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The development and validation of the creep damage constitutive equations for P91 Alloy

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Abstract - This paper presents research on the validation of a set of creep damage constitutive equations for P91 alloy under multi-axial states of stress, and its applicability under lower stress level. Creep damage is one of the serious problems for the high temperature industries and computational creep damage has been developed and used, complementary to the experimental approach, to assist safe operation. In creep damage mechanics, a set of constitutive equations needs to be developed and validated. Recently, a mechanism-based approach for the developing creep damage constitutive equation for this type of high Cr alloy has merged and several versions of creep damage constitutive equations have been proposed. However, so far, they are limited to uni-axial case under medium to high stress level. In fact, multi-axial states of stress and lower stress level are more pertinent to the real industrial applications. That is the objective of this research. This paper contributes to the methodology and specific knowledge.

Keywords: P91, Creep mechanism, CDM Model

1. Introduction

Scientists estimate that the world power requirement will increase by up to 50% in the next 20 years. Hence, it is essential to develop the advanced energy resources which must be cost effective, sustainable and environmental friendly [1]. The Cr-Mo steels have been the material of choice for using in the power generation plants [2]. During 1960s, the Ferriticmartensitic steels with 9-12 wt% Cr were developed for fossil-fuel-fired power plants [3], and used for boiler tube in the advanced gas-cooled reactors [4, 5] later on. P91 (9Cr-1Mo-V-Nb) steel is mostly used in thermal power plants because of its high strength at high temperatures and it has already about ten years for its practical application. Because of concerns about the age-degradtion in the mechanical properties at elevated temperatures of structural components manufactured, more and more research have been conducted to predict the creep life and residual life of base metal of P91 steel [6].

Recently, continuum damage mechanisms modeling were applied to simulate the creep behavior of modified 9Cr-1Mo steel. Firstly, the Orowan Equation was employed to relate the density of mobile dislocations and their glide velocity. Blum et al. (2002) said that the evolution of dislocations was estimated based on a model proposed [7]. Secondly, Orowan's equation was modified by adding the contributions of influences of various creep damage mechanisms such as solid solution depletion, precipitate coarsening, and cavitation. Creep cavitation (nucleation, growth, and coalesces) is another mechanism which affects creep strain, creep damage and rupture. Yin and Faulkner (2006) [8] advanced the approach of continuum creep damage mechanics modelling of McLean and Dyson (2000) [9] by introducing a specific formula to count for the creep cavity damage for 9Cr alloy. Recently, Yunxiang and Ke Yang (2011) [10] have developed a set of creep damage constitutive equations for P91 alloy under the medium and high stress level, following the similar approach, and they have included strain hardness, solute depletion, and particle coarsening, ignoring the multiplication of mobile dislocations.

In this paper, the objectives are respectively divided into below three aspects:

1. To understand the creep damage, continuum creep damage mechanisms, effectively use the numerical method of Euler integration by software of Excel.

2. To validate a set 3D creep damage constitutive equations generalized from Chen Yunxiang and Ke Yang (CK formulation) for P91 at 600 under high stress.

3. To extend the uniaxial creep damage constituteve equations of Chen Yunxiang and Ke Yang for P91 at $600\Box$ under plane stress condition and plane strain condition and apply the uniaxial model from high stress for middle and low stress.

2. Continuum creep damage mechanics modeling

The theory of continuum mechanics is the establishment of the basis of the hypothesis of presented continuous research on realizable on law of motion. The theory of continuum mechanics has a great advantage on the mathematical modeling. Therefore, there are many existing with some microscopic defects inside of materials, such as dislocation, inclusions, cavitation at el. In order to describe the effects of the microscopic defects, Kachanov provided the concept of continuous damaged mechanics. The development and evolution of the continuum damage modeling is based on the concept later on. The main microstructural changes of P91 (high Cr) alloy is summarized below:

2.1. Solid solution depletion (Ds)

The alloying elements are added to enhance the resistance for dislocation motion, which increase the creep resistance of the material. The experimental data on 9Cr-1Mo have shown the creep resistance of precipitation is decreasing during Fe2Mo laves phase. During the conditions of long term high temperature and stress exposure, the Mo depletion in the subgrain matrix produced the decreasing of creep resistance. The element of Mo is added to the material in order to increase the mechanism of solid solution strengthening. There is no helping for the dislocations motion decreasing by the large size of the Laves phase of Fe2Mo and the low volume fraction [1]. The large size Laves phases at grain boundaries are the most likely source of cavity nucleation and the intergranular fracture. This mechanism is described the damage evolution of void nucleation and crack formation. According to Y.F. Yin (2006) [8], the damage owing of the solute depletion (Ds) is defined:

$$Ds = 1 \Box \frac{\Box}{\Box}$$
(1)

where Co is the initial concentration of solid solution in the matrix, and initial is their average concentration at time t. In addition, the rate of change of Ds by Dyson's approach follow by Wert-Zener equation [11] is

$$\dot{\Box}_{\rm s} = {\rm KsDs}^{1/3} (1 \Box \Box_{\Box}) \tag{2}$$

where the parameter of constant Ks is defined as:

$$\mathbf{Ks} = [48 \square^{(}\mathbf{C}_0 \square \stackrel{\square}{=} \square^{1/3} \mathbf{n}^{2/3} \mathbf{D}]$$
(3)

where D is the diffusion coefficient of Mo in matrix, the n is the number of precipitate particles and C_{β} is the concentration of solid solution in the precipitate of Laves. The values of Co and Ce using Thermo-Calc and found Co = 0.56 mol% and Ce= 0.33 mol% [1].

2.2. Precipitate particle coarsening (Dp)

In Dyson's approach, creep damage is owing to particle

coarsening which is because of the interparticle spacing of the hardening particles [12]. The modifying of the precipitate coarsening of 9Cr-1Mo steel plays an important role in the creep resistance of this material that Nakajima et al. (2003) studied the coarsening of $M_{23}C_6$ and MX precipitates in T91 steel during creep processes. The stress, which required for dislocations to climb over precipitates, is decreased by the increased interparticle spacing. Following the damage because of the coarsening of $M_{23}C_6$ precipitate particles following Dyson's approach [12], Dp is defined as

$$\Box_{\Box} = 1 \Box \frac{\Box_{\Box}}{\Box_{\Box}} \tag{4}$$

where Po is the initial particle diameter and Pt is the particle size at any time t. It is a supposed that the coarsening of the particles obeys Livshitz-Wagner equation:

$$\square \square \square \square \qquad (5)$$

where the K is a constant determined by diffusivity, interfacial energy, equilibrium solute concentration. The above equation just only could apply to intragranular spherical particles such as MX, but could not for $M_{23}C_6$.

The rate of precipitate particle coarsening is described by

Where Kp is the rate constant normalized by K and the third power of the initial particle size. As a result, 0 < Dp < 1.Using a constant Kp and an activation energy parameter Qp, the below equation is shown the relationship of Kp and temperature T.

$$\Box \Box = \Box \Box_{1} \Box \Box \Box \Box \Box \frac{\Box_{1}}{\Box_{1}}$$
(7)

Where the R is the universal gas constant, the T is the temperature; the Qp is an activation energy parameter.

2.3. Void nucleation and crack formation (Dn)

Creep damage of 9Cr-1Mo steel is dependent on different mechanisms such as void nucleation and cavity formation [1]. The damage parameter (Dn), which is for cavity nucleation and growth, is defined as the fraction of grain boundary facets cavitation [8]. The below equation shows the evolution of Dn:

$$\dot{\Box}_{\Box} \Box \frac{\Box_{\Box}}{\Box_{\Box \Box}} \dot{\Box}$$
(8)

Where the ε_{fu} is the uniaxial strain at fracture and the k_n is a limit value blew 1/3. It is mean the damage of cavitation in proportion to strain rate.

Yin and Faulkner [8] proposed the rate of evolution of D_n for P91 alloy as:

$$\dot{\Box}_{n} = \mathsf{A}' \dot{\Box} \Box^{\square} \tag{9}$$

where the material constant of A and B are a function of temperature and stress. Where A' (A'=AB) and B' (B'=B-1) are large strains and high strain rates, Dn may be equal to or larger than one. This will cause a divergence in the computation at high stress and strain; so, the magnitude of Dn should not reach one, thus 0 < Dn < 1.

2.4. Dimensionless parameter of strain harding

(H)

The model of primary creep [13] is a modification of that suggested by Ion et al. [14]. The dimensionless parameter H is defined as

$$\Box \Box = \frac{\Box}{\Box}$$
(10)

Where σ is the stress and σ is an internal back stress generated during stress redistribution within strain Harding as inelastic strain accumulates. The H is as follows

The value of H is ranging from zero to a microstructure dependent maximum of H^* ($H^* < 1$). The constant $h' = E\Phi$, where E is the Young's modulus and Φ is the volume fraction.

3. Creep damage constitutive equations

Kachanov and Robotnov's equations

In order to descript the influence of the micro defect for mechanical properties of materials, Kachanov [15] originally put forward the fundamental theory of continuous damaged mechanics, and Rabotnov [16] lead damage fraction (D) to macroscopic constitutive equation in order to represent the damage state of materials characterized by distributed cavities in terms of appropriate mechanical variables (internal state variables), and then to establish mechanical behaviour of damaged materials.

$$\dot{\Box} = \dot{\Box}_0 \left[\frac{\Box}{\Box \Box \Box \Box} \right]^{\rm v} \tag{13}$$

where the \Box is the creep rate during the process of creep; σ is the applied stress for materials during the process of creep. The symbol with the mark of zero is the initial state; n is the constant of materials and normally named stress exponent. Where \square and \square_0 are respectively meaning the change of creep rate in the materials during the creep processes and the creep rate at the beginning of the creep; the v is the material constant.

3.2. Ion's equations

During the secondary creep, it will occur strain hardening and recovery. Ion et.al [14] leads in the dimensionless parameter of H to the creep constitutive

equations in order to present the influence of the working hardening. The creep constitutive equations of Robotnov will be changed and shown in below:

$$\Box = \Box_0 \left[\underbrace{-} \prod_{n=1}^{n} \right]^n \tag{14}$$

where \Box is the creep rate during the process of creep; σ is the applied stress for materials during the process of creep. The symbol with the mark of zero is the initial state; n is the constant of materials and normally named stress exponent; H is the dimensionless parameter.

$$\dot{\Box} = \dot{\Box}_0 \left[\frac{\Box \Box \Box \Box \Box}{\Box \Box \Box \Box \Box} \right]^{\rm v} \tag{15}$$

where \square and \square_0 are respectively meaning the change of creep rate in the materials during the creep processes and the creep rate at the beginning of the creep; the v is the material constant; H is the dimensionless parameter.

3.3. Dyson's equations

The creep constitutive equation of Robotnov is based on the phenomenological theory. Using the D to indicate many microdefects such as solid solution depletion, precipitate coarsening, void nucleation and crack formation et.al, it is too simple to show the influence of multiple microdefects for the process of creep. Dyson modified the CDM model, and summarized the effects of creep rate including particle coarsening (Dp), solute depletion (Ds), cavity nucleation and growth (Dn) and dislocations (Dd) et.al creep damage mechanisms [2]. The physically based CMD model of Dyson shows below:

$$\Box = \Box_{0} \xrightarrow{\square} \Box_{1} \Box_{1} \Box_{1}$$

$$\Box = = \underbrace{\Box}_{0} (1 \Box_{1} \Box_{1}) \Box,$$

$$\Box_{s} = KsDs^{1/3}(1 \Box_{1}),$$

$$\Box_{p} = \underbrace{\Box}_{0} \Box_{1} \Box_{1} \Box_{2},$$

$$\Box_{n} = A' \Box \Box^{2}.$$
(16)

3.4. Chen Yunxiang and Yang Ke's equations

where the σ is engineering stress, the \Box is creep rate.

4. Methodolagy

Firstly, to collect all the parameters used in the creep modeling for P91 at 600°C with stress above 130MPa from the paper of Chen Yunxiang and Ke Yang [10]. The software of Excel is mainly computation tool for analysis the creep damage constitutive equations of Chen Yunxiang and Ke Yang for P91

at $600\square$ under middle and high stress.

Secondly, to develop, validate, and use the Excel software. The computational software for uniaxial case was developed and validated against the published creep strain rate against time under 130 MPa [10]. Further detailed the damage evolutions and their contributions have been obtained.

Thirdly, to generalize 3D version of the creep damage constitutive equations and validate it. The generalization is based on the classical assumption in plasticity/creep theory that the relationship between effective creep strain and effective stress is the same as that of creep strain and stress under uni-axial case. The validation is limited to plane stress and plain strain cases due to the limited experimental data.

Finally, to assess the applicability of the model of Chen Yunxiang and Ke Yang's creep damage constitutive equations for P91 under lower stress level.

5. Development and validation

Table1. Materials constants

5.1. Development and validation of the Excel Software for uni-axial Case

The creep constitutive damage equations for P91 steel proposed by Chen Yunxiang and Ke Yang, the uniaxial creep constitutive damage equations is in third part of three. Creep damage constitutive equations.

 \Box_0 , H^{*}, h', n, Kp, Ks, A and B are the material constants which are calculated by the experiment date and collected together in Chen yunxiang and Ke Yang's paper from different papers and literatures [10]. The table below is the values and units of those material constants.

Term	Value	Unit
H*	0.269	
h'	10000	Mpa
Кр	1.5□10^-7	s ⁻¹
Ks	5 🗆 10^-8	s ⁻¹
А	1.5	
В	2	
A'	2.9	
B'	0.95	
n	10.186	
σ	200	Мра
	5.7□10^-6	s ⁻¹

The model of creep damage constitutive equations for P91 at $600\square$ under uniaxial stress is calculated by the Euler integration method using the science tool of Excel. For example, the parameter H for describing primary creep is solved numerically at each time interval as follows [8]:

$$\Delta H = \frac{\Box}{\Box} (1 \Box \Box \Box \Box) \Delta \epsilon_{i-1}$$
(18)
$$H_{i} = H_{i-1} + \Delta H$$
(19)

The subscript i and i-1 indicate the current and the previous time step respectively. The eluations of H , i , ip and i are calculated once by incremental time i hour, the new results of those will be inset into the eluation of ε , it gets the current creep rate and the current strain, and then can be calculate according the below equation:

$$\boldsymbol{\varepsilon}_{i} = \boldsymbol{\varepsilon}_{i-1} + \boldsymbol{\Box} \Delta t \tag{20}$$

Based on the data produced by the software of Excel, the graphs of strain against time and stress against time under different middle and high stress could be drawn out and shown in below:



Figure 1. The curve of strain rate vs. time at $600 \square$ under 130MPa

From the comparison of the results obtained from the current Excel Software, shown by Figs 1 to 3, with that published in [10], it is concluded that the Excel software has been developed correctly. Furthermore, detailed evolution and damages and their contributions to the creep strain rate and creep strain have been obtained. Due to the limit of space, they will not be reported here.



Figure2. The curve of strain vs. time at 600 under 145MPa







Figure 4. The comparison of the curve of strain vs. time at 600 under different middle and high stress

5.2. 3D generalization and validation

The multi-axial creep damage constitutive equations are based on the uniaxial creep damage constitutive equations of Chen Yunxiang and Ke Yang, the uniaxial stress is replaced by the effective stress (equivalent stress). The multi-axial creep damage constitutive equations are shown below:

 $\Box = \Box_{0} \underbrace{\Box}_{n} \Box \left[\underbrace{\Box}_{n} \Box \Box \Box \right]^{n},$ $\Box = \underbrace{\Box}_{n} (1 \Box \underbrace{\Box}_{n}) \Box_{n},$ $\Box_{s} = KsDs^{1/3}(1 \Box \Box_{n}),$ $\Box_{p} = \underbrace{\Box}_{n} \Box \Box \Box \Box \Box,$ $\Box_{n} = A', \Box \Box \Box \Box \Box,$ (21)

For practical validation under plane stress and plain strain conditions, the von Mises stress has been derived explicitly and given bellow.

$$\boldsymbol{\sigma}_{e} = 1/\sqrt{\Box} \left[\left(\boldsymbol{\sigma}_{1} \cdot \boldsymbol{\sigma}_{2}\right)^{2} + \left(\boldsymbol{\sigma}_{2} \cdot \boldsymbol{\sigma}_{3}\right)^{2} + \left(\boldsymbol{\sigma}_{3} \cdot \boldsymbol{\sigma}_{1}\right)^{2} \right]^{1/2}$$
(22)

1. To calculate the biaxial stress σ_1 and σ_2 under plane stress, the relationship between σ_1 and σ_2 is tangent function, and the value of σ_3 is zero.

$$\tan \alpha = \frac{\alpha}{\alpha}; \sigma_3 = 0$$
 (23)

Submitting the two equations into the equation of the effective stress will get:

2. To calculate the biaxial stress σ_1 and σ_2 under plane strain, the relationship between σ_1 and σ_2 is tangent function, and the value of σ_3 is shown in below equation:

$$\sigma_3 = \frac{1}{\alpha}, \tan \alpha = \frac{1}{\alpha}$$
(25)

Submitting the two equations into the equation of the effective stress will get:

$$\sigma_{\rm e} = \sigma_1 \Box \Box \pm \Box \pm \Box \pm \Box \pm \Box = \Box = \Box \qquad (26)$$

The model of multi-axial creep damage constitutive equations is repeatedly operating at interval of every $5\Box$ with the first principle stress calibrated to yield the same failure time with uniaxial model. After the above steps, the result is the isochronous rupture locus shown in below graph; a boundary representation of the stress at any angle that produces the creep failure of the material in the same time period.



Figure 5. Isochronous rupture loci for multi-axial formulation under plane stress condition for P91 at $600 \square$



Figure6. Isochronous rupture loci for multi-axial formulation under plane strain condition for P91 at 600°C

Figure6 shows that under high (not even pure) hydrostatic pressure, the creep strength is extremely high, which is not true: the hydrostatic pressure does promote the creep cavity and rupture.

This problem is rooted by the adoption of the classic/traditional assumption that the plastic/creep strain rate is controlled by the effective stress, and the creep damage evolution is controlled by the creep strain.

5.3. Application of the equations of Chen Yunxiang and Ke Yang for P91 at 600°C for middle and high stress to low stress

This set of creep damage constitutive equations has been applied to lower stress level, beyond to its original range of application. The lifetime and stress relationship has been obtained as shown in Figure 7.



Figure7. The graph of strain against time under low stress

6. Discussion

6.1. Uni-axial creep simulation for middle and high stress

The numerical simulation of uni-axial creep case under middle and high stress level has been produced successfully. The key feature of this set of creep damage constitutive equation [10] is the inclusion of various creep damage mechanisms, particularly the creep cavity law. A parametric study of their influence and significance on the lifetime reveals the significance of creep cavity damage Dn.

6.2. Multi-axial generalization and validation

A multi-axial version of the creep damage constitutive equations [10] has been proposed. This generalization seems not questionable as apparently it only adopted the classic/traditional assumption of that the effective creep strain is controlled by the effective stress in the creep cavity damage evolution law. However, the numerical prediction of lifetime from the multi-axial constitutive equations is not consistent with the experimental observation. Similar deficiency was revealed in KRH formulation by Xu [17], as illustrated by Figure8 (b). Current work suggests the need to examine further the validity of the creep cavity evolution law, at least under multi-axial and how it is coupled with creep deformation and rupture for the specific material, as well as a general method for continuum creep damage mechanics.

6.3. Extension to lower stress level

Due to the apparent success of this type of creep damage constitutive equations (uni-axial version only) under middle and high stress level [9, 8, 10], it is nature to hope that it will work under the lower stress level. This research has examined this. The authors are not ignorant about the breakdown concept and phenomena, generally and specifically to this alloy.

It seems that the shape of the creep curve under lower stress is not the right type as the leading to rupture is not sharp enough to be observed as brittle type.

The detailed results on the predicted individual creep damage evolutions provide the basis for future improvement. Research work on this aspect is ongoing and will be reported in future.



Figure8. (a) Isochronous rupture loci under plane stress conditions, (b) Isochronous rupture loci under plane strain conditions (Q. Xu, 2001) [17]

7. Conclusion

Significant progress has been noted in the developing creep damage constitutive equations, in terms of generic methodology of mechanism-based approach from Dyson's work, or its specific applications to P91 alloy [8, 9, and 10]. One of the key ingredients for the success is the creep cavity damage evolution law. However, the progress is limited to medium and high stress level and uni-axial case.

This research has proposed a multi-axial version creep damage constitutive equations based on the classic/traditional plasticity/creep theory that the creep strain is controlled by the effective stress and bears the same relationship of creep strain and stress under uni-axial case, in the creep cavity damage evolution law. The validation exercise conducted in this research revealed that this approach was not successful. It shows that further research on the precise nature of creep cavity evolution, hope to leading rupture, and the coupling between creep damage and creep deformation.

A simple extension exercise has confirmed that further dedicated research is needed for the developing of creep damage constitutive equation for lower stress level; it cannot be achieved as a byproduct for high stress level.

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