

# THE EFFECT OF INITIAL ESTIMATED POINTS ON OBJECTIVE FUNCTIONS FOR OPTIMIZATION

Mahdi Soltani  
Annalisa Pola

Dip. di Ingegneria Meccanica e Industriale (DIMI)  
Università degli Studi di Brescia  
Brescia, Italy  
[mahdi.soltani@unibs.it](mailto:mahdi.soltani@unibs.it)  
[annalisa.pola@unibs.it](mailto:annalisa.pola@unibs.it)

Qiang Xu

School of Computing and Engineering  
The University of Huddersfield  
Huddersfield, UK  
[Q.Xu2@hud.ac.uk](mailto:Q.Xu2@hud.ac.uk)

## KEYWORDS

Component, Optimization, initial estimated points, Creep constitutive Equations.

## ABSTRACT

Research progress on the optimization in order to obtain the value of material constants for a set of creep damage constitutive equations was presented, including (1) a brief review of continuum creep damage modeling and the designs of objective functions; (2) case study reporting the influence of the initial start points on the final results; and (3) discussion and conclusion. As far as the authors know, there is no any published paper addressing specifically on the influence of starting values on the final results. In order to overcome the difficulty or inaccuracy it is suggested in this paper to (1) check the accuracy of a particular set of experimental data, (2) review the method to depict the relationship between the stress level and minimum strain rate, (3) to design a better objective functions so that the convergence is ensured to all the stress levels.

## INTRODUCTION

Constitutive equations, the mathematical description of material behaviour, are crucial for academic and industry. Hence, it is extremely important to be able to determine the best values for the material constants for a given set of constitutive equations

The aim of optimization processes is to determine the material constants of a set of constitutive equations with the best fits experimental data, typically using the least squares method. The principle of the least squares approximation to optimize a problem minimizes the sum of the squares of deviation between predicted values and experimental values (Ortega, 1994) (whittle, 1984).It could supply an improved procedure to determine "Direction Vector" to generate a sequence of points by the use of optimization-technique introduced by Numerical algorithms group (NAG) Library.

Creep damage mechanics has been developed and applied for dealing with the creep damage failure in high temperature industries where the core is the development of a set of creep damage constitutive equations. It is in this context, the determination of creep damage constants has been an issue for research community.

The creep experimental data described by (Hayhurst, et al., 2003) for 316 stainless steel at 550°C for six stress levels of 320, 300, 280 MPa (as high stress levels) and 231.65, 200.78, 169.6 MPa (as low stress levels) are used in the optimization and analysis with special initial estimated points (Table 1).

Table 1: Constant Starting Points for Objective functions (OF) within optimization process for 316 stainless steel at 550°C

	<i>A</i>	<i>B</i>	<i>H*</i>	<i>h</i>
<i>IEP</i>	1.53758E-07	0.009979478	0.50004175	47743.527

Although a recent research addressed that objective functions algorithms for optimization could be commenced from any unsystematic starting values without manual selection of initial points (Lia, et al., 2002), this paper tries to illustrate how change in initial Estimated Points (IEP) could lead to changes in the calculated constant material within creep constitutive equations (Table 2). Change in IEP in objective functions (OF) for components under lower stress levels, primarily, have experienced far less marked rather than the higher stress levels, as changing IEP (even less than 10%) could have a significant effect on the creep deformations under high stress levels. Table 2 shows 4 calculated models in different situation:

1. IEP increase by 10%; (A, B, H\*, h)
2. IEP increase by 10%; just only in A and B
3. IEP decrease by 10%; (A, B, H\*, h)
4. IEP decrease by 10%; just only in A and B

Table 2: Change in Starting Points for Objective functions (OF) within optimization process

<i>Model</i>	<i>A</i>	<i>B</i>	<i>H*</i>	<i>h</i>
base	1.53E-07	0.009	0.5	4.77E+04
1	1.69E-07	0.010	0.55	5.25E+04
2	1.69E-07	0.010	0.5	4.77E+04
3	1.38E-07	0.008	0.4	4.30E+04
4	1.38E-07	0.008	0.5	4.77E+04

## CONTINUUM DAMAGE MECHANISMS BASED MODELLING

The material science and engineering research have been established a reasonable understanding of the major creep deformation and damage mechanisms. Nevertheless, according to each class of materials, there are various approaches to use the different mechanisms for creep damage constitutive and evaluation equations have been formulated of the power law functions of stress to give an account of the creep behaviour under uniaxial and multi-axial states of stress over the various temperature ranges. There are several uniaxial creep design methods basing on the Continuum Damage Mechanisms (CDM). CDM-based methods have been used to predict creep damage, the lifetime of creep deformation, the residual strength and rupture strain by utilizing the various constitutive equations.

### Mechanisms-Based Model

Mechanisms-Based Model has a capability to utilize, practically, an alternative solution of the prominent problems in creep behaviours. Hence, the continuum approaches has merit of implementing a numerical method to simulate the processes of damage evolutions during the development in finite elements methods. (Barboza, et al., 2004) One of the proposed models is based upon the relation between Sine hyperbolic stress law and the impression velocities is pertinent to the technical analysis of creep deformations in the different ranges of stress and temperature (Yang, et al., 1995). The mechanisms-based model identified by the reproduction kinetics of dislocation motion using the finite element methods introduced for different materials such as for 0.5Cr-0.5Mo-0.25V ferritic steel under uniaxial over the temperature range of 600-675°C (Perrin & Huyhurst, 1996).

The effect of strain hardening through the primary-creep,  $H$ , has been formulated on the constitutive equations. Moreover, the cavities nucleate often occur on the grain boundaries so there is another variable introduced damage state,  $\omega$ , that it is the inter-granular creep constrained cavitation damage. Furthermore, the effects of temperature on the creep constitutive equation have been considered (equation 1).

$$\begin{cases} \dot{\epsilon} = \frac{A}{(1-\omega)^n} \sinh[B\sigma(1-H)] \\ \dot{H} = \frac{h\dot{\epsilon}}{\sigma} \left(1 - \frac{H}{H^*}\right) \\ \dot{\omega} = D\dot{\epsilon} \\ n = B\sigma(1-H) \coth(B\sigma(1-H)) \end{cases} \quad (1)$$

Where  $A$ ,  $B$ ,  $H^*$  and  $h$  are introduced as the creep constant material. The numerical optimization methods need to be used to determine the material constants with the best fits experimental data for finding the best optimum of a problem by using the least squares method. In many problems, it is trying to approximate a set of data by a best fit (Perrin & Hayhurst, 1996) (Perrin & Huyhurst, 1996). Constitutive Equations corresponding

to the creep behaviours under multi-axial stress could be completed.

### Kachanov-Rabotnov Model

The theory of creep damage mechanics was developed by Kachanov and Rabotnov in the 1960s that it has applied for analysing of creep rupture in different range of materials, although it has been modified within these years. They established a modern procedure introducing new parameters which describe the “continuity” ( $\Psi$ ) and the “damage” ( $\omega$ ) of the components (MacLachlan & Knowles, 2001). There are several different modified finite elements based on K-R creep model in the various mechanical software packages such as ANSYS and ABAQUS (Ling, et al., 2007).

### OPTIMIZATION MODE

The least squares optimization concentrated more on the stress levels (high stress levels and low stress levels) have been proposed on the suggested different creep constitutive equations. The objective function is usually specified to optimize a problem minimizing the sum of the squares of the deviation between predicted and experimental values. The following will demonstrate the put forward points more.

### Objective function

Reference (Lia, et al., 2002) characterized the difficulties in determining the material constants via the principle of the least squares approximation experimental data. Moreover, it was expected that the Objective functions algorithms for optimization could be commenced from any unsystematic starting values inasmuch manual selection of initial points do not need to be used, hence, the objective functions carry out better than binary genetic algorithms suggested previously (Lin & Yangb, 1999). It is introduced two ways for determining the objective functions for optimization:

#### Objective function I (OFI):

The errors could be determined by the shortest distance between calculated and experimental data. Meanwhile, in order to develop the sensitivity, one extra term needs to be introduced (Lia, et al., 2002). Thus the objective function,  $f(X)$ , is defined by:

$$f(X) = \sum_{j=1}^{n_1} \sum_{i=1}^{m_j} w_{ij} d_{ij}^2 + \sum_{j=1}^{n_1} W_j \left( t_{m_j}^t - t_{m_j}^m \right)^2 \quad (2)$$

We need to introduce the definitions of the different terms used in the above equation;

#### Objective function II (OFII):

Where the errors could be determined by time only:

$$F(X) = \sum_{j=1}^{n_1} \sum_{i=1}^{m_j} W_j \left( t_{m_j}^t - t_{m_j}^m \right)^2 \quad (3)$$

## The Overall Optimization for Creep Constitutive Equation

The recommended Objective functions includes the integration of square of the residual value of predicted and experimental strain for each points corresponding to different stress levels (equation 4), and for increasing the sensitivity, two extra terms are introduced, the residual value of computational and experimental lifetimes and minimum creep-strain rates (equation 5) [9]. The Overall Optimization for Creep constitutive Equation identified by (Hayhurst, et al., 2003):

- The Least Square optimization:

$$LS = \sum_{i=1}^{MS} \left\{ \left[ \sum_{j=1}^{a_i} (\varepsilon_j^{\text{pred}} - \varepsilon_j^{\text{exp}})^2 \right] + Z_i (t_i^{\text{pred}} - t_i^{\text{exp}}) / t_i^{\text{exp}} + \alpha_i \{ (\dot{\varepsilon}_{\text{min}}^{\text{pred}} - \dot{\varepsilon}_{\text{min}}^{\text{exp}}) / \dot{\varepsilon}_{\text{min}}^{\text{exp}} \}_i \right\} \quad (4)$$

- The modified Least Square optimization:

$$LS^* = \sum_{i=1}^{MS} \left\{ \left[ \sum_{j=1}^{a_i} \left( \frac{\varepsilon_j^{\text{pred}} - \varepsilon_j^{\text{exp}}}{\varepsilon_{a_i}^{\text{exp}}} \right)^2 \right] + Z_i (t_i^{\text{pred}} - t_i^{\text{exp}}) / t_i^{\text{exp}} + \beta_i \{ (\varepsilon_f^{\text{pred}} - \varepsilon_f^{\text{exp}}) / \varepsilon_f^{\text{exp}} \}_i + \alpha_i \{ (\dot{\varepsilon}_{\text{min}}^{\text{pred}} - \dot{\varepsilon}_{\text{min}}^{\text{exp}}) / \dot{\varepsilon}_{\text{min}}^{\text{exp}} \}_i \right\} \quad (5)$$

If all parts of the creep deformation curves for each stress levels (High stress and also low stress with long lifetime) have been available to investigate, therefore, the least-square optimization will be able to improve greatly; in this situation, different stages of the creep curves could be conventionalized with respect to the experimental-values at the end of each of the corresponding stages, thus the new suggested optimization model is divided into different parts which each part will be pertinent to one stage of the creep curves. (Primary and secondary creep curves) (2005).

## Changing Accuracy in Optimization Process

Any changes in accuracy with different starting points lead to marked changes in calculated constant materials. This study try to illustrates the information about percentage of changes in computed results with different accuracy demanded after 10% increase or decrease in starting points either A and B or all four creep constant materials (A, B, H\* and h).

In this situation, there are some different ‘‘Amplification factors’’ which could control optimization process. Amplification factors could supply an improved procedure to determine ‘‘Direction Vector’’ to generate a

sequence of points by the use of optimization - techniques implanted in the NAG routine.

Albeit, the accuracy of linear minimizations leads to decrease the number of iterations executed by NAG, it would cause an increase in the number of invoked subroutine relevant to Least Square optimization (NAG, 2011). In this situation, the number of iterations required depends on:

- the number of variables of constitutive equations,
- the number of the residual value of computational and experimental data
- the behaviour of  $F(X)$  that  $X = x^{(k)} + \alpha^{(k)} p^{(k)}$ ,
- the accuracy required,
- the distance of the starting point from the solution.

NAG library has determined two different parameters (ETA, XTOL) are the key factors to determine the accuracy demanded. It supposed to change the amount of two mentioned parameters, separately, to achieve a same point.

- ETA indicates how precisely the linear minimizations are to be performed. (Equation 4) is an approximate minimum with respect to  $\alpha^{(k)}$ ; in this Subroutine,  $\alpha^{(k)}$  plays a role in specifying how accurate in the linear-minimization is to be done.

$$F(x^{(k)} + \alpha^{(k)} p^{(k)}) \quad (6)$$

- XTOL indicates the preciseness in x to which the solution is required (NAG, 2011). If  $x_{\text{true}}$  is the true value of x at the minimum, then  $x_{\text{sol}}$ , the estimated position prior to a normal exit, is such that

$$\|x_{\text{sol}} - x_{\text{true}}\| < XTOL \times (1.0 + \|x_{\text{true}}\|) \quad (7)$$

NAG library introduces a controller parameter (is called ETA) that the user can specify the accuracy of minimum with respect to  $\alpha^{(k)}$ . Obviously, it will be located more precisely for small values of ETA (say 0.01) than for large values. Although it reduces the number of iterations carried out by NAG, it will increase the number of calls of Least-Square Optimization made. Changing in accuracy in liner minimizations (ETA) with different starting point at such as 0.5, 0.1, 0.01 and 1.0E-4 at a demanded accuracy in x such as 1.0E-4 lead to a noticeable change in calculated material constant (Table 3 and 4).

Table 3: The Percentage of Change between Initial Calculated Constant materials and calculated results with different IEP when ETA: 0.5(A), and ETA: 0.1(B), XTOL=1.0E-04

ETA=0.5 and XTOL=1.0E-04				
Model	A	B	H*	h
1	-22%	12%	-3%	-15%
2	-76%	17%	-23%	4%
Base	(A)			
3	20%	-3%	-7%	-1%
4	19%	-3%	-2%	-2%
ETA=0.1 and XTOL=1.0E-04				
Model	A	B	H*	h
1	-4%	5%	-1%	-32%
2	-22%	10%	-14%	-37%
Base	(B)			
3	18%	-2%	-7%	6%
4	31%	-6%	3%	-6%

Table 4: The Percentage of Change between Initial Calculated Constant materials and calculated results with different IEP when ETA: 0.01(c), and ETA: 1.0E-4(d); XTOL=1.0E-04

ETA=0.01 and XTOL=1.0E-04				
Model	A	B	H*	h
1	20%	-6%	13%	-21%
2	-8%	7%	-12%	-43%
Base	(C)			
3	31%	-8%	0%	-10%
4	26%	-7%	-2%	-26%
ETA=1.0E-4 and XTOL=1.0E-04				
Model	A	B	H*	h
1	23%	-11%	17%	-29%
2	-36%	14%	-18%	-27%
Base	(D)			
3	27%	-9%	1%	-22%
4	22%	-7%	-2%	-34%

### ANALYSIS

Choosing more appropriate starting values for each material constant within the creep constitutive equations (equation 1) manage to provide a better possibility to converge to one of the local minimum than to a global one (Mustata & Hayhurst, 2005).

When some new experimental creep data (with two new stress levels; 240MPa, 185.3MPa) are added to the last mentioned collection, obviously, all of the previous calculated results will be changed. This paper tries to show that if there is a change in the previous starting points (even by 10 per cent) within this new collection, it could lead to changing significantly in the calculated constant material, especially in high stress levels (Figure 1).

The calculated material constants for creep constitutive equations under low stress levels (for example 231.65MPa, 200.78MPa, 185.3MPa and 169.67MPa), primarily, when initial estimated points for all constant material (A, B, H\*, h) are changed by 10%, the final calculated strain will increase generally less than 15% thus it is expected that the optimization process could be started from any random starting points as the final result

especially in low stress level (Figure 2).

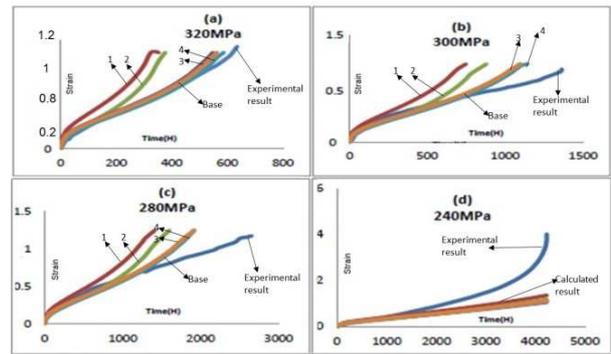


Figure 1: Creep Deformation Curves with Different IEP under higher Engineering Stress Levels

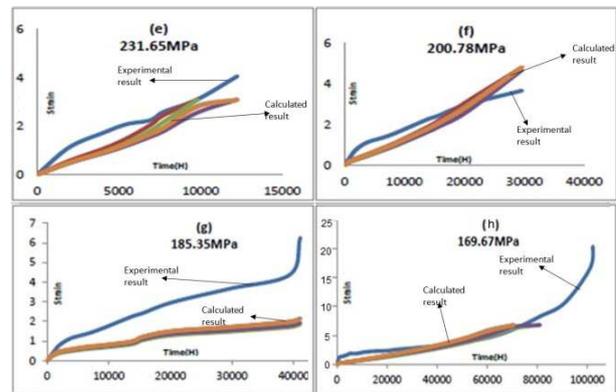


Figure 2: Creep Deformation Curves with Different IEP under lower Engineering Stress Levels

However, this effect is much considerable, especially, for high stress levels (for example 320MPa, 300MPa, 280MPa and 240MPa). The final calculated strain will increase primarily more than 25% (such as 320MPa, at the tertiary creep stages, changes accounted for a significant increase by even more than 50%).

As the creep primary stage for high stress levels is more significant than that under lower stress levels, the reduction of percentages in calculated variables corresponding to the strain hardening through the primary-creep for higher stress levels has a consequential effect on the calculated strain and creep deformation curves (Figure 1). Therefore, these changes could not be neglected, thus using of different starting points lead to different results for objective functions within optimization process.

More fundamentally, careful observation of the numerical predicted creep curves shown in following Figures reveals that: the numerical predictions for high stress level are essentially larger than the experimental ones while the predicted creep curves for low stress level is essential underestimated. As long as the required accuracy for optimisation is achieved, the programme will stop resulting significantly different sets of final material constants. This consequently raises the question of how to design a better objective function to ensure the

agreement at different stress level is ensured rather than just the global agreement.

## CONCLUSION

In this paper, the analysis of changing initial estimated points in optimization process has been proposed for different stress levels. This is achieved by using objective function within an advanced optimization techniques for a creep constitutive equations, which are as follows.

- Any changes in entered experimental data with the change in IEP could lead to a significant change in the calculated constants for materials within creep constitutive equations especially for material under higher stress levels.
- The effect of different accuracy in for the linear minimizations has been performed to approach to accurate local minima than a global minimum.

## REFERENCES

- Barboza, M. J., Neto, C. M., and Silva, C. R. 2004. "Creep mechanisms and physical modeling for Ti-6Al-4V. *Materials Science and Engineering*", 369(1-2), 201-209.
- Hayhurst, D. R., Vakili-Tahami, F., and Zhou, J. Q. 2003. "Constitutive equations for time independent plasticity and creep of 316 stainless steel at 550 °C. *International Journal of Pressure Vessels and Piping*", 80(2), 97-109.
- Lia, B., Lin, J., and Yaoc, X. 2002. "A novel evolutionary algorithm for determining unified creep damage constitutive equations. *International Journal of Mechanical Sciences*", 44(5), 987-1002.
- Lin, J., and Yang, J. 1999. "GA-based multiple objective optimisation for determining viscoplastic constitutive equations for superplastic alloys". *International Journal of Plasticity*, 15(11), 1181-1196.
- Ling, X., Zheng, Y., You, Y., and Chen, Y. 2007. "Creep damage in small punch creep specimens of Type 304 stainless steel." *International Journal of Pressure Vessels and Piping*, 84(5), 304-309.
- MacLachlan, D. W., and Knowles, D. M. 2001. "Modeling and prediction of the stress rupture behaviour of single crystal super alloys." *Materials Science and Engineering*, 302(2), 275-285.
- Mustata, R., and Hayhurst, D. 2005. "Creep constitutive equations for a 0.5Cr 0.5 Mo 0.25V ferritic steel in the temperature range 565 °C-675 °C." *International Journal of Pressure Vessels and Piping*, 82(5), 363-372.
- NAG. 2011. "Numerical Algorithms Group". Tratto il giorno 03 15, 2011 da <http://www.nag.co.uk/index.asp>
- Ortega, J. 1994. "An introduction to FORTRAN 90 for science computing (1st ed.)." *Sunders College Publishing*.
- Perrin, I. J., and Hayhurst, D. R. 1996. "A method for the transformation of creep constitutive equations". *International Journal of Pressure Vessels and Piping*, 68(3), 299-309.
- Perrin, I. J., and Huyhurst, D. 1996. "Creep constitutive equations for a 0.5Cr 0.5 Mo 0.25V ferritic steel in the temperature range 565 °C-675 °C." *Journal of Strain Analysis*, 31(4).
- whittle, P. 1984. "Prediction and Regulation by Linear Least-Square Methods (2nd ed.)." oxford: basil blackwell.
- Yang, F., Li, J. C., and Shih, C. W. 1995. "Computer simulation of impression creep using the hyperbolic sine stress law." *Materials Science and Engineering A*, 201(1-2), 50-57.
- Yang, F., Li, J. C., and Shih, C. W. 1995. "Computer simulation of impression creep using the hyperbolic sine stress law." Volume 201, Issues 1-2, October 1995, Pages , 201(1-2), 50-57.