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Implementation of thermo-viscoplastic constitutive equations into the finite element code ABAQUS

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Abstract

Sophisticated viscoplatic constitutive laws describing material behavior at high temperature have been implemented in the general-purpose finite element code ABAQUS to predict the viscoplastic response of structures to cyclic loading. Because of the complexity of viscoplastic constitutive equation, the general implementation methods are developed. The solution of the non-linear system of algebraic equations arising from time discretization is determined using line-search and back-tracking in combination with Newton method. The time integration method of the constitutive equations is based on semi-implicit method with efficient time step control. For numerical examples, the viscoplastic model proposed by Chaboche is implemented and several applications are illustrated.

1. Introduction

The finite element method is widely employed in the nuclear engineering. The conventional approach, based on material strength concepts, and possibly on elastic analysis by the finite element method, is more and more often being replaced by inelastic analysis to take the effects of stress concentration, plastic or viscoplastic strain, and damage into account, simultaneously or successively.

During last decades there have been many advances in descriptions of viscoplastic material behavior [1]. The progresses of the computer hardware enable the sophisticated constitutive equations to be applied into the analysis of the structure. So the development of the program for life prediction of the structure are more necessary than ever.

The transition of constitutive laws from a laboratory or academic context to industrial use demands the development of appropriate algorithms. In combination with the finite element code, this transition can be applied to general structural analysis. The purpose of this paper is to present the implementation procedure for such sophisticated constitutive laws into the general-purpose finite element code ABAQUS.

The viscoplastic response of materials requires the time integration of system of non-linear first order differential equations. This can be done by either explicit or implicit techniques. Explicit methods are conditionally stable and it needs very small time step by consideration of accuracy. On the contrary, implicit methods are unconditionally stable and time step can be much larger than that of the explicit method without losing accuracy. However, the implicit methods solve the equations with the iterative way and the implementation is more difficult than that of the explicit methods [2].

In viscoplasiticy, the constitutive equation might become very complicated to evaluate depending upon their degree of non-linearity. Both the various types of the loading and the complexity of the constitutive laws ask a stable and efficient algorithm. In this study, the semi-implicit method with efficient time step control is adapted.

The implementation of such an algorithm is illustrated by several numerical examples. The constitutive law proposed by Chaboche is adapted in numerical examples. The problems of a cylindrical notched bar subjected to a several mechanical loadings are treated.

2. Implementation of the constitutive equation

In order to perform the nonlinear structural analysis, the several requirements should be satisfied. At first, the finite element code should be programmed and the implementation algorithm of the constitutive equation into FE code should be established. Because developing the FE code demands a lot of work and time, the structural analysis including new developed constitutive equation may be very difficult work in industrial or research area.

Fortunately, the general-purpose FE codes, such as ABAQUS, MARC and ADINA, supply the user-defined subroutines to supplement the special analysis, not covered by FE code. Using these routines, the material behavior can be implemented and the structure made of new types of materials can be analyzed. In the case of ABAQUS, the 'UMAT' subroutine is the material definition subroutine and asks the information about the constitutive equation, such as stress increments, state variable increments and the tangent modulus.

The implementation procedures of viscoplastic constitutive equations into ABAQUS are made up the integration of the constitutive equations and the derivation of the consistent tangent modulus. ABAQUS gives the value of the initial state variable and the strain increment and then the final state variable and tangent modulus are returned to ABAQUS [3]. At the first iteration of the equilibrium where the displacement fields are unknown, the explicit methods are activated and the continuum tangent modulus is determined. From the next iteration, the implicit methods are activated and the proposed algorithms are executed.

2.1. Constitutive equations in thermo-viscoplasticity

Viscoplastic equation basically consists of the evolution law of state variables divided into external state variable and internal state variable. External state variables are direct-measurable quantities such as stress, strain and temperature. On the contrary, internal state variables can not be observed directly and they are associates with the internal change of the material, such as plastic strain, kinematic hardening, isotropic hardening and damage etc.

Because the complex constitutive equations contain many internal variables, the conventional methods applied to classical kinematic hardening or isotropic hardening models cannot be adapted. For instance, the Chaboche viscoplastic model contains three tensorial variables and three scalar variables[4]. So the implementation procedure are generalized for arbitrary evolution laws represented in the function of the state variables.

It is assumed that the total strain rate $\dot{e}$ can be separated into elastic $\dot{e}^{e}$, viscopalstic $\dot{e}^{p}$ and thermal $\dot{e}^{th}$ components as

$$\dot{e} = \dot{e}^{e} + \dot{e}^{p} + \dot{e}^{th} \tag{1}$$

where the elastic strain rates are related to the total stress rates by Hooke's law

$$\dot{s} = \mathbf{E}\dot{e}^{e} \tag{2}$$

where **E** is the elasticity matrix and the thermal strain rates are given by

$$\dot{e}^{th} = \mathbf{A}\dot{T} \tag{3}$$

where **A** is the matrix of thermal dilatation coefficients and $\dot{T}$ is the temperature rate.

The viscoplastic strain rate can be represented as a product of the accumulated plastic strain rate $\dot{p}$ and the plastic strain direction **n**

$$\dot{e}^{p} = \dot{p}\mathbf{n} \tag{4}$$

and each component is the function of the state variables.

$$\dot{p} = \dot{p}(s, \mathbf{X}, R) \tag{5}$$

$$\mathbf{n} = \mathbf{n}(s, \mathbf{X}) \tag{6}$$

where s is the matrix of the current stresses and $\mathbf{X}$ is the tensorial internal variables such as the internal stresses associated to kinematic hardening. R is the scalar internal variable such as internal stresses associated to isotropic hardening.

The notation implies

$$\dot{p} = \sqrt{\frac{2}{3}\dot{e}^{p} : \dot{e}^{p}}$$

By combining Eq. (5), Eq. (6) and Eq. (10), the flow rule can be rewritten as

$$\dot{e}^{p} = \mathbf{f}(s, \mathbf{X}, R) \tag{7}$$

and inserting Eq. (7) into Eq. (2) gives

$$\dot{s} = \mathbf{E}\dot{e} + \mathbf{f}^{*}(s, \mathbf{X}, R, T) \tag{8}$$

where $\mathbf{f}^{*} = (-)\mathbf{E}\mathbf{f}(s, \mathbf{X}, R, T)$.

The description of internal state variable can be generalized as the functions of the current state variables.

$$\dot{\mathbf{X}} = \mathbf{g}(s, \mathbf{X}, R, T) \tag{9}$$

$$\dot{R} = h(s, \mathbf{X}, R, T) \tag{10}$$

Equation (9) means the evolution law of the tensorial internal variable. It may be associated with the kinematic hardening or the anisotropic damage etc. Similarly, equation (10) means the evolution law of the scalar internal variables such as isotropic hardening, isotropic damage etc. Here, the detailed explanations about the evolution law of internal variables are abbreviated so that the various types of constitutive equations can be covered.

2.2. Time integration of the viscoplastic constitutive equations

Equation (8) to (10) show that the viscoplastic material behavior is governed by a system of non-linear first order differential equations. They can be summarized in the general form

$$\dot{y} = f(t, y) \tag{11}$$

where y represents the vector of state variables, i.e., the stress and the hardening internal variables.

To minimized computational costs, it appears necessary to choose an algorithm of integration that requires a minimum number of evaluations of the constitutive equations. The method chosen in this study is a semi-implicit method. Much of the theoretical and practical aspects of this method have been covered by several authors such as [5], [6].

Using trapezoidal rule, the increment of the state variable is expressed as

$$\Delta y = \left[(1-\theta)\dot{y}_t + \theta\,\dot{y}_{t+\Delta t}\right]\Delta t \tag{12}$$

By adding this increment into the initial state variable y_t, the final state variable $y_{t+\Delta t}$ is written as

$$y_{t+\Delta t} = y_t + \left[(1-\theta)\,f(t, y_t) + \theta\,f(t+\Delta t, y_t + \Delta y)\right]\Delta t \tag{13}$$

With respect to value of midpoint parameter θ, the integration methods are classified as forward gradient method(θ = 1), backward gradient method(θ = 0) and Crank-Nicolson method (θ = 1/2). If midpoint parameter θ is the arbitrary value on $0 < \theta \le 1$, that case is called semi-implicit method [2].

The increment of the state variables can be written as

$$\Delta s = \mathbf{E}\Delta e + [(1-\theta)\mathbf{f}_t^* + \theta\mathbf{f}_{t+\Delta t}^*]\Delta t \tag{14}$$

$$\Delta\mathbf{X} = [(1-\theta)\mathbf{g}_t + \theta\mathbf{g}_{t+\Delta t}]\Delta t \tag{15}$$

$$\Delta R = [(1-\theta)h_t + \theta h_{t+\Delta t}]\Delta t \tag{16}$$

The notation implies that

$$f_t = f(s_t, \mathbf{X}_t, R_t, T_t), \quad f_{t+\Delta t} = f(s_{t+\Delta t}, \mathbf{X}_{t+\Delta t}, R_{t+\Delta t}, T_{t+\Delta t}).$$

The final state variables can be deduce as

$$s_{t+\Delta t} = s_t + \mathbf{E}\Delta e + \left[(1-\theta)\mathbf{f}_t^* + \theta\mathbf{f}^*(s_{t+\Delta t}, \mathbf{X}_{t+\Delta t}, R_{t+\Delta t}, T_{t+\Delta t})\right]\Delta t \tag{17}$$

$$\mathbf{X}_{t+\Delta t} = \mathbf{X}_t + \left[(1-\theta)\mathbf{g}_t + \theta\mathbf{g}(s_{t+\Delta t}, \mathbf{X}_{t+\Delta t}, R_{t+\Delta t}, T_{t+\Delta t})\right]\Delta t \tag{18}$$

$$R_{t+\Delta t} = R_t + \left[(1-\theta)h_t + \theta h(s_{t+\Delta t}, \mathbf{X}_{t+\Delta t}, R_{t+\Delta t}, T_{t+\Delta t})\right]\Delta t \tag{19}$$

Since the initial state variables are all known value, the unknown values of the equation (17) to (19) are final state variables $s_{t+\Delta t}, \mathbf{X}_{t+\Delta t}, R_{t+\Delta t}, T_{t+\Delta t}$ and the strain increments Δe. In the case of the displacement-based finite element method, the strain increments are prescribed in the beginning of the increment. For uncoupled analysis, the temperature changes are solved at previous heat transfer analysis. (The formulation for the coupled analysis with the thermal and force equilibrium must be considered the change of the temperature as an unknown variable.) Thus the variables to be determined are reduced to $s_{t+\Delta t}, \mathbf{X}_{t+\Delta t}, R_{t+\Delta t}$. Following the semi-implicit method, the time integration of the constitutive equations is converted to the root finding of the set of nonlinear equations.

The Newton's method is usually adapted for solving the nonlinear simultaneous equations. In spite of rapid convergence near the root points, invalid selection of the initial guess can induce the divergence. In this study, the initial values of the state variables are determined by explicit methods within the limit of deviation.

$$\mathrm{Res} = y^*_{t+\Delta t} - \left\{ y_t + \left[(1-\theta) f(t, y_t) + \theta f(t+\Delta t, y^*_{t+\Delta t}) \right] \Delta t \right\} \tag{20}$$

where $y^*_{t+\Delta t}$ is the final state variable predicted by explicit method.

If the residuals exceed the tolerance limit, the time increment for forward gradient method are divided in several shorter parts and the improved initial guess are determined. The line search and back tracking are used to prevent the divergence of the root. These theoretical and practical aspects of these methods are explained in the reference [7].

2.3. Consistent tangent modules

In viscoplastic constitutive equations, the tangent modulus **H** can be defined as

$$\mathbf{H} = \frac{\partial(\Delta s)}{\partial(\Delta e)} \quad \text{or} \quad \Delta s = \mathbf{H}\Delta e \tag{21}$$

The tangent modulus should be obtained through the way consistent with the time integration method. By using it, the quadratic converge rate of the equilibrium iteration can be obtained.

Taking derivative of equation (17) to (19),

$$\begin{aligned} d(\Delta s) &= ds_{i+1} \\ &= \mathbf{E} de_{i+1} + \theta \left[\left.\frac{\partial \mathbf{f}^*}{\partial s}\right|_{i+1} ds_{i+1} + \left.\frac{\partial \mathbf{f}^*}{\partial \mathbf{X}}\right|_{i+1} d\mathbf{X}_{i+1} + \left.\frac{\partial \mathbf{f}^*}{\partial R}\right|_{i+1} dR_{i+1} \right] \Delta t \end{aligned} \tag{22}$$

$$d(\Delta \mathbf{X}) = d\mathbf{X}_{i+1} = \left[\left.\frac{\partial \mathbf{g}}{\partial s}\right|_{i+1} ds_{i+1} + \left.\frac{\partial \mathbf{g}}{\partial \mathbf{X}}\right|_{i+1} d\mathbf{X}_{i+1} + \left.\frac{\partial \mathbf{g}}{\partial R}\right|_{i+1} dR_{i+1} \right] \Delta t \tag{23}$$

$$d(\Delta R) = dR_{i+1} = \left[\left.\frac{\partial h}{\partial s}\right|_{i+1} ds_{i+1} + \left.\frac{\partial h}{\partial \mathbf{X}}\right|_{i+1} d\mathbf{X}_{i+1} + \left.\frac{\partial h}{\partial R}\right|_{i+1} dR_{i+1} \right] \Delta t \tag{24}$$

The subscript ‘i’ and ‘i+1’ mean respectively, the derivative at initial state (t) and the derivative at final state (t+Δt). Combining equation (22) to (24) gives

$$d\mathbf{y} = \Delta t \left[\frac{\partial \mathbf{P}}{\partial \mathbf{y}} \right] (d\mathbf{y}) + \mathbf{E}^* d¥å \tag{25}$$

where $d\mathbf{y} = (ds_{i+1}\ d\mathbf{X}_{i+1}\ d\mathbf{R}_{i+1})^{\mathbf{T}}$, $\mathbf{P} = (\,\mathbf{f}\ \mathbf{g}\ h\,)^{\mathbf{T}}$, $\mathbf{E}^* = [\mathbf{E} \quad \mathbf{0} \quad 0]^{T}$.

By solving equation (25), the tangent modulus is derived as

$$(d\mathbf{y}) = \left[\mathbf{I} - \Delta t \left[\frac{\partial \mathbf{P}}{\partial \mathbf{y}} \right] \right]^{-1} \mathbf{E}^* de = \mathbf{H}^* de \tag{26}$$

The matrix **H*** contains all the relations between the state variable increments and the strain increments as following.

$$\mathbf{H}^* = [\mathbf{H}_\sigma \quad \mathbf{H}_X \quad \mathbf{H}_R]^{T} \tag{28}$$

$$ds = \mathbf{H}_\sigma de \tag{29}$$

$$d\mathbf{X} = \mathbf{H}_X de \tag{30}$$

$$dR = \mathbf{H}_R de \tag{31}$$

The tangent modulus is $\mathbf{H}_\sigma$ and used at equilibrium iteration of the whole system.

3. Numerical examples

The numerical example considered is illustrated in Fig. 1. It consists of several material tests with the notched specimen. The bar is modeled by 110 quadrilateral elements with axi-symmetric conditions. The constitutive equation used in this example is proposed by Chaboche[4] for a stainless steel alloy of type AISI 316. The brief description of Chaboche model is listed in Appendix and the material parameters are given in Table.1. The simulations are performed about tension test, cyclic test, creep test and stress recovery test.

Fig.2 represents the strain rate dependency of the viscoplastic material at simple tension test. The label ‘x/d’ means that the relative distance from the center of the specimen where ‘d’ is the radius of the specimen. The strain rates are different with respect to the distance from the center and the stress levels are proportional to the strain rate.

Fig.3 represents the hysteresis curve under cyclic loading. After 4 cycles, the hysteresis curve is stablized. The creep behavior are simulated and displayed in Fig.4. It can be found that the stress concentration near notch accelerates the creep deformation. Fig.5 shows that stress levels at constant strain degrade gradually due to the dynamic recovery. The main characteristics of viscoplastic material are successfully simulated and the applicability of developed program into viscoplastic materials is verified.

Table.1. Material constants for 316 stainless steel at 600 ^oC [4]

Symbol	Constant	Symbol	Constant
E	144000	B	12
α	2.e6	M_1	4807
n	24	M_2	58480
k	10	m_1	4
K_0	116	m_2	4
α_K	1.5	γ	0.2e-6
α_R	0.35	M	2
a_1	67.5	η	0.06
c_1	1300	μ	19
a_2	80	Q_0	30
c_2	45	Q_r^*	455
Φ_0	.5	Q_{max}	200

4. Conclusions

In the present investigation, the supplementary program for implementing of constitutive equations into ABAQUS was developed. The time integration of constitutive equations was performed by the semi-implicit method. The solution of the non-linear system of algebraic equations arising from time discretization was determined using line-search and back-tracking in combination with Newton method. The effective calculation procedure for consistent tangent modulus was developed with the consideration of general description of constitutive equations. The viscoplastic constitutive equations proposed by Chaboche were implemented for numerical examples and material behaviors under several loading conditions were simulated to demonstrate the efficiency and applicability of the present implementation.

Reference

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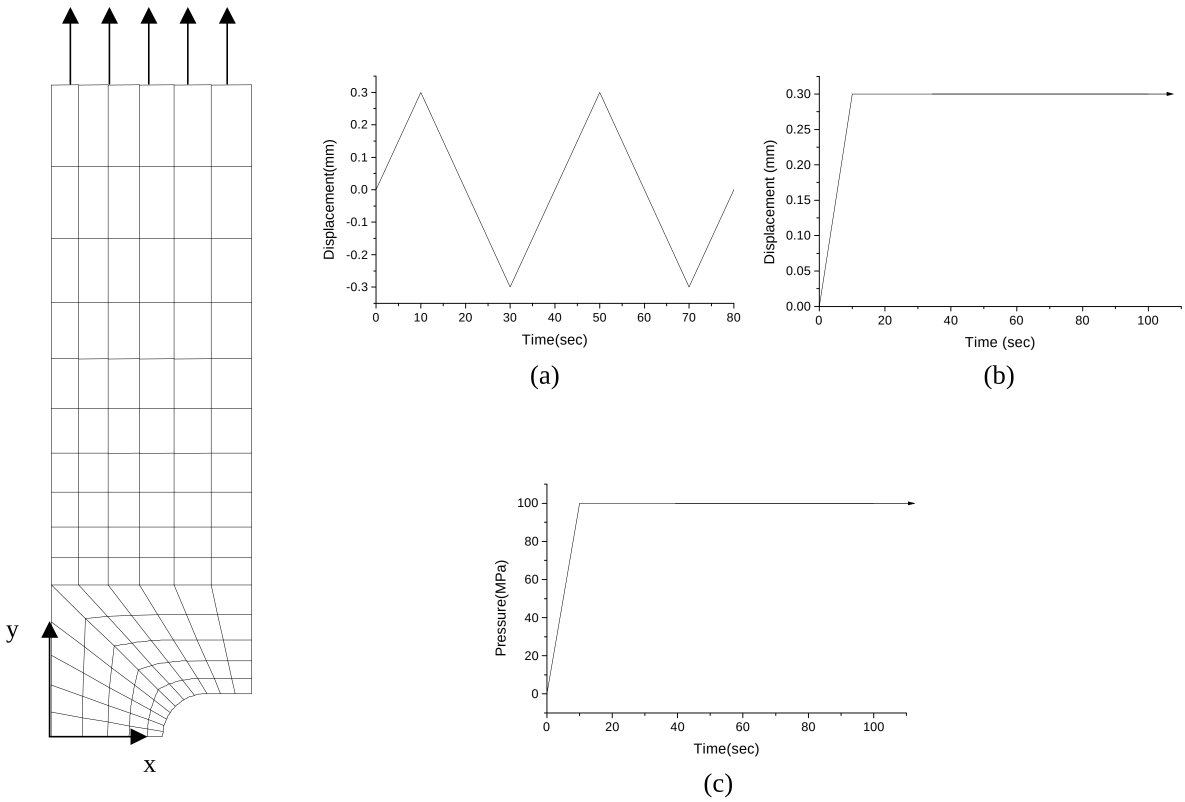
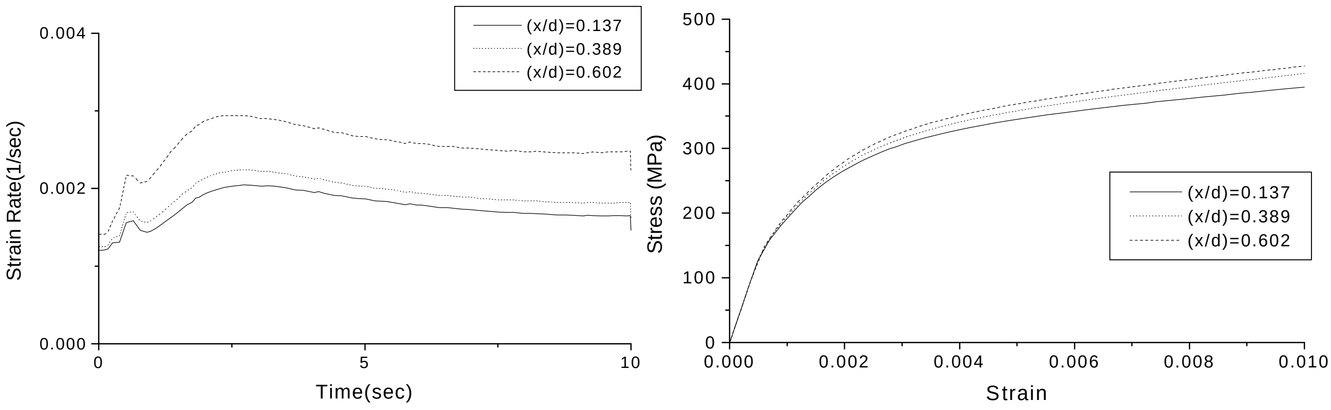


Fig. 1. The finite element model and the loading history

(a) cyclic tension-compression loading, (b) strain-hold loading, (c) stress-hold loading



(a) (b)

Fig. 3. The strain rate sensitivity of the specimen

(a) the strain rate history of tension stroke, (b) the stress-strain curve of tension stroke

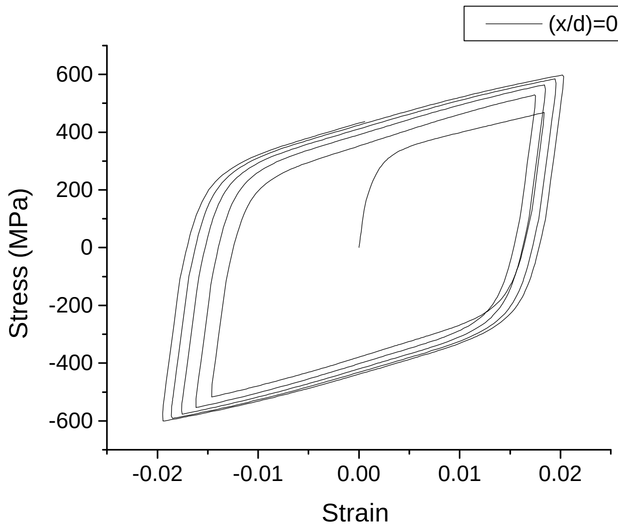


Fig. 4. The hysterisis curve of cyclic tension-compression test

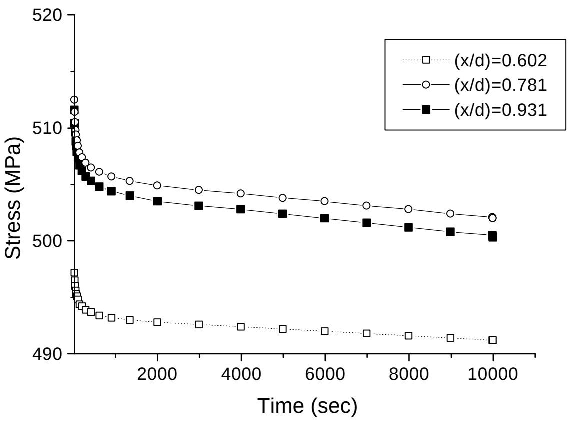


Fig. 5 The stress history of the recovery test

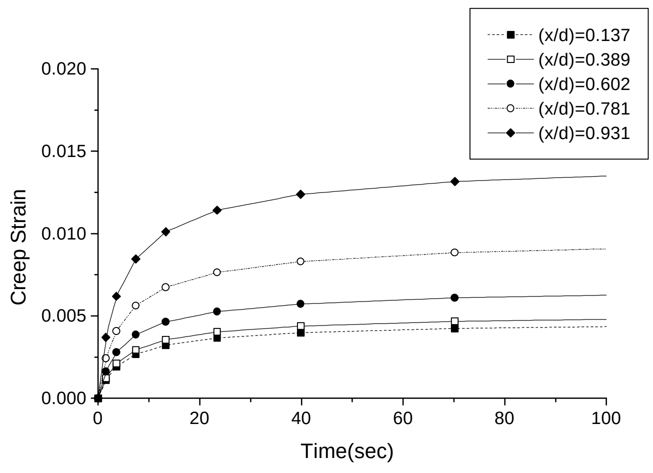


Fig. 6 The creep strain curve versus time

Appendix

The Constitutive equations proposed by Chaboche[4]

Viscopalstic strain rate:

$$\dot{e} = \frac{3}{2}\dot{p}\frac{\mathbf{s}-\mathbf{X}}{J(\mathbf{s}-\mathbf{X})} \tag{A.1}$$

$$\dot{p} = \left\langle \frac{J(\mathbf{s}-\mathbf{X})-\alpha_R R - k}{K_0+\alpha_K R} \right\rangle^n \tag{A.2}$$

where **s** implies the deviatoric stress tensor.

The notation implies that

$$J(\mathbf{s}-\mathbf{X}) = \sqrt{\frac{3}{2}(\mathbf{s_{ij}}-\mathbf{X_{ij}})(\mathbf{s_{ij}}-\mathbf{X_{ij}})}$$

Kinematic hardening and time recovery :

$$\mathbf{X} = \mathbf{X_1} + \mathbf{X}_2 \tag{A.3}$$

$$\dot{\mathbf{X}}_i = \frac{2}{3}a_i c_i \dot{e}_p - a_i \Phi(p)\mathbf{X}_i \dot{p} - \left[\frac{J(\mathbf{X})}{M_i}\right]^{m_i} \mathbf{X}_i \tag{A.4}$$

$$\Phi(p) = \Phi_0 + (1-\Phi_0)e^{-bp} \tag{A.5}$$

Isotropic hardening and time recovery :

$$\dot{R} = b(Q-R)\dot{p} + \gamma|Q_r - R|^{m-1}(Q_r - R) \tag{A.6}$$

$$\dot{Q} = 2\mu(Q_{max} - Q)\dot{q} \tag{A.7}$$

$$Q_r = Q - Q_r^*\left[1-\left(\frac{Q_{max}-Q}{Q_{max}}\right)^2\right] \tag{A.8}$$

Plastic strain memorization :

$$\dot{q} = \eta H(F) < \mathbf{n} : \mathbf{n}^* > \dot{p} \tag{A.9}$$

$$\dot{x} = \sqrt{\frac{3}{2}}(1-\eta)H(F) < \mathbf{n} : \mathbf{n}^* > \dot{p}\mathbf{n}^* \tag{A.10}$$

$$F = \frac{2}{3}J(e_p - x) - q \tag{A.11}$$

$$\dot{\mathbf{n}} = \sqrt{\frac{3}{2}}\frac{\mathbf{s}-a}{J(\mathbf{s}-a)}, \quad \dot{\mathbf{n}}^* = \sqrt{\frac{3}{2}}\frac{e_p - x}{J(e_p - x)} \tag{A.12}$$

In the above equations K_0, k, α_K, α_R , n, c_1, a_1, M_1, m_1, c_2, a_2, M_2, m_2, Φ_0, b, γ, m, Q_r^*,Q_{max}, μ, η are the material constants which are function of temperature to be identified from the experimental data.