NUMERICAL CONSIDERATIONS IN THE DEVELOPMENT AND IMPLEMENTATION OF CONSTITUTIVE MODELS

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Several unified constitutive models were tested in uniaxial form by specifying input strain histories and comparing output stress histories. The purpose of the tests was to evaluate several time integration methods with regard to accuracy, stability, and computational economy. The sensitivity of the models to slight changes in input constants was also investigated. Results are presented for IN100 at 1350°F and Hastelloy-X at 1800°F.

INTRODUCTION

The characterization of the constitutive behaviour of metals has its roots in the early work of Tresca, Levy, vonMises, Hencky, Prandtl, Reuss, Prager, and Ziegler (Refs. 1-8). These early models are incremental in nature, assume that plasticity and creep can be separated, and they incorporate a yield function, flow rule, and hardening rule to define the plastic strain increment. These original incremental theories have been expanded and modified by many researchers so that they provide adequate, and often very good predictions of rate-independent plastic flow (see for example Refs. 9-10). However, they are sometimes criticized as having no formal micromechanical basis upon which to make the assumption of an uncoupling of the inelastic strain into rate-independent (plastic) and rate-dependent (creep) strain components. Nevertheless, the classical incremental theories are widely used.

During the last ten years, a number of unified constiutive models have been proposed which retain the inelastic strain as a unified quantity without aritifical separation into plasticity and creep components. These include the models developed by Bodner (Refs. 11-13), Stouffer (Refs. 14-15), Krieg (Ref. 16), Miller (Ref. 17), Walker (Refs. 18-19), Valanis (Refs. 20-21), Krempl (Ref. 22), Cernocky (Ref. 23-24), Hart (Ref. 25), Chaboche (Ref. 26), Robinson (Ref. 27), Kocks (Ref. 28), and Cescotto and Leckie (Ref. 29). The applicability of these viscoplastic constitutive theories (mostly to high temperature applications) has been investigated by several researchers. Walker (Ref. 19) compared the predictive capability of several models (Walker, Miller and Krieg) for Hastelloy-X at 1800°F. More recently, Milly and Allen

(Ref. 30) provided a qualitative as well as quantitative comparison of the models developed by Bodner, Krieg, Walker and Krempl for IN100. Both Refs. 19 and 30 conclude that these models generally provide adequate results for elevated isothermal conditions, they provide poor and overly-square results at low temperature, the material constants are often difficult to obtain experimentally, the resulting rate equations are "stiff" and sensitive to numerical integration, and the models do not provide any satisfactory transient temperature capability. Beek, Allen, and Milly (Ref. 31) have shown that all the unified viscoplastic models mentioned above can be cast in a functionally similar form (in terms of internal state variables).

None of the published literature provides a thorough evaluation of current viscoplastic constitutive models with comparison to experimental response for complex input histories. Such an evaluation is difficult at present for many reasons, namely: 1) Material constants for most models are usually available only for a single material and often for a single temperature; 2) The experimental procedures given by model developers for determining material constants from experimental data are often sketchy at best; 3) Material constants for some models are often obtained by trial-and-error and are not based on experiments; and 4) There is a lack of good experimental data against which the models can be evaluated (that is, test data which is significantly different from that used to generate the material constants).

The purpose of the present paper is to report some preliminary evaluations of several of the unified viscoplastic models (Bodner, Krieg, Miller, and Walker). These four models are evaluated with regard to 1) their sensitivity to numerical integration and 2) their sensitivity to slight changes in input material constants.

CONSTITUTIVE MODELS CONSIDERED

The constitutive theories which have been studied to date include Bodner's (Refs. 11-15), Krieg's (Ref. 16), Miller's (Ref. 17), and Walker's (Refs. 18-19). These particular models were selected for this initial study because material constants for Hastelloy-X were available for three of the models. Other models are currently being considered as material constants become available. Each model is listed below in uniaxial form using a consistent notation as presented by Beek, Allen and Milly (Ref. 31). In Ref. 31, it is shown that all of the current viscoplastic models considered may be written in uniaxial form as

$$\sigma = E(\varepsilon - \alpha_1 - \varepsilon^T) \quad (1)$$

where σ is stress, E is Young's modulus, ε is strain, α_1 is the inelastic strain (internal state variable), and ε^T is the thermal strain. Each viscoplastic theory postulates a particular growth law for the internal state variable(s) and the inelastic strain is obtained by time integration of the growth law for α_1, i.e.

$$\alpha_1 = \int_{-\infty}^{t} \dot{\alpha}_1(t')dt' \qquad (2)$$

where

$$\dot{\alpha}_1 = \frac{d\alpha_1}{dt} = \dot{\alpha}_i(\varepsilon, T, \alpha_2, \alpha_3, \ldots, \alpha_m) \qquad (3)$$

In equations (2) and (3), t is time, T is temperature, α_2 is the back stress (related to the dislocation arrangement and produces kinematic hardening or the Bauschinger effect), and α_3 is the drag stress (which represents the dislocation density and produces isotropic hardening).

Bodner's Theory

The growth law for the inelastic strain in Bodner's model may be written in uniaxial form as

$$\dot{\alpha}_1 = \frac{2}{\sqrt{3}} D_o \exp\left[-\left(\frac{n+1}{2n}\right)\left(\frac{\sigma}{\alpha_3}\right)^{-2n}\right] \mathrm{sgn}(\sigma) \qquad (4)$$

where

$$\dot{\alpha}_3 = m(Z_1 - \alpha_3)\dot{W}_p - AZ_1\left(\frac{\alpha_3 - Z_I}{Z_1}\right)^r \qquad (5)$$

$$\dot{W}_p = \sigma\,\dot{\alpha}_i \qquad (6)$$

The quantities E, D_o, n, m, Z_I, A, Z_1 and r are material constants. As noted before, the variable α_3 is similar to the drag stress used in many models (a measure of isotropic hardening or dislocation density). It is noted that the model contains no parameter representing the back stress and cannot account for the Bauschinger effect in kinematic hardening materials. The material constants are tabulated for IN100 at 1350°F (732°C) in Table 1 (taken from Ref. 14).

Krieg's Theory

The inelastic strain growth law for the model developed by Krieg and coworkers may be written in terms of state variables representing back stress and drag stress:

$$\dot{\alpha}_1 = C_1 \left(\frac{|\sigma - \alpha_2|}{\alpha_3} \right)^{C_2} \mathrm{sgn}(\sigma - \alpha_2) \tag{7}$$

$$\dot{\alpha}_2 = C_3 \dot{\alpha}_1 - C_4 \alpha_2^2 [\exp(C_5 \alpha_2^2) - 1] \mathrm{sgn}(\alpha_2) \tag{8}$$

$$\dot{\alpha}_3 = C_6 |\dot{\alpha}_1| - C_7 (\alpha_3 - \alpha_{3_o})^n \tag{9}$$

The model contains ten constants (C_1, C_2 . . . , C_7, E, α_{3_o}, and n). These have been evaluated by Walker (Ref. 19) for Hastelloy-X at 1800°F (982°C) and are tabulated in Table 2. It should be noted that equations (7), (8) and (9) form a coupled set of ordinary differential equations.

Miller's Theory

The growth laws for Miller's model may be written in uniaxial form as

$$\dot{\alpha}_1 = B\theta' \left[\sinh \left(\frac{|\sigma - \alpha_2|}{\alpha_3} \right)^{1.5} \right]^n \mathrm{sgn}(\sigma - \alpha_2) \tag{10}$$

$$\dot{\alpha}_2 = H_1 \dot{\alpha}_1 - H_1 B\theta' [\sinh (A_1 |\alpha_2|)]^n \mathrm{sgn}(\alpha_2) \tag{11}$$

$$\dot{\alpha}_3 = H_2 |\dot{\alpha}_1| \left(C_2 + |\alpha_2| - \frac{A_2}{A_1} \alpha_3^3 \right) - H_2 C_2 B\theta' \left[\sinh \left(A_2 \alpha_3^3 \right) \right]^n \tag{12}$$

Miller's theory contains nine constants which are tabulated for Hastelloy-X at 1800°F (982°C) in Table 3 (see Ref. 19).

Walker's Theory

Walker's nonlinear viscoplastic theory can be cast in the following uniaxial form

$$\dot{\alpha}_1 = \left(\frac{|\sigma - \alpha_2|}{\alpha_3}\right)^n \text{sgn}(\sigma - \alpha_2) \tag{13}$$

$$\dot{\alpha}_2 = (n_1 + n_2)\dot{\alpha}_1 - (\alpha_2 - \alpha_{2_o} - n_1\alpha_1)\left\{|\dot{\alpha}_1| \frac{\partial}{\partial R}\left[(n_3 + n_4 R)\ln\left(\frac{n_5 R}{1+n_6 R} + 1\right)\right] + n_7 |\alpha_2 - \alpha_{2_o}|^{m-1}\right\} \tag{14}$$

$$\dot{\alpha}_3 = n_8 |\dot{\alpha}_1| - n_9 |\dot{\alpha}_1|\alpha_3 - n_{10} (\alpha_3 - \alpha_{3_o})^q \tag{15}$$

where R is the cumulative inelastic strain

$$R = \int_o^t \left|\frac{\partial \alpha_1}{\partial t'}\right| dt' \tag{16}$$

The general model requires sixteen constants (E, n, m, q, n_1, n_2, . . . , n_{10}, α_{2_o} and $\alpha_3(t=0)$. In determining the constants for Hastelloy-X at 1800°F (982°C), Walker made several simplifying assumptions [including α_3 = constant = $\alpha_3(t=0)$] which reduces the number of parameters to those shown in Table 4 (see Ref. 19). Further, the constants reported in Ref. 19 were developed from tests using strain rates in the range 10^{-3} to 10^{-6} sec^{-1} and strain ranges of ±0.6%.

NUMERICAL TIME INTEGRATION STUDY

The integration of the constitutive relationship given by equations (1), (2) and (3) forms an integral and extremely important part in any numerical solution of a nonlinear field problem. It has been observed by many researchers that the coupled system of ordinary differential equations defining the state variables may be locally "stiff" and thus are sensitive to the time step size and numerical algorithm. The accurate integration of these stiff equations can be accomplished by various means: use of small time steps, higher-order or multi-point integration schemes, subincrementation procedures (Refs. 33-35), "smart" algorithms which attempt to select appropriate time steps in order to achieve accuracy and stability (Refs. 36,37), algorithms tailored for individual constitutive theories (Refs. 32,37), or combinations of these approaches. In general, the computation time required for the accurate solution of materially nonlinear problems is directly related to the numerical integration scheme used.

Regarding the constitutive models reviewed herein, Walker (Ref. 32) uses a stable, iterative implicit scheme which takes advantage of the functional form of the integrand in the development of the reccurence relation. Miller originally used Gear's method (Ref. 36) to integrate the stiff equations in his theory but later concluded in Ref. 37 that an implicit backward difference method was more economical and preferable to either Gear's method or the explicit Euler forward integration method. The type of numerical integration scheme used by Bodner and Krieg is not known.

The selection of an appropriate time integration scheme to be used in a computer code is very important but is often based on the answers to such questions as: "What is available in the present code?", "What will work most of the time?", "What can we use that most users will understand?", "What is the cheapest and easiest to use?", and the like. The usual response given is "it depends on the problem being solved!"

In general, equation (3) may be integrated between time t and $t + \Delta t$ by writing

$$\int_t^{t+\Delta t} d\alpha_1 = \int_t^{t+\Delta t} \dot{\alpha}_1 \, dt \qquad (17)$$

or

$$\Delta\alpha_1 = \alpha_1(t + \Delta t) - \alpha_1(t) = \int_t^{t+\Delta t} \dot{\alpha}_1 \, dt \qquad (18)$$

where $\dot{\alpha}_1$ is defined by the particular constitutive theory being used. The present investigation considers four integration schemes: explicit Euler forward integration, implicit trapezoidal method, trapezoidal predictor-corrector (iterative) method, and Runge-Kutta 4th order method. The approximations for each of these methods is given in Table 5.

Each of the integration schemes in Table 5 were used to obtain stress-time and stress-strain responses for the four constitutive models considered herein when subjected to the uniaxial, alternating square-wave strain-rate history shown in Fig. 1. Figure 1 shows the 35 second response obtained by Krieg's theory for Hastelloy-X at 1800°F using a time step of 0.1 seconds. For this time step, the Euler and trapezoidal predictor-corrector methods provide essentially the same results and are virtually identical to that obtained for all methods using a time step of 0.005 seconds. The 4th order Runge-Kutta method generally overestimates the peak response while the trapezoidal method underestimates the response. Figure 2 presents results for three integration methods such that the total computation time for a 35 second response solution is approximately the same. For equivalent computation times, the Euler method provides the most accurate results although smaller time steps are required. Similar results are observed for Miller's model.

Figures 3 and 4 illustrate that various constitutive models may behave appreciably different using the same integration method (in this case the Euler method). In Fig. 3, Miller's theory (for Hastelloy-X at 1800°F) gives considerable oscillatory response for a time step of 0.005 seconds while Walker's theory shown in Fig. 4 gives a much smoother response for the same time step. Comparing Figs. 3 and 4, it is seen that a smaller time step is required (with Euler integration) in Miller's theory than in Walker's theory.

Figure 5 presents results for IN100 at 1350°F using Bodner's model. Time steps were chosen for each integration scheme to obtain solutions which required approximately equal computation times. These results, when compared to solutions with much smaller time steps, indicate that the Euler method provides the most accurate results. Again, the time step used is smaller than that for the other methods but the computation time is the same (for integrating the constitutive equations).

SENSITIVITY STUDY FOR MATERIAL CONSTANTS

In the previous section, results were presented which showed how the numerical integration method used to integrate the constitutive equations could affect the accuracy and computation times of predicted results for stress-time and stress-strain responses. In this section, we consider another important parameter in the application of any constitutive theory. Namely, "how does the accuracy to which material constants are determined from experimental test data affect the predicted response?"

Figures 6 and 7 present results for Walker's model (Hastelloy-X at 1800°F subjected to an alternating square-wave strain-rate history as shown) wherein specified input material constants have been adjusted by 5%. Figure 6 shows the effect of a -5% change (error) in the stress exponent n (the most sensitive parameter). Figure 7 shows that a +5% error in all test data required to compute material constants results in significant predicted response errors, up to 30% over-prediction in the stress at a time of 35 seconds (during the relaxation period).

Figures 8 and 9 present similar results for Krieg's model (Hastelloy-X at 1800°F) and Bodner's model (IN100 at 1350°F), respectively. Both results indicate that the most sensitive parameter is the stress exponent "n" and that a 5% error in specifying n may produce significant errors in the predicted response. Miller's model appears to be much less sensitive to errors in input material parameters.

Figure 10 provides a comparison of the Miller, Krieg, and Walker models for the Hastelloy-X test at 1800°F (using constants obtained by Walker for all models). The Euler method was used with a time step of 0.0005 seconds which provides a solution with no significant truncation error. The results obtained here show approximately 10-15% differences in peak stress amplitudes between the three constitutive models. Since no experimental results are available at this time, no conclusions can be drawn as to which model more accurately represents observed test data. However, the results do point out that significant differences (greater than 15%) can be obtained for stress peaks and stress relation values through the use of different constitutive models.

CONCLUSIONS AND FUTURE WORK

The results of this study are not complete since only a portion of the available constitutive models and numerical integration schemes have been considered. However, some tentative conclusions can be reached. First, it appears clear from the present investigation, and the work of others, that simple integration schemes (like the Euler forward defference method) are often preferable to more complex schemes from the standpoint of accuracy, computation time, and ease of implementation. Although not reported herein, our work in progress indicates that Euler's method used with a simple subincrementation strategy provides the most accurate and economical solution for most constitutive models.

The sensitivity study on material constants indicates that most viscoplastic constitutive models are significantly sensitive to one or more material constants derived from laboratory tests. It has been shown that a 5% "error" in laboratory measurements may lead to errors of 25%, or greater, in predicted stress responses. Although most model developers have fine-tuned their models and input material constants for specific material/temperature/strain-rate combinations, it is not clear that end-users will be able to do so when called upon to develop material constants for a new situation. The problem can be negated to some extent by defining more explicit testing procedures for obtaining material constants and by guidelines defining which constants are most sensitive to experimental error.

Our current and future work concerns the application of several integration schemes to the other constitutive theories, investigation of subincremental strategies, and consideration of "smart" integration methods which detect local "stiffness" and adjust time steps but without significant computational expense. The material parameter sensitivity study will be continued by considering other constitutive theories, and more importantly, by comparison with laboratory tests which involve complex thermomechanical loadings including transient temperature inputs.

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Table 1. Material Constants Used in Bodner's Model for IN100 at 1350°F (732°C)

Bodners notation	Beek and Allen's notation	Numerical Value
E	E	$21.3\text{x}10^{6}$ psi
n	n	0.7
Z_1	Z_1	$1.105\text{x}10^{6}$ psi
m	m	$2.57\text{x}10^{3}$ psi^{-1}
D_o	D_o	10^{4} sec^{-1}
A	A	$1.9\text{x}10^{-3}$ sec^{-1}
r	r	2.66
Z_I	Z_I	$0.6\text{x}10^{6}$ psi
ε^p (t=0)	α_I(t=0)	0.0
Z_o	α_3(t=0)	$0.915\text{x}10^{6}$ psi

Table 2. Material Constants Used in Krieg's Model for Hastelloy-X at 1800°F (982°C)

Walker's notation for Krieg's constants	Beek and Allen's notation	Numerical Value
	C_1	1.0
n	C_2	4.49
A_1	C_3	1.0×10^6 psi
A_2	C_4	6.21×10^{-6} psi^{-1} sec^{-1}
A_3	C_5	4.027×10^{-7} psi^{-2}
A_4	C_6	100 psi $sec^{1/n}$
A_5	C_7	4.365 psi^{1-n} $sec^{1/n-2}$
E	E	13.2×10^6 psi
K_o	α_{3_o}	59,292 psi $sec^{1/n}$
n	n	4.49
c(t=0)	$\alpha_1(t=0)$	0.0
$\Omega(t=0)$	$\alpha_2(t=0)$	0.0
K(t=0)	$\alpha_3(t=0)$	59,292 psi

Table 3. Material Constants Used in Miller's Model for Hastelloy-X at 1800°F (982°C)

Miller's notation	Beek and Allen's notation	Numerical Value
n	n	2.363
$B\theta'$	$B\theta'$	2.616×10^{-5} sec^{-1}
H_1	H_1	1×10^6 psi
A_1	A_1	1.4053×10^{-3} psi^{-1}
H_2	H_2	100 psi $sec^{1/n}$
C_2	C_2	5,000 psi
A_2	A_2	4.355×10^{-12} psi^{-3}
E	E	13.2×10^6 psi
$\varepsilon(t=0)$	$\alpha_1(t=0)$	0.0
R(t=0)	$\alpha_2(t=0)$	0.0
D_o	$\alpha_3(t=0)$	8,642 psi

Table 4. Material Constants Used in Walker's Model for Hastelloy-X at 1800°F (982°C)

Walker's notation	Beek and Allen's notation	Numerical Value
$\overset{\circ}{\Omega}$	α_2	-1,200 psi
n_1	n_1	0 psi (not used)
n_2	n_2	1×10^6 psi
n_9	*	312.5
n_7	n_7	2.73×10^{-3} psi^{1-m} sec^{-1}
n	n	4.49
m	m	1.16
E	E	13.2×10^6 psi
c(t=0)	α_1(t=0)	0.0
Ω(t=0)	α_2(t=0)	0.0
K(t=0)	α_3(t=0)	59,292 psi
	n_8,n_9,n_{10},q	0 (not used)

$$* = \frac{\partial}{\partial R}\left[(n_3 + n_4R)\ \ell n\left(\frac{n_5R}{1+n_6R} + 1\right)\right]$$

Table 5. Numerical Integration Approximation for $\Delta\alpha_1 = \int_t^{t+\Delta t}\dot{\alpha}_1\,dt$

Method	Approximation
Euler Forward Difference	$\Delta\alpha_1 = \Delta t\ \dot{\alpha}_1(t)$
Trapezoidal Rule	$\Delta\alpha_1 = \frac{\Delta t}{2}[\dot{\alpha}_1(t) + \dot{\alpha}_1(t+\Delta t)]$
Trapezoidal Predictor-Corrector	Same as trapezoidal except iterate
Runge-Kutta 4th Order	$\Delta\alpha_1 = \frac{1}{6}(K_1 + 2K_2 + 2K_3 + K_4)$
	$K_1 = \Delta t\ \dot{\alpha}_1(t,\alpha_1(t))$
	$K_2 = \Delta t\ \dot{\alpha}_1(t+\Delta t/2,\alpha_1(t)+K_1/2)$
	$K_3 = \Delta t\ \dot{\alpha}_1(t+\Delta t/2,\alpha_1(t)+K_2/2)$
	$K_4 = \Delta t\ \dot{\alpha}_1(t+\Delta t,\alpha_1(t)+K_3)$

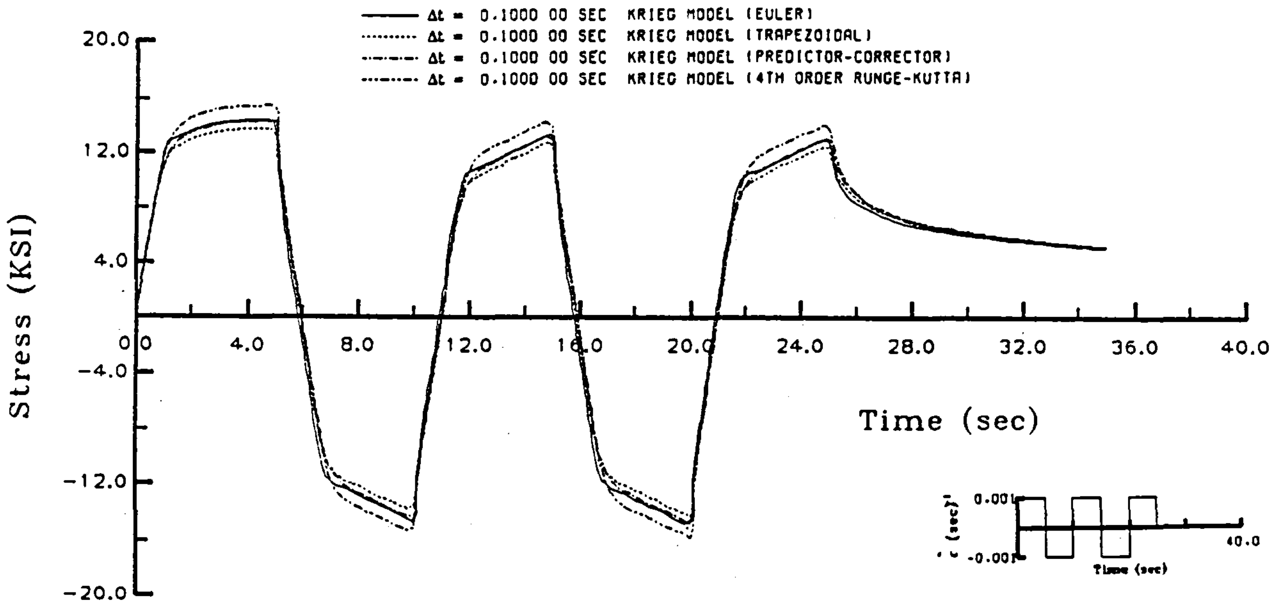

Fig. 1 Comparison of integration methods for Krieg's theory (Hastelloy-X at 1800°F)

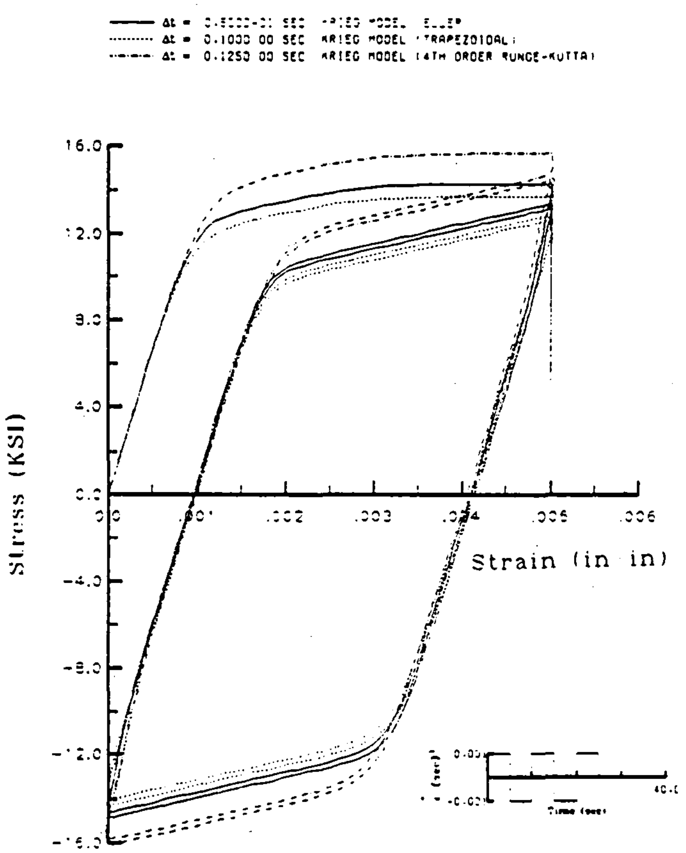

Fig. 2 Comparison of integration methods for Kreig's thoery with equal computation time allowed for each method (Hastelloy-X at 1800°F)

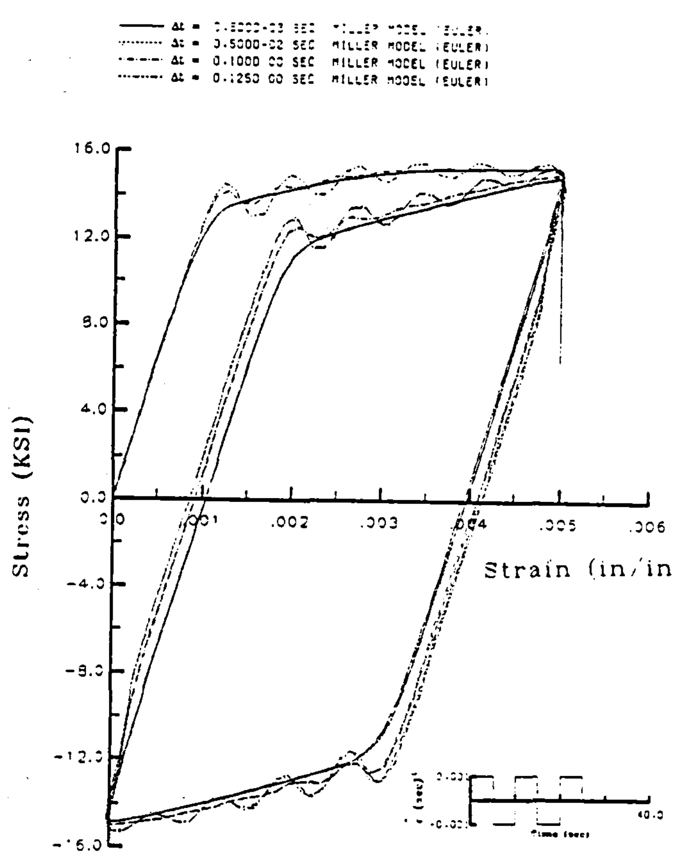

Fig. 3 Stability and accuracy of Euler's method for Miller's theory (Hastelloy-X at 1800°F)

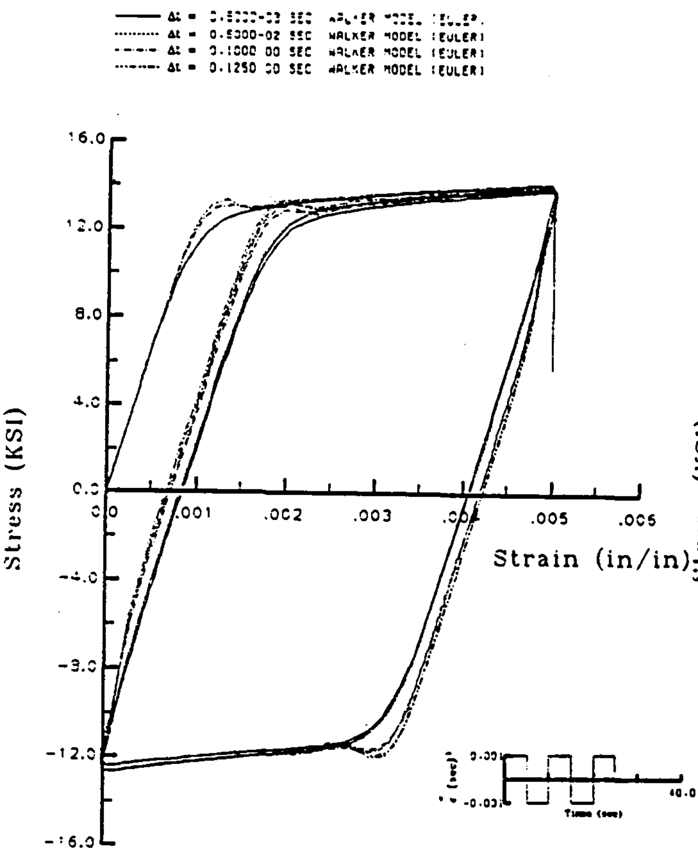

Fig. 4 Stability and accuracy of Euler's method for Walker's theory (Hastelloy-X at 1800°F)

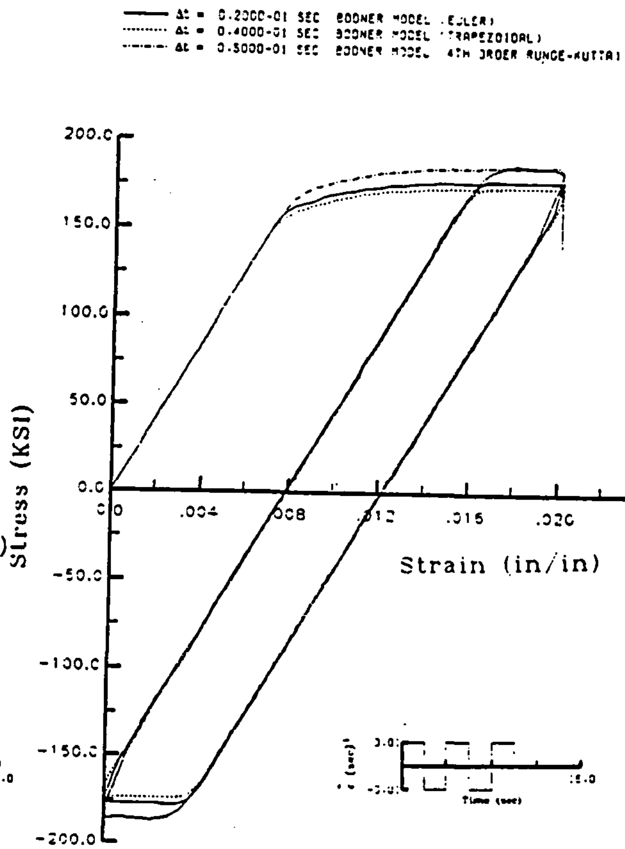

Fig. 5 Comparison of integration methods for Bodner's theory with equal computation time allowed for each method (IN100 at 1350°F)

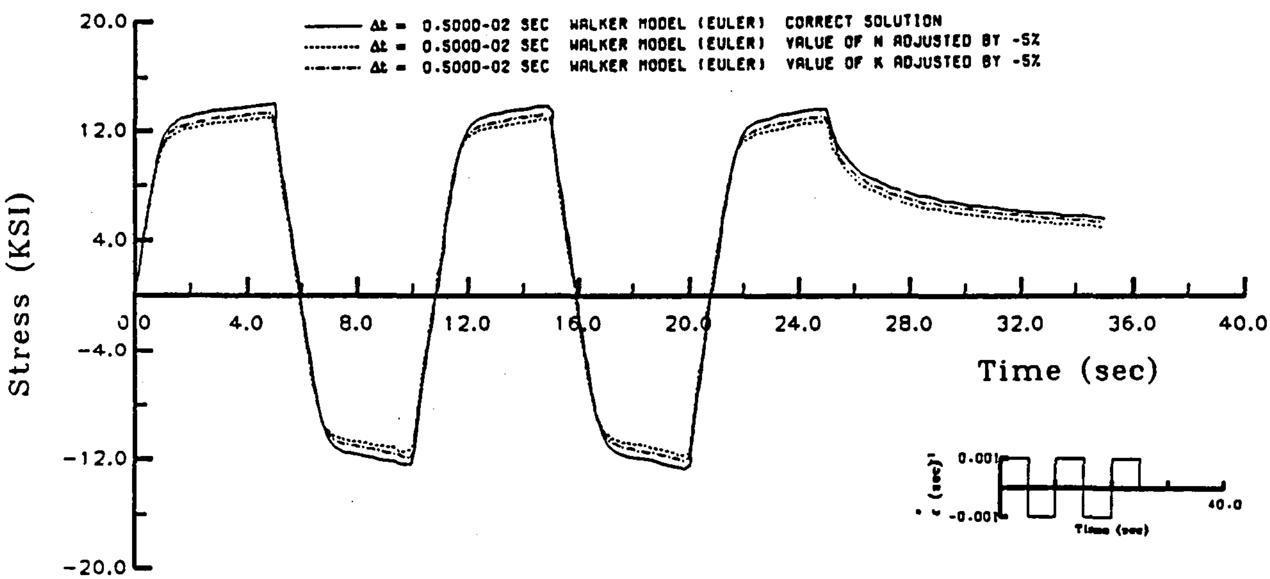

Fig. 6 Sensitivity of Walker's theory to -5% change in input constants (Hastelloy-X at 1800°F)

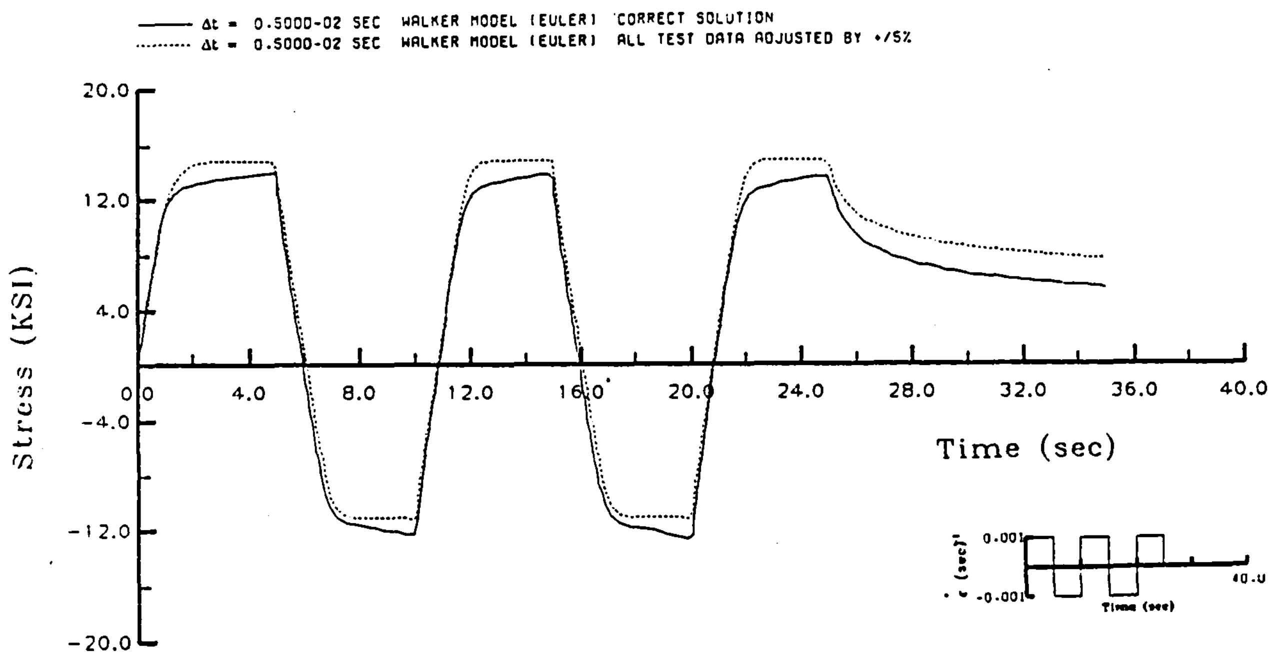

Fig. 7 Sensitivity of Walker's theory to 5% change in experimental test data used to generate constants (Hastelloy-X at 1800°F)

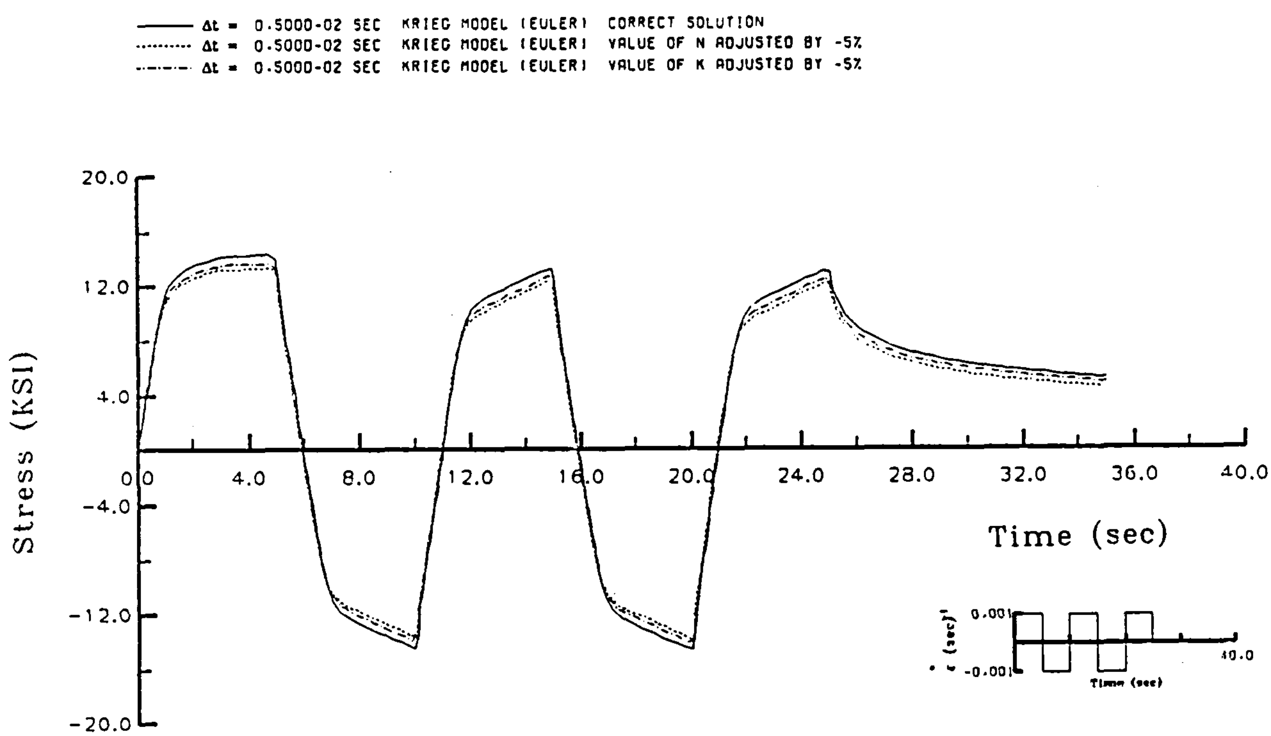

Fig. 8 Sensitivity of Krieg's theory to -5% change in input constants (Hastelloy-X at 1800°F)

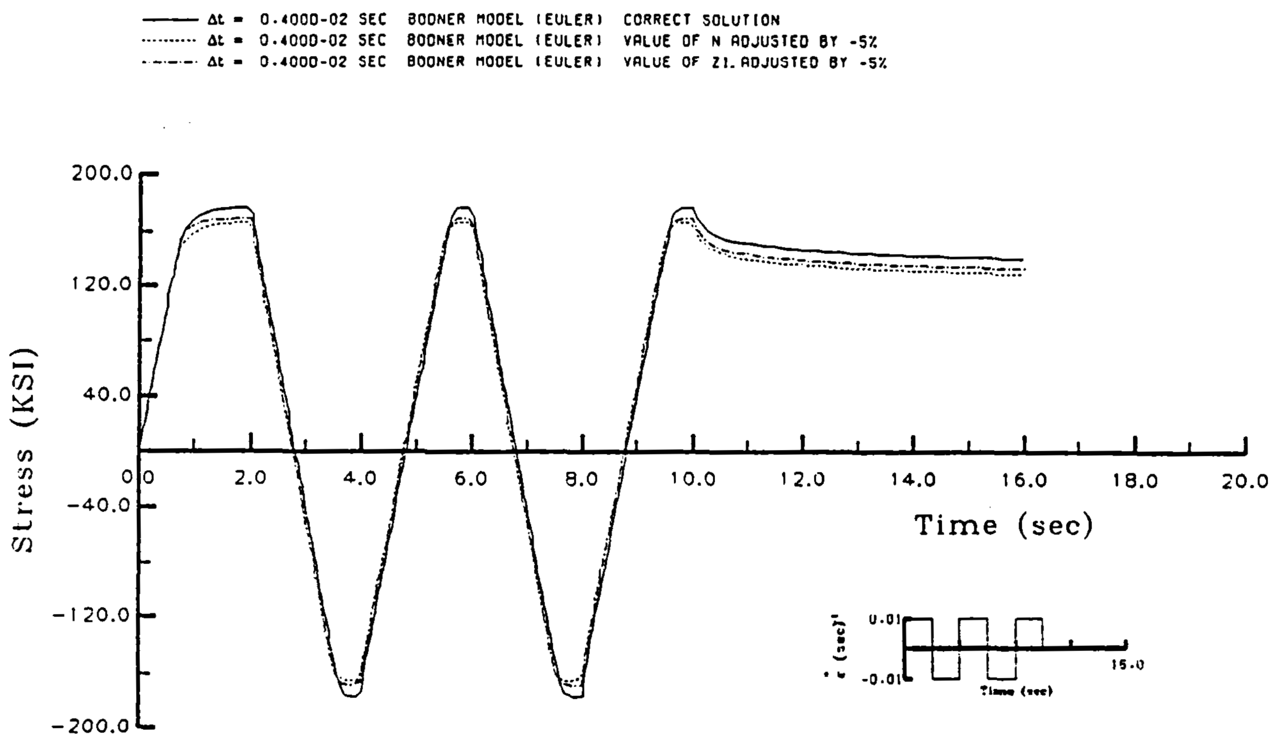

Fig. 9 Sensitivity of Bodner's theory to -5% change in input constants (IN100 at 1350°F)

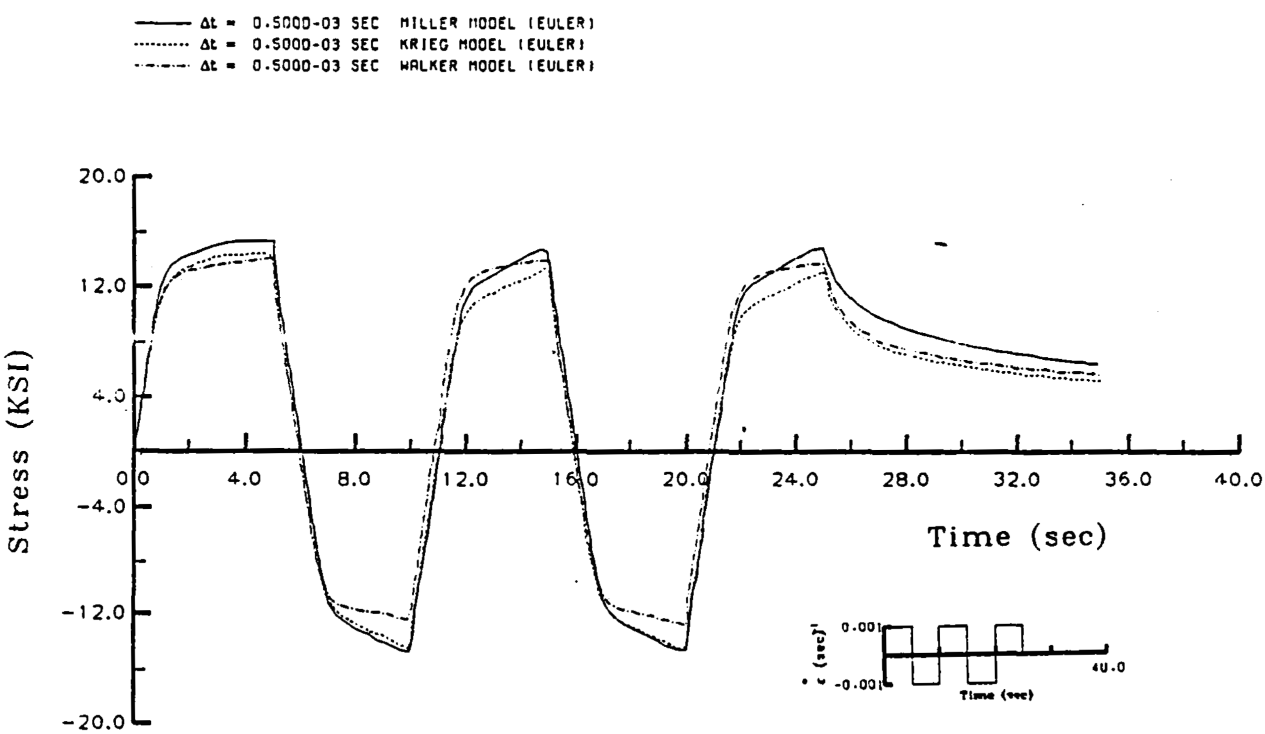

Fig. 10 Comparison of stress-time predictions for Miller, Krieg and Walker theories (Hastelloy-X at 1800°F)