementation

The increment in effective plastic strain is obtained using an implicit integration scheme. In order to update all the required quantities in terms of the increment in effective plastic strain-rate, the von...
Mises equivalent stress, $\sigma_e$, is defined as a function of the trial stress and the increment in effective plastic strain-rate as [15]:

$$J_2(\sigma - \chi) = \sigma_{tr}^e - 3G\Delta p$$

(20)

where $G$ is the shear modulus, $\Delta p$ is the increment in effective plastic strain and $\sigma_{tr}^e$ is the von Mises equivalent trial stress, defined as:

$$\sigma_{tr}^e = \left[ \frac{3}{2} (s^{tr} - \chi) : (s^{tr} - \chi) \right]^{1/2}$$

(21)

Thus, the constitutive equation for the increment in effective accumulated plastic strain-rate, given in equation (1), may be rewritten as:

$$\dot{\rho} = \phi(\Delta p, \chi, R) = \alpha \sinh \beta (\sigma_{tr}^e - 3G\Delta p - R - k)$$

(22)

Rearranging equation (22) and writing it incrementally in a form suitable for a Newton iterative method yields [15]:

$$\varphi(\Delta p, \chi, R) = \Delta p - \phi(\Delta p, \chi, R)\Delta t = 0$$

(23)

Applying the Newton iterative method then results in:

$$\varphi + \frac{\partial \varphi}{\partial \Delta p} d\Delta p + \frac{\partial \varphi}{\partial \chi} d\chi + \frac{\partial \varphi}{\partial R} dR = 0$$

(24)

Evaluating the partial derivatives in equation (24) gives:

$$\varphi + \left(1 - \frac{\partial \phi}{\partial \Delta p}\Delta t \right) d\Delta p - \frac{\partial \phi}{\partial \chi} \Delta t d\chi - \frac{\partial \phi}{\partial R} \Delta t dR = 0$$

(25)

Thus, evaluating the partial derivatives and rearranging equation (25) to obtain the iterative increment in effective plastic strain yields:

$$d\Delta p = \left[ \varphi - (\Delta p/\Delta t) - Zn: C_1 \frac{\partial G}{\partial T} dT - Z \left( \frac{1}{b} \frac{\partial b}{\partial T} + \frac{1}{Q} \frac{\partial Q}{\partial T} \right) RdT \right]$$

(26)

$$\left[ \frac{1}{\Delta t} + 3GZ + ZC_1 - Zn: C_1 \chi_1 + Zb(Q - R) \right]$$

where

$$Z = \alpha \beta \cosh \beta (\sigma_{tr}^e - 3G\Delta p - R - k)$$

(27)

And the increment in effective plastic strain is:

$$\Delta p = \Delta p + d\Delta p$$

(28)

Equation (28) is updated until convergence is obtained. The tolerance within the present study is set at $1 \times 10^{-10}$ and convergence is checked against the numerator of equation (26).

The material model is implemented within a UMAT user material subroutine for use with the commercial FE code Abaqus. A flowchart depicting the main processes within the UMAT is shown in
Figure 6. To ensure that unloading occurs elastically within the material model, the following conditions represent viscoplastic behaviour in 3D stress space:

\[ f > 0 \text{ and } (\partial f / \partial \sigma) : \varepsilon > 0 \]  

(29)

The increment in plastic strain is determined using the flow rule of equation (15). The increment in stress is calculated as:

\[ \Delta \sigma = \Lambda : (\Delta \varepsilon - \Delta \varepsilon^\text{pl} - \Delta \varepsilon^\text{th}) \]  

(30)

where \( \Lambda \) is the elasticity tensor. The material model is also implemented uniaxially in a standalone computer program as a material parameter calibration tool and to validate the UMAT implementation.

3 Results

3.1 Determination and Calibration of Material Parameters

The model requires a total of twelve temperature-dependent material parameters in three groups of material parameters, namely: (i) the elastic material parameters, which consist of Young's modulus, \( E \), the coefficient of thermal expansion, \( \alpha_{\text{COE}} \), and Poisson's ratio, \( \nu \), (ii) the cyclic plasticity material parameters related to isotropic hardening (\( h \) and \( Q \)) and kinematic hardening (\( C_1 \), \( C_2 \), \( \gamma_1 \) and \( \gamma_2 \)), as well as the initial, cyclic, yield stress value, \( k \), and (iii) the temperature-dependent cyclic viscoplastic material parameters \( \alpha \) and \( \beta \). The material parameters are calibrated from experimental data via a three step process using the standalone uniaxial code.

Step 1: Elastic Material Parameters

The elastic constants for Young's modulus are calibrated from the initial monotonic portion of the cyclic test data and the values of the coefficient of thermal expansion are taken from published ASME data \[65\], with an assumed linear dependence on temperature in the 400 °C to 600 °C temperature range. Poisson's ratio, \( \nu \), is taken to have a constant value of 0.3 throughout the simulations and the elastic material parameters for 'as new' P91 steel are shown in Table 3.

Step 2: Cyclic Plasticity Material Parameters

The isotropic and kinematic hardening evolution equations are similar to those used in Saad et al.\[37\], except for the additional anisothermal terms of the present model. Hence, the hardening parameters have been adopted from the latter, with algebraic manipulation to suit the specific formulation used here. The cyclic plasticity parameters for the 400 °C to 600 °C temperature range are presented in Table 4.

Step 3: Creep Related Material Parameters

The cyclic viscoplastic material parameters \( \alpha \) and \( \beta \), of equation (1), are intrinsically linked to the viscous (creep) behaviour of the material, and should ideally be obtained from long term creep data, similar to the experimental data of Figure 1. Plotting stress against strain-rate on a log-log axis for the creep loading case enable curve fitting to the data using the following expression for the minimum creep rate:
where $\alpha_{CR}$ and $\beta_{CR}$ are the secondary creep constants and $\sigma$ is the uniaxial stress. Figures 7 and 8 illustrate the excellent correlation achieved with the experimental data of Haney et al. [57] and Klueh et al. [58] and the fit obtained using equation (31), further highlighting the importance and capability of the hyperbolic sine constitutive equation. However, the conditions present in modern plant operating under increased flexibility and the unified nature of the current material model dictates that the effects of rate-independent cyclic plasticity must also be accounted for through the use of cyclic viscoplastic material parameters, namely $\alpha$ and $\beta$ of equation (1). Hence, the values of $\alpha_{CR}$ and $\beta_{CR}$ need to be adjusted using a data fitting process to fit the isothermal fatigue test data and the experimental stress relaxation results. This process uses the constants obtained from the long term creep data as a starting position. A relationship between the viscoplastic parameters in a pure creep loading condition ($\alpha_{CR}$ and $\beta_{CR}$) and the cyclic viscoplastic material parameters ($\alpha$ and $\beta$) has been identified to allow the value of $\beta$ to be obtained from creep data. This relationship is:

$$\beta_{CR} \equiv \beta$$

so that $\alpha$ may be scaled as:

$$\alpha = \frac{\alpha_{CR} \sinh \beta \sigma}{\sinh \beta f} = A\alpha_{CR}$$

where $A$ is the cyclic viscoplastic scaling factor. As equation (33) includes the cyclic plasticity terms, $\chi$ and $R$, the value of $\alpha$ is fitted to data from stress relaxation tests using a theoretical approach supplemented by the standalone uniaxial code. For an isothermal, uniaxial stress relaxation test, once the load has been applied to its maximum value, $\sigma_0$, and held at this displacement for a period up to time $t$, the theoretical strain history is given by:

$$\frac{d\sigma}{\sinh \beta f} = -\alpha E dt$$

where $E$ is Young's modulus. The uniaxial stress, $\sigma$, may be then written as a function of time:

$$\sigma = \frac{2}{\beta} \tanh^{-1} \left( \tanh \left( \frac{\beta (\sigma_0 - \chi - R - k)}{2} \right) e^{-\alpha \beta E (t-t_0)} \right) + \chi + R + k$$

where $t_0$ is the time at which the load has reached its maximum value, i.e. at the start of the hold period, and hence, a value of $\alpha$ may be obtained. In equation (35), the initial decay rate of the stress relaxation test is predominately controlled by $\beta$ and the level of stress obtained increases with decreasing values of $\alpha$ and/or $\beta$. Figures 7 and 8 illustrate the relationship between the secondary creep material parameters and the cyclic viscoplastic material parameters, for 500 °C and 600 °C respectively, with more creep behaviour observed at 600 °C as a closer relationship between the creep and cyclic viscoplastic material parameters is predicted. The cyclic viscoplastic material parameters are given in Table 5.

**Calibration Process**

The calibration process is based on data at 400 °C, 500 °C and 600 °C and at a cyclic strain-rate of 0.1 %/s only. For the temperatures in the present study, the results of the viscoplastic material parameter calibration process are contained in Figures 9 to 12. Figure 9 depicts the calibrated fit obtained with
the stress relaxation data of Koo and Kwon [36] at temperatures of 500 °C and 600 °C respectively. Figure 10 illustrates the excellent fit achieved with the cyclic data of Saad et al. [37] at 400 °C and a strain-rate of 0.1 %/s for the initial and stabilised cycles, i.e. capturing the evolution (softening) of the cyclic responses. Figures 11 and 12 show the calibration results at 500 °C and 600 °C respectively, where once again an excellent fit with the experimental data (also including the cyclic softening) is obtained.

3.2 Material Model Validation
To analyse the performance of the material model, validation is conducted against a range of experimental data intermediate to or outside of the range of the calibration data in Section 3.1 (see Figures 9 to 12). Hence, application of the model to other temperatures and strain-rates constitutes validation with respect to temperature and strain-rate sensitivity and interpolation or extrapolation. The validation model setup employs an axisymmetric FE implementation of a test specimen gauge length. As an initial step in the validation process, it was first established that the standalone uniaxial code and the UMAT implementation gave identical results for uniaxial loading conditions. The model results presented below are those of the UMAT and the loading conditions applied to the FE model are based on the isothermal fatigue experiments conducted by [36, 37, 42] and the TMF data of [37], as summarised in Table 6. Within the present study, piece-wise linear interpolation is used to account for the variation of the material parameters as a function of temperature.

Stress Relaxation Tests
To assess the strain-rate sensitivity of the material model (and the strain-rate independence of the material parameters), the predicted FE results are compared with stress relaxation tests conducted at a variety of different loading conditions, temperatures and hold times. The experimental results are obtained from data available in the literature [37, 52] for temperatures of 500 °C and 550 °C. Validation is obtained by comparison with two different hold times of 120 s and 3500 s, which are simulated at the displacements corresponding to the maximum stress in Figure 13. The results in Figure 13 illustrate excellent agreement with the experimental data for the range of conditions simulated.

Isothermal Loading
For cyclic loading under isothermal conditions, the performance of the material model was compared with experimental data at temperatures of 500 °C and 550 °C. The material model was validated at strain-rates of 1 %/s to 0.01 %/s, which lie above and below the strain-rate used for calibration, with strain ranges of ±0.35 % to ±0.6 % respectively. Validation is achieved by comparison with experimental data available from two different sources in the literature [36, 42]. Figure 14 illustrates the result obtained at a temperature of 500 °C for the initial and stabilised cycles where a good fit is obtained with the experimental data of Koo and Kwon [36]. Figures 15 and 16 demonstrate the interpolation performance of the material model with respect to temperature and strain-rate. The results show excellent correlation with the experimental data.

Anisothermal Loading
Anisothermal loading conditions are also simulated to validate the improved model against TMF tests from [37], within the 400 °C to 600 °C temperature range. Both in-phase and out-of-phase TMF loading conditions are simulated, as depicted in Figure 17. For in-phase loading, Figure 18 shows the excellent fit achieved with TMF test data for the 400 °C to 500 °C case and Figure 19 also illustrates
good correlation for the out-of-phase case. The results of the 400 °C to 600 °C in-phase loading simulations are contained in Figure 20, where a good fit with the experimental data is again obtained.

4 Discussion

This study presents an improved (hyperbolic sine) unified cyclic viscoplastic material model, which is capable of capturing the complex high temperature material behaviour of 9Cr steels under cyclic loading conditions. The material model has been implemented in a UMAT user material subroutine for use with Abaqus and has been successfully validated for a range of uniaxial loading conditions. The benefit of using the hyperbolic sine material model is its ability to capture the measured strain-rate sensitivity of stress, as illustrated in Figures 7 and 8 and hence enables the identification of material parameters which are independent of strain-rate. This contrasts with the more conventional (Chaboche) power law unified viscoplastic model [30-33, 36, 37], which is limited to a narrow range of strain-rates via the constraint of constant strain-rate sensitivity.

The results of the validation process illustrate that the material model is successful at determining the constitutive behaviour of high Cr steels across a broad range of strain-rates and strain ranges. This ability is typified by Figure 13, which portrays the relaxation behaviour of P91 steel, obtaining excellent agreement with the experimental data at 500 °C and a reasonable fit with the experimental data at the intermediate temperature of 550 °C. The results depicted in Figures 14 to 16 show that the material model is capable of reproducing the isothermal cyclic constitutive behaviour for the test conditions of Koo and Kwon [36] and Fournier et al. [42], to a high degree of accuracy at strain-rates of 0.01 %/s and 1 %/s respectively, which lie outside the range of calibration. These results conclude that the hyperbolic sine material model presented here can accurately capture the strain-rate effect observed in high Cr steels under high temperature loading, to facilitate accurate interpolation and extrapolation from the limited range of experimental data typically available. This is important for simulating the requirement for flexible conditions of modern [13] and next generation plant.

The novel method for the calibration of the cyclic viscoplastic material parameters, $\alpha$ and $\beta$, identifies another benefit of the new material model. The identification of pure creep material parameters, $\alpha_{CR}$ and $\beta_{CR}$, and the subsequent determination of a scaled value of the cyclic viscoplastic parameter $\alpha$, represents a method of reconciling long- and short-term creep data. Also, this process of cyclic viscoplastic parameter identification is the key step to capturing the strain-rate effect. The choice of the isotropic hardening model described in equation (17), coupled with a negative $Q$ value, as highlighted in Saad et al. [37], allows for the cyclic softening behaviour of martensitic steels to be modelled, with reductions of up to 22 % observed in the experimental work conducted by Saad and co-workers [37].

From Figures 18 to 20, the FE predicted results show excellent correlation with the TMF test data of Saad et al. [37], particularly for the initial cycles and the in-phase loading conditions. The slight over-prediction of the stress range, by approximately 5 % for the TMF-OP, 400 °C to 500 °C temperature range, is attributed to non-optimised material parameters, including the coefficient of thermal expansion, and the use of a piece-wise linear interpolation scheme. Within the current material model, the opportunity exists for the development of more complex global optimisation techniques, such as conducted by Gong et al. [66], Huber et al. [67] or Mahmoudi et al. [68], which may be used to obtain more precise values of the twelve material parameters. The inclusion of an Arrhenius type function, as conducted in [20, 25, 26], may generate further improvements and simplification in the interpolation
of material parameters as a function of temperature. Furthermore, the impact of the inclusion of temperature rate terms in equations (17) and (19) is found to have a beneficial (albeit small) impact for the conditions simulated here.

This development of a hyperbolic sine material model represents completion of the first key step in developing a multi-scale advanced materials capability, which can accurately predict the life of modern and next generation plant components. Future work will address multi-axial validation of the material model, via comparison with experimental results from notched specimen testing, similar to Ha et al. [69] and Kupkovits and co-workers [70], or small punch tests as conducted by Milička and Dobeš [54].

5 Conclusions

The key novel contributions of this study are as follows:

- An improved unified cyclic viscoplasticity model, via a hyperbolic sine flow rule with cyclic evolution of nonlinear isotropic and kinematic hardening, to achieve significantly improved strain-rate sensitivity for high temperature fatigue applications. This is important for life prediction of modern power plant in significantly more flexible operation modes.
- Multi-axial implementation of the material model in a UMAT user subroutine, incorporating cyclic evolution of isotropic and kinematic hardening and creep effects under anisothermal loading conditions, using an implicit integration scheme.
- Development of a novel (cyclic) viscoplastic parameter identification process to effectively 'unify' long- and short-term creep data and application to P91 steel in the 400 °C to 600 °C temperature range.
- The modelling of TMF test conditions via temperature rate terms in the evolution equations of the hardening variables and temperature dependent material parameters, identified from isothermal test data.
- Uniaxial validation of the performance of the material model against isothermal fatigue, stress relaxation and TMF test data.

Acknowledgements

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References


Appendix A

The thermodynamic framework for this material model is predominately based upon the first law (the conservation of energy), and second law of thermodynamics. The conservation of energy is defined as [18, 33, 38, 49]:

$$\rho \dot{\varepsilon} = \sigma : \dot{\varepsilon} + r_{vd} - \text{div} \mathbf{q} \tag{A1}$$

where $e$ is the specific internal energy, $r_{vd}$ is the volumetric density of internal heat production and $\mathbf{q}$ is the heat flux. The second law of thermodynamics is defined as [33]:

$$\rho \frac{ds}{dt} + \frac{\text{grad} \mathbf{q}}{T} - \frac{r_{vd}}{T} \geq 0 \tag{A2}$$

where $s$ is the specific entropy. Combining the first and second laws of thermodynamics and multiplying by $T > 0$ yields:

$$\rho \left( T \frac{ds}{dt} - \frac{de}{dt} \right) + \sigma : \dot{\varepsilon} - \mathbf{q} \frac{\text{grad} T}{T^2} \geq 0 \tag{A3}$$

The rate form of the specific free energy, $\Psi$, is given as [33]:

$$\Psi = \frac{de}{dt} - T \frac{ds}{dt} - s \frac{dT}{dt} \tag{A4}$$

The Clausius-Duhem inequality may then be obtained by rearranging and inserting equation (A4) into the second law of thermodynamics [33]:

$$\sigma : \dot{\varepsilon} - \rho \left( \frac{\partial \Psi}{\partial r} \right) - \mathbf{q} \frac{\text{grad} T}{T^2} \geq 0 \tag{A5}$$

For the material model within the present study, the specific free energy, $\Psi$, may be decomposed into its elastic and inelastic components as:

$$\Psi = \Psi_{ei}(\varepsilon^{ei}, T) + \Psi_{pl}(\alpha_1, \alpha_2, r, T) \tag{A6}$$

From equation (A6), the thermodynamic variables related to the hardening terms are given as:
Using a Legendre-Fenchel transformation [33], the dual form of the dissipation potential, which represents the flux variables as a function of the dual variables, may be obtained as:

\[ \Omega = \Omega (\sigma, \chi_1, \chi_2, R; T, \alpha_1, \alpha_2, r) \]  

(A9)

Thus, the resulting complementary laws are of the form:

\[ \dot{\varepsilon} = \frac{\partial \Omega}{\partial \sigma} \]  

(A10)

\[ \dot{\alpha}_i = -\frac{\partial \Omega}{\partial \chi_i} \]  

(A11)

\[ \dot{r} = -\frac{\partial \Omega}{\partial R} \]  

(A12)

The free energy is given by [33, 48]:

\[ \rho \Psi = \rho \Psi_{\text{el}} + \sum_{i=1}^{2} \frac{1}{3} C_i \alpha_i \chi_i + h(p) \]  

(A13)

and the isotropic hardening term, \( h(p) \), is defined as [33]:

\[ h(p) = Q_p - \frac{Q}{b} [1 - \exp(-bp)] \]  

(A14)

Thus, the associated thermodynamic variables (see equations (A7) and (A8)) may be rewritten as:

\[ R = \frac{\partial h(p)}{\partial p} \]  

(A15)

\[ \chi_i = \frac{2}{3} C_i \alpha_i \]  

(A16)

From Lemaitre and Chaboche [33], the dissipation potential, \( \Omega \), is:

\[ \Omega = \Omega \left( J_2(\sigma - \chi) - R - k + \frac{1}{2} \frac{\gamma_i(p)}{C_i} J_2(\chi_i) - \frac{2}{9} C_i \gamma_i(p) J_2(\chi_i) \right) \]  

(A17)

such that the complementary laws of equations (A10) to (A12) become [33, 43, 44]:

\[ \dot{\varepsilon} = \frac{\partial \Omega}{\partial \sigma} = \frac{\partial \Omega}{\partial f} \frac{\partial f}{\partial \sigma} = \frac{\partial \Omega}{\partial f} n \]  

(A18)
Combining equation (A11) and equation (A19) allows for the kinematic hardening evolution law described in equation (19) to be obtained and such that the dissipation potential reduces to [33]:

\[ \Omega = \Omega \left( J_2 (\sigma - \chi) - R - k; T, \nu \right) \]  

(A21)
Tables

Table 1: Chemical composition of P91 steel [6].

<table>
<thead>
<tr>
<th>Element</th>
<th>C</th>
<th>Mn</th>
<th>P</th>
<th>S</th>
<th>Si</th>
<th>Cr</th>
<th>Mo</th>
<th>Ni</th>
<th>V</th>
<th>Nb</th>
<th>N</th>
<th>Al</th>
</tr>
</thead>
<tbody>
<tr>
<td>Weight (%)</td>
<td>0.08-0.012</td>
<td>0.30-0.60</td>
<td>0.02 max</td>
<td>0.01 max</td>
<td>0.20-0.50</td>
<td>8.00-9.50</td>
<td>0.85-1.05</td>
<td>0.4 max</td>
<td>0.18-0.25</td>
<td>0.06-0.10</td>
<td>0.03-0.07 max</td>
<td>0.04</td>
</tr>
</tbody>
</table>

Table 2: The dissipation variables within the material model written in terms of the flux variables and the dual variables.

<table>
<thead>
<tr>
<th>Dissipation Variables</th>
<th>Flux Variables</th>
<th>Dual Variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\dot{\varepsilon}^p$</td>
<td>$\sigma$</td>
<td></td>
</tr>
<tr>
<td>$-\dot{\alpha}$</td>
<td>$\chi_i$</td>
<td></td>
</tr>
<tr>
<td>$-\dot{\gamma}$</td>
<td>$R$</td>
<td></td>
</tr>
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</table>

Table 3: Elastic material parameters.

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Young's Modulus (GPa)</th>
<th>Thermal Expansion (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>400</td>
<td>184</td>
<td>$12.95 \times 10^{-6}$</td>
</tr>
<tr>
<td>500</td>
<td>180</td>
<td>$13.31 \times 10^{-6}$</td>
</tr>
<tr>
<td>600</td>
<td>142</td>
<td>$13.59 \times 10^{-6}$</td>
</tr>
</tbody>
</table>

Table 4: Cyclic plasticity material parameters [37].

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>$Q$ (MPa)</th>
<th>$b$</th>
<th>$C_1$ (MPa)</th>
<th>$\gamma_1$</th>
<th>$C_2$ (MPa)</th>
<th>$\gamma_2$</th>
<th>$k$ (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>400</td>
<td>-55.0</td>
<td>0.45</td>
<td>352500.0</td>
<td>2350.0</td>
<td>48600.0</td>
<td>405.0</td>
<td>96</td>
</tr>
<tr>
<td>500</td>
<td>-60.0</td>
<td>0.60</td>
<td>215872.6</td>
<td>2191.6</td>
<td>48235.29</td>
<td>460.7</td>
<td>90</td>
</tr>
<tr>
<td>600</td>
<td>-75.4</td>
<td>1.00</td>
<td>106860.0</td>
<td>2055.0</td>
<td>31159.90</td>
<td>463.0</td>
<td>43</td>
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</table>

Table 5: Identified cyclic viscoplasticity parameters.

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>$a$ (s$^{-1}$)</th>
<th>$\beta$ (MPa$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>400</td>
<td>$1.4 \times 10^{-6}$</td>
<td>0.07</td>
</tr>
<tr>
<td>500</td>
<td>$8.0 \times 10^{-7}$</td>
<td>0.064</td>
</tr>
<tr>
<td>600</td>
<td>$1.0 \times 10^{-7}$</td>
<td>0.055</td>
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</table>

Table 6: Isothermal fatigue experimental test conditions.

<table>
<thead>
<tr>
<th>Source</th>
<th>Strain-Rate (%/s)</th>
<th>Strain Range (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fournier et al.[42]</td>
<td>1.00</td>
<td>$\pm 0.35$</td>
</tr>
<tr>
<td>Saad et al.[37]</td>
<td>0.10</td>
<td>$\pm 0.50$</td>
</tr>
<tr>
<td>Koo and Kwon[36]</td>
<td>0.01</td>
<td>$\pm 0.60$</td>
</tr>
</tbody>
</table>
**Figures**

**Figure 1:** Measured relationship between strain-rate and stress for P91 steel at high temperature (600 °C).

**Figure 2:** Generic deformation map for a typical steel.
Figure 3: Typical stress-strain-rate behaviour of the mechanisms of deformation for P91 steel and a hyperbolic sine fit to the dominant creep process.

Figure 4: Elastic and viscoplastic domains in 3D stress space with the back stress tensor representing the centre of the elastic domain.
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Figure 7: Comparison of theoretical model to long term creep data illustrating the effect of the creep and cyclic viscoplastic parameters at a temperature of 500 °C.

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Figure 9: Calibration of the cyclic viscoplasticity material parameters from stress relaxation tests [36], at temperatures of (a) 500 °C and (b) 600 °C.

Figure 10: Calibration of material parameters from measured evolving stress-strain data [37] at 400 °C and a strain-rate of 0.1 %/s for (a) the initial cycle and (b) after 800 cycles.

Figure 11: Calibration of material parameters from measured evolving stress-strain data [37] at 500 °C and a strain-rate of 0.1 %/s for (a) the initial cycle and (b) after 600 cycles.
Figure 12: Calibration of material parameters from experimental data [37] at 600 °C and a strain-rate of 0.1 %/s for the initial and 300th cycles.

Figure 13: Comparison of predicted FE results with experimental stress relaxation data at (a) a temperature of 500 °C for 120 s [37] and (b) at a temperature of 550 °C for 3500 s [52].

Figure 14: Comparison of FE-predicted and measured evolving stress-strain data [36] at 500 °C and a strain-rate of 0.01 %/s for (a) the initial cycle and (b) after 130 cycles.
Figure 15: Comparison of FE-predicted and measured evolving stress-strain data [36] at 550 °C and a strain-rate of 0.01 %/s for (a) the initial cycle and (b) after 103 cycles.

Figure 16: Comparison of FE-predicted and measured evolving stress-strain data [42] at 550 °C and a strain-rate of 1 %/s for (a) the initial cycle and (b) after 2000 cycles.

Figure 17: Loading conditions for (a) TMF-IP loading and (b) TMF-OP loading conditions.
Figure 18: Comparison of FE-predicted and measured [37] hysteresis loops for 400-500 °C, TMF-IP loading for (a) the initial cycle and (b) after 100 cycles.

Figure 19: Comparison of FE-predicted and measured [37] hysteresis loops for 400-500 °C, TMF-OP loading for (a) the initial cycle and (b) after 100 cycles.

Figure 20: Comparison of FE-predicted and measured [37] hysteresis loops for 400-600 °C, TMF-IP loading for (a) the initial cycle and (b) after 3 cycles.