Transactions of the 15th International Conference on
Structural Mechanics in Reactor Technology (SMiRT-15)
Seoul, Korea, August 15-20, 1999

G04/2

Implementation of Thermo-Viscoplastic Constitutive Equations into the Finite Element Code

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ABSTRACT

Sophisticated viscoplastic 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 the structure to a cyclic loading. With the consideration of the complexity and variety of viscoplastic constitutive equation, a general implementation method is developed. The solution of a non-linear system of algebraic equations arising from time discretization is determined using Newton's method in combination with line-search and back-tracking. The time integration method of the constitutive equations is based on the semi-implicit method with efficient time step control. For numerical examples, the viscoplastic model proposed by Chaboche is implemented and the problem of thick-walled cylinder subject to internal pressure was analyzed. The results of finite element analysis were in a good agreement with those of the analytic solution.

1. INTRODUCTION

The finite element method is widely employed in engineering analysis. The conventional approach, based on material strength concepts and possibly on elastic analysis by the finite element method, is often being replaced by inelastic analysis to take the effects of strain hardening, viscosity and damage into account, simultaneously. During last decades there have been many advances in descriptions of viscoplastic material behavior[1]. The developments of the computer hardware enable the use of the sophisticated constitutive equations in the analysis of the structure. The development of the program for life prediction of the structure is more necessary than ever. The application of constitutive laws from a laboratory or academic context to industrial use requires the development of appropriate algorithms. In combination with the finite element code, these algorithms 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 material are mathematically expressed as a system of the non-linear first order differential equations and very complicated, depending upon their degree of non-linearity. Those equations are solved with the time integration algorithm, either explicit or implicit. Explicit methods are conditionally stable and needs very small time step for accuracy. On the contrary, implicit methods are unconditionally stable and time step of this method is much larger than that of the explicit method without sacrificing the accuracy. However, the implicit methods solve the equations iteratively and the implementation is more difficult than that of the explicit methods[2]. In this study, the semi-implicit method with efficient time step control is adapted. The constitutive law proposed by Chaboche[3] was implemented and applied to the problem of a thick-walled cylinder subjected to both mechanical and thermal loading.

2. IMPLEMENTATION OF THE CONSTITUTIVE EQUATION

In order to perform the nonlinear structural analysis, several requirements should be satisfied. At first, the finite element codes which can be applied to nonlinear materials should be programmed and the algorithm to implement the constitutive equation into finite element code should be accomplished. Because developing the finite element code requires a lot of efforts, the structural analysis including newly developed constitutive equation can be very difficult job in industrial area.

Fortunately, the general-purpose finite element codes, such as ABAQUS, MARC, ANSYS and ADINA, supply the user-defined subroutines to supplement the special analysis, not covered in finite element code. The behavior of new types of materials can be implemented and the structural analysis with this routine can be performed. In the case of ABAQUS, the 'UMAT' subroutine is the material definition subroutine and consists of the information about the constitutive equation, such as stress increments, state variable increments and tangent modulus[4].

2.1. Constitutive Equations in Thermo-Viscoplasticity

The viscoplastic constitutive equations basically consist of the evolution law of state variables, divided into the external state variable and the internal state variable. External state variables are direct-measurable quantities such as stress, strain and temperature. On the contrary, the internal state variables can not be observed directly and they are associated 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 should be expanded into general description of constitutive equations.

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

$$\dot{\varepsilon} = \dot{\varepsilon}^e + \dot{\varepsilon}^p + \dot{\varepsilon}^{th} \quad (1)$$

and the thermal strain rates are usually given by

$$\dot{\varepsilon}^{th} = \mathbf{A}\dot{T} \quad (2)$$

where **A** is the matrix of thermal dilatation coefficients and $\dot{T}$ is the temperature rate. The viscoplastic strain rate can be represented as function of the stress and internal state variables

$$\dot{\varepsilon}^p = \dot{\varepsilon}^p(\sigma, \xi, T) \quad (3)$$

where ξ means internal state variables to describe the internal change of material. It means that the viscoplastic strain rate can be described only by the current state variables.

By combining Eqs. (1), (2) and (3), the elastic strain rate can be written as

$$\dot{\varepsilon}^e = \dot{\varepsilon} - \dot{\varepsilon}^p - \dot{\varepsilon}^{th} = \dot{\varepsilon} - \dot{\varepsilon}^p(\sigma,\xi,T) - \alpha(T)\dot{T} \tag{4}$$

and reformed as a function form.

$$\dot{\varepsilon}^e = \dot{\varepsilon}^e\left(\sigma,\xi\,;\,\varepsilon,T,\dot{\varepsilon},\dot{T}\right) \tag{5}$$

The semicolon in Eq.(5) divides independent variables into unknown part and known part. In displacement-based finite element code, the values of the strain and temperature are given and then corresponding stress and other state variables should be calculated. The former parts of variables, σ and ξ, are unknown variables and the latter parts, ε and T, are given or already known. The Hooke's law can relate the stress rate with the elastic strain rate in Eq.(5).

$$\dot{\sigma} = \mathbf{E}(T)\cdot\dot{\varepsilon}^e\left(\sigma,\xi\,;\,\varepsilon,T,\dot{\varepsilon},\dot{T}\right) \tag{6}$$

where **E** is the elastic stiffness matrix. For convenience of notation, the description of stress rate are shown as the function of the state variables.

$$\dot{\sigma} = \mathbf{f}\left(\sigma,\xi\,;\,\varepsilon,T,\dot{\varepsilon},\dot{T}\right) \tag{7}$$

The evolution law for the internal state variable can be also described as the similar form of Eq.(7).

$$\xi = \mathbf{g}(\sigma,\xi\,;\varepsilon,T,\dot{\varepsilon},\dot{T}) \tag{8}$$

Note that the detailed explanations about the evolution law of the internal variables are not referred and thus Eq.(8) can be used for scalar or any order tensorial variables.

2.2. Time Integration of the Viscoplastic Constitutive Equations

The constitutive equations, Eqs.(7) and (8), show that the viscoplastic material behavior is governed by a system of non-linear first order differential equations. There have been a variety of methods for the integration of the ordinary differential equation, such as Euler Method, Runge-Kutta Method, Gear method and Stoer-Blush method, etc. However, there are some restrictions for these methods to be implemented to the finite element code. In implicit finite element analysis, the nonlinear behavior of local elements should be linearized and are combined into the stiffness matrix of the whole system, used for solving the equilibrium equation. The one step methods, such as Euler method, are applicable in implicit finite element code, for instance, ABAQUS. To minimize computational costs, it is necessary to choose an algorithm for the integration that requires the minimum number of evaluations. The method chosen in this study is a semi-implicit method and the theoretical and practical aspects of this method have been covered by several references[5, 6].

The system of the ordinary differential equation is summarized as following.

$$\dot{y} = \mathbf{f}(t,y) \tag{9}$$

where y represents the vector of state variables, i.e., the stress and the internal hardening variables. Using trapezoidal rule, the increment of the variable is expressed as

$$\Delta y = \left[(1-\theta)\dot{y}_t + \theta\dot{y}_{t+\Delta t}\right]\Delta t \tag{10}$$

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

$$\mathbf{y}_{t+\Delta t} = \mathbf{y}_t + \left[(1-\theta)\,\mathbf{f}(t,\mathbf{y}_t) + \theta\,\mathbf{f}(t+\Delta t, \mathbf{y}_t + \Delta \mathbf{y})\right]\Delta t \tag{11}$$

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

Following the same procedure, the viscoplastic constitutive equations, Eqs.(7) and (8), can be integrated

$$\sigma_{t+\Delta t} = \sigma_t + \left[(1-\theta)\,\mathbf{f}(\sigma_t, \xi_t) + \theta\,\mathbf{f}(\sigma_{t+\Delta t}, \xi_{t+\Delta t})\right]\Delta t \tag{12}$$

$$\xi_{t+\Delta t} = \xi_t + \left[(1-\theta)\,\mathbf{g}(\sigma_t, \xi_t) + \theta\,\mathbf{g}(\sigma_{t+\Delta t}, \xi_{t+\Delta t})\right]\Delta t \tag{13}$$

Eqs.(12) and (13) have the unknown variables σ and ξ to be obtained by numerical iteration. Consequently, the time integration of the constitutive equations is converted to the problem of solving the set of nonlinear equations.

The Newton's method is usually adapted for solving the nonlinear equations. In spite of rapid convergence near the root points, invalid selection of the initial guess can result in the divergence of the roots. To avoid such divergence, we use an algorithm that combines the rapid convergence of Newton's method with a globally convergent strategy that will guarantee some progress towards the solution at each the iteration. The theoretical aspects of this method are explained in the reference[7].

The initial guess of the state variables is determined by Euler forward method and the iterations are continued until the error, defined in Eq.(14), becomes below the tolerance limit.

$$\text{Error} = \left| \frac{{}^{(i+1)}\mathbf{y}_{t+\Delta t} - {}^{(i)}\mathbf{y}_{t+\Delta t}}{{}^{(i)}\mathbf{y}_{t+\Delta t}} \right| \tag{14}$$

where ${}^{(i+1)}\mathbf{y}_{t+\Delta t}$, ${}^{(i)}\mathbf{y}_{t+\Delta t}$ are state variables induced in 'i+1'th iteration and 'i'th iteration respectively. The notation $|\mathbf{x}|$ means the norm of the vector $\mathbf{X}$.

2.3. Consistent Tangent Modules

The tangent modulus matrix $\mathbf{H}$ of inelastic material can be defined as

$$\mathbf{H} = \frac{\partial(\Delta\sigma)}{\partial(\Delta\varepsilon)} \quad \text{or} \quad \Delta\sigma = \mathbf{H}\Delta\varepsilon \tag{15}$$

and should be obtained through the consistent way with the time integration method. By using it, the quadratic convergence rate of the equilibrium iteration can be obtained.

Taking derivative of Eqs.(12) and (13),

$$\begin{aligned} d\sigma_{i+1} = \Delta t\left[(1-\theta)\left(\left.\frac{\partial \mathbf{f}}{\partial \varepsilon}\right|_i d\varepsilon_{i+1} + \left.\frac{\partial \mathbf{f}}{\partial T}\right|_i dT_{i+1}\right) + \theta\left(\left.\frac{\partial \mathbf{f}}{\partial \varepsilon}\right|_{i+1} d\varepsilon_{i+1} + \left.\frac{\partial \mathbf{f}}{\partial T}\right|_{i+1} dT_{i+1}\right)\right] \\ + \theta\Delta t\left[\left.\frac{\partial \mathbf{f}}{\partial \sigma}\right|_{i+1} d\sigma_{i+1} + \left.\frac{\partial \mathbf{f}}{\partial \xi}\right|_{i+1} d\xi_{i+1}\right] \end{aligned} \tag{16}$$

$$d\xi_{i+1} = \Delta t\left[(1-\theta)\left(\left.\frac{\partial \mathbf{g}}{\partial \varepsilon}\right|_{i} d\varepsilon_{i+1} + \left.\frac{\partial \mathbf{g}}{\partial T}\right|_{i} dT_{i+1}\right) + \theta\left(\left.\frac{\partial \mathbf{g}}{\partial \varepsilon}\right|_{i+1} d\varepsilon_{i+1} + \left.\frac{\partial \mathbf{g}}{\partial T}\right|_{i+1} dT_{i+1}\right)\right] \quad ,$$
$$+\theta\Delta t\left[\left.\frac{\partial \mathbf{g}}{\partial \sigma}\right|_{i+1} d\sigma_{i+1} + \left.\frac{\partial \mathbf{g}}{\partial \xi}\right|_{i+1} d\xi_{i+1}\right] \qquad (17)$$

where the subscripts 'i' and 'i+1' mean the derivative at initial state 't' and the derivative at final state 't+Δt' respectively. Note that the initial stress rates depend upon the final strain and temperature because the strain rate and temperature rate at the initial and the final state are the same value as defined in Eq.(18). With the same reason, the initial rate of the internal state variable can depend on the final strain and final temperature.

$$\dot{\varepsilon}_t = \frac{\Delta\varepsilon}{\Delta t} = \dot{\varepsilon}_{t+\Delta t}\,, \quad \dot{T}_t = \frac{\Delta T}{\Delta t} = \dot{T}_{t+\Delta t}\,. \qquad (18)$$

Combining Eqs.(16) and (17) gives

$$\mathbf{A}\begin{pmatrix} d\sigma_{i+1} \\ d\xi_{i+1} \end{pmatrix} = \mathbf{B}\begin{pmatrix} d\varepsilon_{i+1} \\ dT_{i+1} \end{pmatrix} \qquad (19)$$

where

$$\mathbf{A} = \begin{bmatrix} \mathbf{I} - \Delta t\theta \left.\frac{\partial f}{\partial \sigma}\right|_{i+1} & -\Delta t\theta \left.\frac{\partial f}{\partial \xi}\right|_{i+1} \\ -\Delta t\theta \left.\frac{\partial g}{\partial \xi}\right|_{i+1} & \mathbf{I} - \Delta t\theta \left.\frac{\partial g}{\partial \sigma}\right|_{i+1} \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} \Delta t\left((1-\theta)\left.\frac{\partial f}{\partial \varepsilon}\right|_{i} + \theta\left.\frac{\partial f}{\partial \varepsilon}\right|_{i+1}\right) & \Delta t\left((1-\theta)\left.\frac{\partial f}{\partial T}\right|_{i} + \theta\left.\frac{\partial f}{\partial T}\right|_{i+1}\right) \\ \Delta t\left((1-\theta)\left.\frac{\partial g}{\partial \varepsilon}\right|_{i} + \theta\left.\frac{\partial g}{\partial \varepsilon}\right|_{i+1}\right) & \Delta t\left((1-\theta)\left.\frac{\partial g}{\partial T}\right|_{i} + \theta\left.\frac{\partial g}{\partial T}\right|_{i+1}\right) \end{bmatrix}$$

By multiplying both sides of Eq.(19) with the inverse matrix of **A**, the tangent modulus is derived as

$$\begin{pmatrix} d\sigma_{i+1} \\ d\xi_{i+1} \end{pmatrix} = \mathbf{A}^{-1}\mathbf{B}\begin{pmatrix} d\varepsilon_{i+1} \\ dT_{i+1} \end{pmatrix} \qquad (20)$$

where

$$\mathbf{A}^{-1}\mathbf{B} = \begin{bmatrix} \frac{\partial \sigma_{i+1}}{\partial \varepsilon_{i+1}} & \frac{\partial \sigma_{i+1}}{\partial T_{i+1}} \\ \frac{\partial \xi_{i+1}}{\partial \varepsilon_{i+1}} & \frac{\partial \xi_{i+1}}{\partial T_{i+1}} \end{bmatrix}$$

The first row-first column element of matrix $\mathbf{A}^{-1}\mathbf{B}$ is tangent modulus used for equilibrium iteration of the whole system. The first row-second column element is the ratio of the stress increment and the temperature increment and is necessary for a coupled temperature-displacement analysis.

3. NUMERICAL EXAMPLES

In order to verify the accuracy and the applicability of the developed program, the implementation was applied to a multiaxial problem and compared with an analytic solution. The constitutive equations used in this example was proposed by Chaboche[3] for a type 316 stainless steel. The brief description of Chaboche model is listed in Appendix I and the material parameters are given in Table 1. The example problem is about the viscoplastic behavior of a thick-wall cylinder subjected to internal pressure under isothermal conditions. The inner and outer radii of the cylinder are taken as 40 mm and 60 mm and the temperature is 600°C. The internal pressure is 0 MPa initially and increased up to 26 MPa in 10 seconds. The cylinder is modeled by 80 axi-symmetric quadrilateral elements. In order to impose the plane strain condition(ε_z=0), the distance between upper side and bottom side of the finite element model are constrained to be constant

The results of these computations have been plotted in Fig.1 to Fig.5 with the symbol such as square, circle, up-triangle and down-triangle. The Symbols in Figs.1, 2, 3 show respectively the radial, hoop and axial stress distribution across the wall of a cylinder using the Chaboche's model and FE code, ABAQUS. The symbols plotted at different values of time show the redistribution of stresses. The radial and hoop strain distribution has been plotted in Figs.4 and 5 at different values of time.

The analytical solution for the problem of a thick cylinder with internal pressure derived by Arya[8] was corrected and used for comparison. The results of finite element analysis and the original solution show considerable discrepancy but the finite element solution shows a good agreement with the corrected solution. In Fig.1 to Fig.5, the results of the analytic solution are plotted in the line form. The excellent agreement of the ABAQUS and the analytic solution verifies the implementation of Chaboche's constitutive equations into FE code, ABAQUS. Thus the developed finite element procedure can be applied to the problems with complex geometry and thermo-mechanical loading quite accurately.

4. CONCLUSIONS

In the present investigation, the supplementary program for implementing of viscoplastic constitutive equations into ABAQUS was developed. The time integration of the constitutive equations was performed by the semi-implicit method. The solution of the non-linear system of algebraic equations arising from time discretization was obtained using Newton's method in combination with line-search and back-tracking techniques. The efficient calculation procedure for consistent tangent modulus was developed and can be applied to various types of constitutive equations. The viscoplastic constitutive equations proposed by Chaboche were implemented and the example problem of a thick cylinder subjected to internal pressure was analyzed. The result using the developed finite element procedure shows a good agreement with the analytic solution.

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Table.1. Material constants for 316 stainless steel at 600 °C [3]

Symbol	Parameter	Symbol	Parameter
E	149.7Gpa	k	6
ν	0.3	C	24800
α	1.86e-5	γ	300
K	150 MPa	Q	80
n	12	b	10

Appendix I. The Viscoplastic Constitutive Equations Proposed by Chaboche[3]

Viscopalstic strain rate

$$\dot{\varepsilon} = \frac{3}{2}\dot{p}\frac{s-X}{J(s-X)}, \quad \dot{p} = \left\langle \frac{J(s-X)-R-k}{K} \right\rangle^{n} \qquad (A.1)$$

Kinematic hardening rules shows

$$\dot{X} = \frac{2}{3}c\dot{\varepsilon}_{p} - \gamma X\dot{p} \qquad (A.2)$$

Isotropic hardening can be expressed as

$$\dot{R} = b(Q-R)\dot{p} \qquad (A.3)$$

where s implies the deviatoric stress tensor and $J(s-X) = \sqrt{\frac{3}{2}(s_{ij} - X_{ij})(s_{ij} - X_{ij})}$.

In the above equations K, k, n, c, γ, b, Q are the material constants.

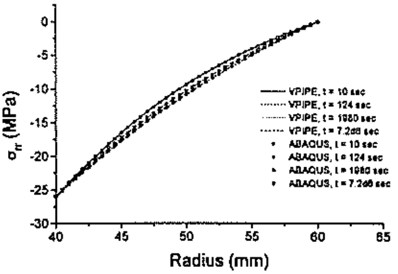

Fig.1. Radial stress distribution in a thick-walled cylinder at 600°C (symbols : FEM analysis, lines : analytic solution)

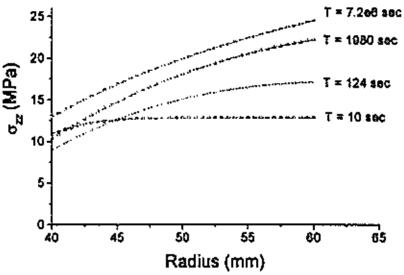

Fig.2. Axial stress distribution in a thick-walled cylinder at 600°C (symbols : FEM analysis, lines : analytic solution)

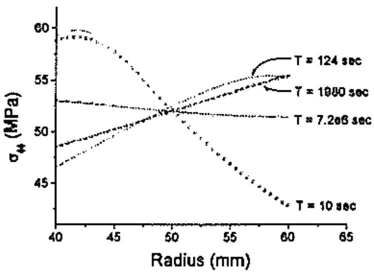

Fig.3. Hoop stress distribution in a thick-walled cylinder at 600°C(symbols : FEM analysis, lines : analytic solution)

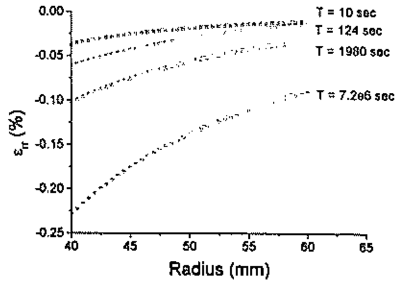

Fig.4. Radial strain distribution in a thick-walled cylinder at 600°C (symbols : FEM analysis, lines : analytic solution)

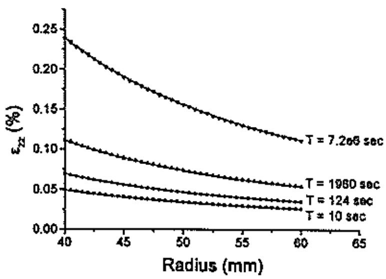

Fig.5. Axial strain distribution in a thick-walled cylinder at 600°C (symbols : FEM analysis, lines : analytic solution)