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Determination of the material constants of creep damage constitutive equations using Matlab optimization procedure

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Abstract- Creep damage constitutive equations based in continuum damage mechanics are characterized by their complexity due to the coupled form of the multi-damage state variables over a wide range of stresses. Thus, the determination of the material constants involved in these equations requires the application of an optimization technique. A new objective function was designed where the errors between the predicted and experimental normalized deformation and lifetime were used in conjunction of the minimal nonlinear least square method from Matlab. Its use is simpler, more compact, and less uncertain and is able to obtain an accurate solution for a sample material (0.5Cr 0.5Mo 0.25V ferritic steel) at the range of 560-590°C. The specific experimental data, the material constants, and all the factors needed are provided as a comparison with the existent investigation of this material. Future works should aim at to further establish the reliability and user-friendness of the method.

Keywords: Creep constitutive equations, ferritic steel, material constants, optimization, Matlab

I. INTRODUCTION

Ferritic steel alloys are extensive utilized for a welded steam pipes in the assembly of power plant components operating under a critical conditions where the creep deformation and possible failure are significant in the design factors requirements such as strain histories, damage field evolution and lifetimes. Continuum damage mechanics describes the creep behavior using physically based creep damage constitutive equations [1, 2]. These equations are developing into more elaborated because new state variables are introduced to describe more accurately the deformation and the damage mechanisms [3, 4]. The accurate determination of the material constants involve in constitutive equations utilizing the experimental data for a range of temperatures and stresses is a challenging and difficult task according to [5, 6].

In the past decades many researchers have investigated this issue, and commonly optimization procedure are utilized to determinate the constants, by applying the minimal least square method to an objective function which compute the errors of simulated and experimental data. Methods were developed for the creep damage [1, 4], and viscoplasticity model [7, 8]. The optimization routines of these approaches need a set of careful chosen starting values in order to achieve global convergence. To solve this problem Lin & Yang [6], and Li, Lin, & Yao [5] Dr Qiang Xu School of Computing and Engineering University of Huddersfield Huddersfield, United Kingdom <u>Q.Xu2@hud.ac.uk</u> ORCID iD <u>0000-0002-5903-9781</u>

developed a global optimization method for superplasticy and creep damage, respectively, using genetic algorithms, which do not need a good starting value for a correct convergence, whereas, the difficulty to implement the objective function is increased considerably, moreover, a higher understanding of complex program code routines are needed.

Gong, Hyde, Sun, & Hyde [7] developed a simple optimization program for determining the material parameters in the Chaboche unified viscoplasticiy model, using Matlab. In this case the optimization routine seeks for the global minimum of the difference between the square sum of the predicted and experimental stresses. Runga-Kutta-Felhberd algorithm was used to solve the ODE's of the model, and the Matlab optimization toolbox function, '*Isqnonlin*' which implement the Levenberg-Marquardt algorithm for each iteration step, was used to solve the nonlinear least square optimization.

Kowalewsky, Hayhurst, & Dyson [2] generated a satisfactory three-stage procedure to estimate the initial estimation of the material constants of the constitutive equations for an aluminum alloy. This equations can be related to the different parts of the creep curve, then, working out them, it can be found a good enough first guess. Later on, a general optimization process is used to estimate the final values. Similarly, Mustata & Hayhurst [1] developed a methodology for a 0.5Cr 0.5Mo 0.25V ferritic steel. The objective function utilized for the optimization is separated in three parts. First, the strain estimated and compared with the experimental, separating, each stage of the curve with a scaling factor, second, a time term with amplification factor, and third, a penalty function with the minimum strain rates. This objective function is significantly complex, the values of the several scaling factors are not given, resulting in uncertainty in its generic application. Furthermore, both approaches utilized a NAG numerical library in FORTRAN to implement the optimization routine, which is not as easily available as Matlab.

This paper reports the determination of the material constants for a set of creep damage constitutive equations, a similar approach of [7] for the viscoplasticity model. It is featured by the design of new objective function where both the differences of creep strain and the time between experimental and prediction are normalized including a weighting function.

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II. OBJECTIVES

The main objective of this paper is to develop a general optimization procedure, using Matlab, to calibrate the material constants of the CDM-based creep constitutive equations for 0.5Cr 0.5Mo 0.25V ferritic steel. The program developed has to be able to reproduce the behavior of the creep mechanics of this material operating at high temperatures.

III. CONSTITUTIVE EQUATIONS

The hardening and softening mechanisms and the initiation and growth damage of the ferritic steel alloy are expressed by CDM-based constitutive equations. The uniaxial from proposed by Dyson, Hayhurst, & Lin [9] for a constant temperature is given by the following set of equations:

$$\frac{d\varepsilon}{dt} = A \sinh\left[\frac{B\sigma(1-H)}{(1-\Phi)(1-\omega)}\right]$$
(1)

$$\frac{dH}{dt} = \frac{h}{\sigma} \frac{d\varepsilon}{dt} \left(1 - \frac{H}{H^*} \right)$$
(2)

 $\frac{\mathrm{d}\Phi}{\mathrm{d}t} = \frac{\mathrm{K}_{\mathrm{c}}}{3} (1 - \Phi)^4 \tag{3}$

$$\frac{d\omega}{dt} = C\frac{d\varepsilon}{dt}$$
(4)

where the state variables represents, Φ , the coarsening of the carbide precipitates, the variable changes from zero to one, ω , the intergranular creep constrained cavitation damage, and also varies from zero (no damage state) to ω_f (failure), and, H, the strain hardening effect, in the beginning, it is zero and increases to a boundary value H^* at steady-state creep. A, B, C, h, H* and Kc are material constants to be calibrated with the optimization method, ε is the deformation, and σ is the stress applied to the material. The material constant can be related to difference stages of the creep curve [3]: 1) h and H^* describe the primary stage, where is produced the hardening process, 2) A and B model the secondary stage, strain rate remains almost constant, 3) C and K_c describe the last stage of the curve, where are localized the damage mechanisms.

IV. OPTIMIZATION METHOD

The identification of a material constants in the CDMbased creep constitutive equations is a reverse process based on experimental data. A nonlinear least square optimization procedure is adopted. The primary aim is to find the value for the material constants which produce a global minimum of an objective function which basically simulate the difference between the predicted and experimental deformation under different stress levels at the same temperature.

$$f(b) = \sum_{i=1}^{m} \left[\sum_{j=1}^{n} \left(\varepsilon(b)_{j}^{\text{pred}} - \varepsilon_{j}^{\text{exp}} \right)^{2} \right]$$
(5)

 $b \in \mathbb{R}^n$; $LB \le b \le UB$ where f(b) is the basic objective function, b is the optimization variable set (a vector of n-dimensional space, \mathbb{R}^n), which for this specific case are

material constants on the CDM-based creep constitutive equations, $b = [A, B, H^*, h, K_c, C]^T$, *LB* and *UB* are the lower and upper boundaries of *b* allowed during the calibration, $\varepsilon(b)_j^{pre}$ and ε_j^{exp} are the model predicted total strain and the experimental measured strain, respectively, at a specific time *j* within the loop of maxim *n*, *i* is the specific curve used in the optimization for *m* number curves with different stress levels.

During the calibration of the boundary constraints has been noticed that for the material at 560°C the upper boundary for the constant A, has to be fixed on 1.00e-9 h⁻¹ for an accurate solution. For the other parameters, it was left a range of variance around them. The values can be seen in the Table 1.

A. Numerical Techniques

The prediction of the creep deformation at specific temperature and stress can be achieved by integrating the set of ODE's for a set of identify material constant vector b. From the set (1) to (4) a first order non-linear system with four differential equations with four variables $x = [\Phi, \omega, H, \varepsilon]^T$ can be identified. Solving the ODE's system by a numerical method such as Runge Kutta-Fehleberg algorithm can be estimated the creep damage characteristics (deformation, lifetime, and rupture strain). The Runge-Kutta-Feheleberg algorithm uses a pair of Runge-Kutta methods to obtain both the computed solution and an estimate of the truncation error [10]. Matlab has a command named as 'ode45' which implement this algorithm directly, it is needed only to specific a range time, initial values for the variables, and a tolerance for the solution [11].

The nonlinear least square optimization algorithm applied here was used satisfactorily by Gong, Hyde, Sun, & Hyde [7], the Levenberg-Marquadt which in Matlab is implemented in the '*Isqnonlin*' command. This function ask for a vector valued function as input:

$$f(b)=[f_1(b) \ f_2(b) \dots f_n(b)]$$
 (6)

where *b* is a vector of the unknown values to be estimated, and $f_n(b)$ are the vectors of the objective function [11]. The output of this command can be represented mathematically as the following nonlinear least square equation:

$$\min_{b} \|f(b)\|_{2}^{2} = \min_{b} [f_{1}(b)^{2} + f_{2}(b)^{2} + \dots + f_{n}(b)^{2}]$$
(7)

where the variables represent the same as in the previous equation.

B. Experimental Data

Experimental data of the uniaxial creep curves from [1] were digitized and shown in Fig.1, and Fig.2 schematically, and numerically in the Table 2, and Table 3. A lack of data is observed from the experimental tests, thus extra points were interpolated for a curve fitting purpose, which were also shown in the Figures and Tables. The new data is represented as dots, and clearly, it can be seen that, specially, for the 85 MPa curve of the material at 560 °C the rebuilt is needed because the data in the primary and tertiary stage is insufficient.

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The experimental lifetimes for the material at 560 °C are 91000, 51900, 31111 hours, for 85, 100, 110 MPa, respectively [1]. For the 590 °C are unknown, thus, they were estimated from the curves being 5100, 2700, 1400 hours, for 100, 110, 120 MPa, respectively.

Table 1. Boundary constraints for the material constants

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Boundary	Material at 560°C		Material at 590°C		
Constraints	LB	UB	LB	UB	
A (h ⁻¹)	1.00E-10	1.00E-09	1.00E-10	5.00E-09	
B (MPa ⁻¹)	1.00E-01	2.00E-01	1.00E-01	2.00E-01	
H* (-)	4.00E-01	8.00E-01	3.00E-01	8.00E-01	
h (MPa)	1.00E+04	2.00E+05	1.00E+04	3.00E+05	
$K_{c}(h^{-1})$	1.00E-06	3.00E-05	1.00E-06	1.50E-04	
C(-)	3	10	2	8	



Figure 1. Real experimental data and interpolated (dotted points) for curve fitting purpose of the material at $560^{\circ}C$



Figure 2. Real experimental data and interpolated (dotted points) for curve fitting purpose of the material at 590°C

C. Initial Guess

How was said in the introduction and according to Kowalewsky, Hayhurst, & Dyson [3] and Mustata & Hayhurst [1] to be successful in the determination of the material constants, it is critical to start with acceptable values for the combined integration/optimization process.

The constants A and B are calculated integrating (1), and applying a linear least square optimization to the variation of the minimum strain rate and the stress. H^* and h are estimated by applying a nonlinear curve fitting for the primary part of the curve. C is calculated by averaging the value of the failure strain, integrating (4) and knowing that $\omega_f=1/3$. Finally, K_c is obtained by applying a similar process to the general optimization, but in this case only is allowed to vary to the *Kc* parameter, keeping the remainders constants [3].

The results obtained for the initial values of the constants for 560°C are demonstrated on the Table 4. For 590°C, the only modification in the constants, is C=2.88, obtained only accounting the stresses 100, 110, and 120 MPa. Also in the Fig.3, and Fig.4 is illustrated the predicted creep curves using these values for the material constants.

The initial guess for the first case clearly shows a good approximation, whereas, for the second case the approximation diverge considerably from the experimental curve that is due to the initial estimation process is only accurate for a specific temperature. Despite of this divergence in the solution, it will keep the initial values for the optimization process with the intention to check the usefulness of the program to predict the creep mechanic behavior, for different operating temperatures.

D. General Objective Function

The new objective function introduced in this paper to be minimized for the nonlinear least square optimization, is a slightly different to (5), a term to involve lifetime has been introduced following the approach utilized by Kowalewsky, Hayhurst, & Dyson [3], conversely, and it is squared to be part of the least square process. When the predicted range time is longer than the equivalent experimental, some of the simulated data cannot be involved, thus, this term compensates these errors. Furthermore, the strain error is normalized by the failure deformation, therefore, the amplification factor in the time term will have a value in the order of 0 to 1, and due to the normalization, and both terms have the same scale. The value of the weight depends on the level of sensitivity of the creep deformation or lifetime in regard to the parameters to be estimated. When the time and strain have the same relevancy for the optimization, the factor is equal to 1, and when is 0 only the strain errors are accounted. The new function can be expressed as:

$$\begin{split} F_{\varepsilon}(b) &= \sum_{i=1}^{m} \left[\sum_{j=1}^{n} \left\{ \left(\frac{\varepsilon(b)_{j}^{pred} - \varepsilon_{j}^{exp}}{\varepsilon_{fi}^{exp}} \right)^{2} \right\} + \\ &+ w_{i} \left(\frac{t(b)_{fi}^{pred} - t_{fi}^{exp}}{t_{fi}^{exp}} \right)^{2} \right] \end{split} \tag{8}$$

where the new terms are: $F_{\varepsilon}(b)$, the new objective function, w_i , a scaling factor for each curve i, $t(b)_{fi}^{pred}$ and t_{fi}^{exp} denote predicted and experimental lifetime for a specific time and curve, respectively, and ε_{fi}^{exp} represents the rupture deformation for a specific stress curve. The second term in the expression is only invoked, when t_f^{pred} is larger than t_f^{exp} . This approach allows to work with values of the same scale, almost guaranteeing an equal contribution in the least square process of each term, and the calibration of the w can be obtained

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straightforward by using a loop to calculate the optimization solution for w = [0.1, 0.2, ..., 1].

Table 2. Real experimental data (shaded cells) and new digitized data for curve fitting purpose of material at 560°C

85 Mpa		100 N	100 Mpa 11		0 Mpa	
	time (hours)	ε (%)	time (hours)	ε (%)	time (hours)	ε (%)
	0	0.000	0	0.000	0	0.000
Γ	390	0.051	164	0.027	82	0.113
Γ	1014	0.089	906	0.179	150	0.127
	3011	0.151	1474	0.165	303	0.179
Γ	4961	0.191	2546	0.268	772	0.231
Γ	6473	0.217	4504	0.326	1114	0.287
Γ	9981	0.268	6581	0.402	2447	0.384
Γ	13596	0.316	8042	0.442	3038	0.418
	16634	0.461	10240	0.534	4393	0.488
	22547	0.430	12184	0.554	5501	0.541
	26223	0.570	14901	0.630	8352	0.672
	29158	0.521	16630	0.769	10239	0.606
	34158	0.597	19218	0.761	12075	0.854
	36658	0.639	22366	0.950	14252	0.841
	38270	0.769	25070	1.058	16873	1.022
	41658	0.730	26954	1.167	18675	1.176
	47448	0.913	28101	1.212	20148	1.320
	50070	0.995	29575	1.257	21130	1.456
	52037	1.058	31705	1.366	22604	1.601
	54823	1.140	33589	1.483	23995	1.863
	57609	1.194	35227	1.601	25058	2.071
	60395	1.239	36947	1.736	25957	2.252
	62936	1.302	38256	1.908	27020	2.496
	67934	1.456	39730	2.071	27428	2.659
	70719	1.574	40630	2.216	28163	2.903
	75962	1.836	42021	2.424	28733	3.193
	78911	2.026	43330	2.632	28894	3.437
	81284	2.379	44475	2.849	29219	3.672
	82465	2.587	45700	3.202	29544	3.943
	83222	2.910	46598	3.572	29605	4.187
	84295	3.312	47494	3.979	29702	4.477
Ľ	84945	3.653	47981	4.404	29745	4.703
	85789	4.201	48058	4.829	29793	4.938
	86389	4.701	48382	5.200	29857	5.191
	87033	5.189	48459	5.643	30017	5.517
1	87610	6.017	48536	6.032	30100	5.906

Table 3. Real experimental data (shaded cells) and new digitized data for curve fitting purpose of material at $590^{\circ}C$

100 Mpa		110 Mpa		120 Mpa	
time (hours)	ε (%)	time (hours) ε (%)		time (hours)	ε (%)
0	0.000	0	0.000	0	0.000
54	0.078	54	0.104	30	0.027
119	0.156	119	0.209	48	0.118
212	0.235	179	0.261	65	0.209
282	0.261	239	0.313	98	0.235
363	0.287	282	0.365	130	0.261
418	0.313	331	0.391	160	0.300
499	0.313	407	0.417	190	0.339
586	0.365	445	0.443	209	0.391
667	0.391	488	0.469	228	0.443
754	0.417	537	0.495	250	0.469
787	0.417	591	0.600	271	0.495
857	0.417	635	0.626	293	0.547
884	0.417	689	0.704	315	0.600
955	0.469	776	0.756	328	0.626
987	0.469	835	0.808	342	0.652
1052	0.521	884	0.873	355	0.665
1080	0.547	933	0.939	369	0.678
1156	0.521	993	1.017	415	0.795
1199	0.547	1052	1.095	461	0.912
1280	0.600	1150	1.199	499	0.991
1318	0.626	1196	1.277	537	1.069
1421	0.678	1242	1.356	597	1.238
1503	0.730	1297	1.434	656	1.408
1606	0.756	1345	1.499	700	1.525
1703	0.808	1394	1.564	743	1.642
1807	0.860	1446	1.655	784	1.773
1904	0.912	1497	1.747	825	1.903
2013	0.965	1543	1.851	868	2.086
2105	1.017	1590	1.955	906	2.242

2213	1.069	1644	2.086	944	2.399
2311	1.121	1698	2.216	968	2.529
2430	1.225	1744	2.320	993	2.659
2528	1.304	1790	2.425	1010	2.757
2626	1.356	1855	2.607	1028	2.855
2729	1.382	1926	2.842	1063	3.050
2805	1.564	1975	2.972	1085	3.220
2913	1.564	2024	3.102	1107	3.389
3011	1.616	2056	3.181	1134	3.598
3098	1.695	2089	3.337	1161	3.806
3201	1.825	2121	3.493	1183	4.041
3282	1.929	2170	3.728	1193	4.178
3385	2.060	2219	3.963	1204	4.315
3505	2.242	2268	4.171	1226	4.588
3613	2.346	2327	4.458	1229	4.595
3700	2.451	2357	4.680	1253	4.875
3765	2.555	2387	4.901	1257	4.970
3863	2.685	2400	5.100	1286	5.345
3949	2.842	2430	5.371	1281	5.372
4042	3.024	2441	5.501	1305	5.775
4145	3.181	2468	5.788	1302	5.789
4231	3.389	2485	6.022	1324	6.205
4329	3.598	2501	6.231	1320	6.114
4410	3.858	2517	6.544	1337	6.439
4497	4.145	2528	6.700	1335	6.394
4579	4.458	2544	6.987	1351	6.674
4660	4.927	2566	7.430	1356	6.831
4741	5.371	2582	7.873	1362	7.091
4779	5.709	2582	8.082	1367	7.352
4839	6.101	2599	8.577	1367	7.847
4931	6.831	2604	9.020	1373	8.343
4969	7.326	2606	9.200	1378	8.838
5013	7.717	2610	9.400	1381	9.073
5018	7.847	2615	9.568	1383	9.307
5034	8.343	2626	9.881	1386	9.607
5072	8.864	2627	10.000	1389	9.907
5078	9.333	2627	10.200	1389	10.155
5094	9.881	2631	10.376	1389	10.402
5094	10.402	2637	10.845	1389	10.845
5099	11.002	2637	11.002	1389	11.002



Figure 3. Predicted deformation using the initial estimated values of the material constants for the material at 560° C

Table 4. Initial estimation of the material constants

Initial guess (b ₀)	Material at 560°C
$A(h^{-1})$	1.00E-09
B (MPa ⁻¹)	1.10E-01
H* (-)	4.26E-01
h (MPa)	5.05E+04
$K_{c}(h^{-1})$	6.86E-06
C(-)	4.311

E. Program Development

The program developed in Matlab to obtain the parameters which give the best curve fitting can be divided in four stages.

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Figure 4. Predicted deformation using the initial estimated values of the material constants for the material at 590° C

First step is to digitize the experimental data and calculate the b_0 , following procedure describe in the sections 4.B and 4.C. Second, the initial conditions are set up, initial values of the state variables x_0 , the tolerances for the optimization solution, and the boundary constraints for the parameters to be optimized. Continuously, it is started a for loop which is utilized to calibrate the value of the time factor w_i , it is decide the number of w tried, N, and the variance on the amplification value Δw , which will vary between 0-1, depending on the different importance of the lifetime in the optimization in each curve. Third, the '*Isqnonlin*' iteration process is started, calling the command '*ode45*', which is used to integrate the ODE's of the constitutive equations (1)-(4), and predict the strain for each b_k , where k is the specific iteration solution. The simulating range time tsim is specified in the initial condition. The value of b and $F_{\varepsilon}(b)$ are obtained and a conditional step comparing with the tolerance says if the optimized solution is achieved. The variable tolerance is identify as λ_1 and function tolerance as λ_2 . Finally, a set of b_p are obtained for the different values of the lifetime factor. The best fitting is achieved by finding the minimal of: normalized residual, error approximation of lifetime, and minimum strain rate, if the experimental values are available. All this process is illustrated at the optimization flow chart at the Fig. 5.

V. RESULTS

A. Ferritic Stainless Steel

The results achieved are demonstrated at the Fig. 6 and Fig. 7, for the material at 560°C and 590°C, respectively. The best values for the lifetime factors are w = [1,1,1] and w = [0.12, 0.12, 1] for the temperatures of 560°C and 590°C, respectively. Matlab does not confirm if a global optimum solution has been accomplished but the high accuracy observed in the creep curve behavior, makes think it does, whereas, with the modification of the initial values a slightly difference in the solution is observed.

The values of the optimized constants for both creep curves are illustrated at the Table 5. It can be identify a high difference in the values, specially, for the constants A, and C, which are quadruple and double for the material at 590°C. That confirms the severe dependency on the material constants value in order to represent accurately the creep mechanical behavior.





Figure 5. General flow chart of the optimization process

How was said in the section 4.C, the initial estimation for the material at 590°C was not a good guess even that, the Fig. 7 shows a high accuracy in the prediction of the creep damage mechanical behavior, meaning that the optimization routine had ran, and optimized the parameters. Similarly, Fig. 6 illustrates the predicted deformation for the material at 560°C, demonstrating an almost perfect fitting with the experimental data.

B. Comparison with Mustata & Hayhurst Solution

In order to a further validation a comparison with the solution obtained for Mustata & Hayhurst [1] for the same material and conditions has been done.

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Figure 6. Prediction of mechanical behaviour of material at 560°C determined with the optimized material constants



Figure 7. Prediction of mechanical behaviour of material at 590°C determined with the optimized material constants

It is generated the Table 6, and Table 7, which, demonstrates the percentage of error approximation between the predicted and experimental lifetimes and minimum strain rate of both approaches. In respect of the prognostic for the material at 560°C of the minimum rates the error of [1] is nearly 12%, a 5% better, whereas, the error of the lifetime forecasted by this project is a 0.5% better. For the material at 590°C, experimental data for the minimum strain rate is not available, thus, only the error approximation of lifetimes is compared. The average error for this report approach is under 2%, whereas, the other authors approach gives over 6% which is more than the triple of error.

Table 6. Error approximations for lifetimes and minimum creep strain rates for the estimated set of constitutive for material at 560°C

T(560°C)	Mustata &	Hayhurst	This project	
Stress	ε _{min} (%)	Lifetime	ϵ_{\min} (%)	Lifetime
(Mpa)		(%)		(%)
85	3.72	0.13	11.21	0.74
100	16.29	6.54	17.53	6.01
110	14.99	2.34	12.64	0.61
% Average	11.67	3.00	13.79	2.45

Table 7. Error approximations for lifetimes for the estimated set of constitutive parameters for material at $590^{\circ}C$

Т(590°С)	Mustata & Hayhurst	This project
Stress (Mpa)	Lifeti	me (%)
100	6.47	1.43
110	8.23	2.66
120	4.76	0.68
% Average	6.49	1.59

VI. CONCLUSION AND FUTURE WORKS

To conclude, it can be said that the main objective of this project has been achieved. The optimization program optimizes the material constants for the ferritic steel in the operating temperatures required, and the creep damage mechanical behavior is reproduced with high accuracy.

The objective function is simpler, more compact, less uncertain and at least as accurate as the past papers presented. However, it must say that the accuracy in the results is dependable in the new digitized points for curve fitting purpose. The initial values has been demonstrated to be a key for obtain accurate solution, however, it was showed for the material at 590°C, that, even without a perfect first guesses the program gives an desirable output.

Future works are required to demonstrate the robustness, reliability and usefulness of the optimization program. Regarding to the program implementation, an upgrade of the Matlab code with the aim to be more user friendly is an expect target.

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