

**CALIBRATING MATERIAL CONSTANTS FROM EXPERIMENTAL
DATA FOR LEAD-FREE SOLDER MATERIALS USING A
PARAMETRIC OPTIMIZATION APPROACH**

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THEME

Automated Optimization Process

KEYWORDS

Optimization, Material calibration, Modified Anand model, Abaqus, Isight

SUMMARY

The material model used in a Finite Element (FE) analysis is one of its most central aspects and must accurately represent the physical behaviour of the material being used. Often, sophisticated material models consist of multiple parameters requiring calibration from different sets of experimentally measured data. The calibration process is both challenging and time consuming due to the complexity of material models being used in today's FE analyses.

In this paper, an automated optimization workflow is presented for calibrating the material constants for the Modified Anand constitutive model. This material model is a prevalent viscoplastic model used by the electronics industry for modeling lead-free solder materials. The work-flow leverages optimization techniques with a non-linear FE solver. This combined methodology results in a calibration of material parameters from multiple sets of experimental stress-strain responses measured at different temperatures and strain-rates. The optimization technique modifies the parameter values of the material model setup inside the nonlinear FE model. The objective is to minimize the differences between the output stress-strain responses and the experimental data sets. The complexity of the optimization task is realized from the comparison of multiple experimental data sets and the material parameters to be calibrated.

In this study, the mechanical behaviour of Sn-3.5Ag (tin-silver) material is calibrated from experimental data sets. The material model corresponds accurately throughout the data range. The study demonstrates the importance of having a simple, graphical user interface with seamless integration of simulation software. The paper illustrates the capability of this process for calibrating material constants for a wide range of material models.

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1: INTRODUCTION

Lead and its compounds have been widely used for many years in the electronics industry, and the long-term reliability for these materials is well understood. However, the global impetus to reduce the use of hazardous materials has compelled electronics manufacturers to evaluate the use of lead-free materials in new products. Lead-free solders in commercial use may contain a variety of elements; most commonly, tin, silver and copper. Most lead-free solder have melting points above 215°C with varying thermal and electrical conductivity, joint strength and thermal fatigue resistance properties. As a result, the transition to lead-free alternative compounds has necessitated the development of new analytical capabilities for estimating the reliability of components with lead-free solder.

Solder joints have been widely used in the ball grid array (BGA) package to provide electrical and mechanical connections between the package and the PCB Board (see Figure 1). A major concern with the solder joints is the effect of temperature cycling on the reliability of electronic packages, since they are mainly subjected to cyclic power and thermal loadings during service life. Mismatch between the thermal expansion behaviours of the various materials may induce severe stresses high enough to cause plasticity and creep. In particular, solder balls are at risk, because they are stressed at temperatures above half of the solder's melting point. At these temperatures, the solder creeps, and after a number of thermal cycles, the accumulation of large inelastic strains may result in failure of the solder joints. As observed in tests [1], thermal fatigue failures usually occur at the interfaces near either the package (die) side or board (substrate) side. Therefore, the creep analysis of solder balls under cyclic thermal loading becomes an important part of the design phase.

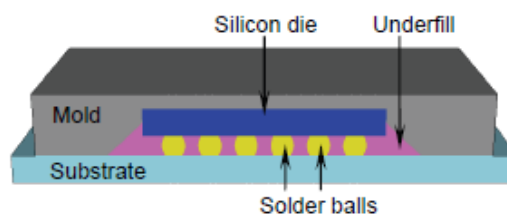


Figure 1: Schematic section view of a typical BGA package

Temperature cycling testing used to study the thermal fatigue of solder joints is a time-consuming and costly process. Employing accelerated life testing methods to obtain reliability estimates can reduce the time required but not the complexity of the experimental process. The maturation of numerical techniques has enabled the use of numerical simulations by designers to accurately predict reliability of solder joints independent of costly

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experimentation. Many companies now rely on numerical simulation to assess electronic component reliability during the design process.

Advanced constitutive models, together with nonlinear solution techniques and thermal-mechanical coupling capability, make commercial FE solvers, such as Abaqus/Standard [2], an ideal tool for analyzing the reliability of electronic components. FE analysis is used to analyze the inelastic strain range and strain energy density of the solder joint due to thermal cycling. The analysis is used to predict the fatigue life for the solder joint.

2: MODIFIED ANAND MODEL

A key aspect to achieving an accurate predictive capability involves understanding the stress-strain response of lead-free solders. Experimental stress-strain curves show that steady-state plastic flow "saturation" stresses are highly dependent on operating temperatures and, to a lesser extent, on strain rates. Figure 2 shows temperature and strain-rate dependence for Sn-3.5Ag solder.

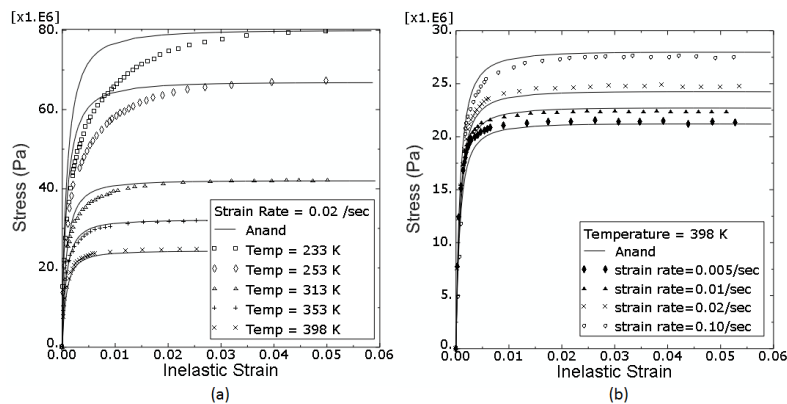


Figure 2: Comparison of experiments and predictions of Anand model for lead-free solder Sn-3.5Ag: (a) stress-strain curves with different temperatures at strain rate 0.02/s, (b) stress-strain curves with different strain rates at temperature 398K[3]

To capture this behaviour, a number of lead-free solder constitutive models have been proposed. For example, Wiese et al. [4] identified two mechanisms for steady state creep deformation of Sn-4.0Ag-0.5Cu (SAC405) solder and adopted a double power law to simulate climb controlled (low stress) and combined glide/climb (high stress) behaviour. Other researchers [5-7] have used the hyperbolic-sine law for modelling the reliability of lead-free solders.

Of particular interest, Chen et al. [3] found (shown in Figure 2) that the Anand model [8-9] cannot accurately describe the material behaviors at small strains for the lead-free material Sn-3.5Ag, especially at relatively low temperatures.

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It is important that the material model exactly replicates this behavior in order to capture the proper inelastic strain range and strain energy density utilized in subsequent damage assessment. Based on understanding of the physically-based parameters, a modification to the Anand model was proposed.

The Anand model [8-9] is a viscoplastic model with a deformation resistance stress incorporated as a state variable. The creep strain rate is given by:

$$\dot{\epsilon}_{cr} = A \exp\left(-\frac{Q}{RT}\right) \left[\sinh\left(\xi \frac{q}{s}\right)\right]^{\frac{1}{m}} \quad (1)$$

where s is the deformation resistance; q is the equivalent deviatoric stress; A , m , and ξ are material constants; Q is the activation energy; T is absolute temperature; R is the universal gas constant. The evolution equation for the deformation resistance s (initially $s=s_0$) is

$$\dot{s} = h_0 |1 - s/s^*|^a \text{sign}(1 - s/s^*) \dot{\epsilon}_{cr} \quad (2)$$

with

$$s^* = \hat{s} \left[\frac{1}{A} \dot{\epsilon}_{cr} \exp\left(\frac{Q}{RT}\right) \right]^n \quad (3)$$

where h_0 , a , \hat{s} , and n are material constants. In particular, h_0 influences the shape of the stress-strain curve by scaling the magnitude of the dynamic strain hardening and recovery processes.

The Modified Anand model [3] allows the initial deformation resistance to vary as a function of temperature

$$s_0 = s_1 + s_2 T + s_3 T^2 \quad (4)$$

and the parameter, h_0 , to depend on temperature and strain rate

$$h_0 = A_0 + A_1 T + A_2 T^2 + A_3 \dot{\epsilon}_{cr} + A_4 \dot{\epsilon}_{cr}^2 \quad (5)$$

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The Modified Anand model describes the mechanical behavior of Sn-3.5Ag and other lead-free solder materials with a high degree of accuracy for a wide range of strains and temperatures.

The constants in Equations (1)-(5) are derived values for Sn-3.5Ag [3] using a five-stage nonlinear least square fitting procedure. The constants are listed in Table 1.

Parameter (unit)	Value for Sn-3.5Ag [3]
Q/R (K)	10278.43 K
A (1/sec)	177016 s ⁻¹
ξ	7.0
M	0.207
\hat{s} (Pa)	52.4 MPa
N	0.0177
A	1.6
S ₁ (Pa)	28.6 MPa
S ₂ (Pa/K)	-0.0673 MPa/K
S ₃ (Pa/K ²)	0
A ₀ (Pa)	-90939.8 MPa
A ₁ (Pa/K)	960.7 MPa/K
A ₂ (Pa/K ²)	-0.956 MPa/K ²
A ₃ (Pa×s)	-3260581.8 MPa×s
A ₄ (Pa×s ²)	24976815.5 MPa×s ²

Table 1. Modified Anand model material constants for Sn-3.5Ag.

The calibrated constants for the Sn-3.5Ag in Table 1 can be used directly in FE simulation models. However, material constants for new, evolving materials being tested for application as solder materials are not readily available in literature. Calibration methods require extensive experimental data. Added to the computational expense of running optimization driven FE simulations, calibration methods can become impractical very quickly. Therefore, it is desirable to implement an optimization process that minimizes both the number of experiments required for the calibration and the overall computational effort.

3: PARAMETRIC OPTIMIZATION APPROACH

We use Isight [10], a commercially available simulation process automation and design optimization software package to execute simulation tools, such as Abaqus [2]. Isight provides engineers with a suite of visual and flexible tools for creating simulation process flows to automate the exploration of design alternatives and to identify optimal performance parameters. Figure 3 illustrates an Isight parametric optimization workflow for material model calibration.

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We outline a methodology for the calibration of temperature and strain rate sensitive creep material models. In this method, the material calibration is posed as an optimization problem. That is, the design variables (the material constants of the constitutive model) are varied with an overall objective to minimize the differences between simulation results and experimental stress-strain data.

Multiple objectives are minimized simultaneously. This is because multiple experimental data sets are compared simultaneously with their corresponding simulation data for calibration; and for every data set, several measures of fit are needed to ensure a robust fit for each data set. Multi-objective techniques implemented in Isight [13] are utilized when competing objective functions are present.

In our methodology, we include a global measure of fit, such as an area difference between experiment and simulation stress-strain plots and a local measure, such as the maximum difference between the same two plots. This ensures a robust comparison between the plots at all points. Also, the simulation data are interpolated to experimental data. Thus, data measured at all time intervals can be compared. Interpolation also provides a smoothing effect on the data. For noisy experimental and simulation data, one of several smoothing filters available in Abaqus can be used.

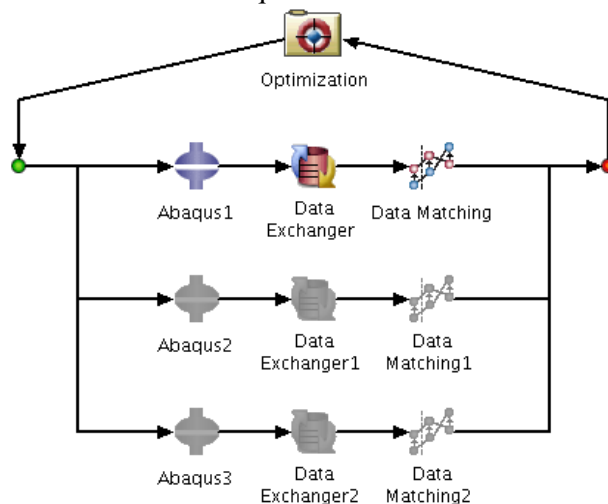


Figure 3: An optimization workflow in Isight. Two parallel paths are disabled for initial estimation with one data set.

We propose the following general method to calibrate material constants from experimental data:

- 1. Identify a robust starting point for the optimization algorithm.**
- 2. Define the design space by constraining the design variables to a physically meaningful range.**
- 3. Determine the minimum number of experimental data sets required for the calibration.**

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4. Select a suitable optimization algorithm for the experimental data set.
5. Calibrate the material model using the minimum number of required experimental data sets.
6. Verify the validity of the material constants at non fitted experimental data sets.
7. Add experimental data sets as necessary.

A robust starting point and a well constrained design space in combination with an appropriate optimization algorithm, enhances the chances of finding a global optimum. Further, this method is found to be computationally efficient as unnecessary design space exploration is avoided, which greatly affects optimizer performance. For instance, FE analyses with unphysical material constants will not converge and produce a highly discontinuous design space.

Finally, in an optimization where the magnitudes of the design variables may vary by many orders of magnitude, care must be taken to ensure that some design variables don't dominate the objective functions due to their orders of magnitude. Similarly, if several objectives are utilized, the analyst must ensure that each objective is treated equally.

4: METHODOLOGY EXAMPLE: MODIFIED ANAND MATERIAL CONSTANTS

Having outlined the general methodology, in this section we show the application of the method to calculate the Modified Anand material constants. Specifically, we calculate the constants A_0 , A_1 , A_2 , A_3 and A_4 that define h_0 , which scales the magnitude of the dynamic strain hardening in the evolution equation for the deformation resistance. (See Equations 2, 5)

1: Identify a robust starting point: Estimate A_0

The Anand model is able to capture the stress-strain behavior of the lead-free solder materials at high temperatures quite well with only a constant scaling of the dynamic strain hardening. (e.g. see stress-strain curve at 0.02 s^{-1} , 398K in Figure 2a). Therefore, we find the constant term in h_0 (which is A_0) by fitting the Modified Anand Model to a single stress-strain curve at a high temperature while neglecting the linear and quadratic terms. ($A_1 = A_2 = A_3 = A_4 = 0$).

Not having found any estimates for A_1 , A_2 , A_3 and A_4 , we retain the initial values of these design variables at 0. The estimate of A_0 along with the zero valued design variables serve as a starting point for our calibration.

2: Define the design space and constrain the optimization

A_0 , the constant term in h_0 , represents the initial scaling of the magnitude of the dynamic strain hardening. Since a negative scaling at a given strain rate and temperature would mean a non-physical behaviour of the model, we constrain our design space to positive values of A_0 . Further, since we have already

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estimated A_0 , a large variation from this estimate would be computationally inefficient.

Next, we constrain the magnitudes of A_1 , A_2 , A_3 and A_4 such that the contribution from each of them to h_0 is, at most, the same order of magnitude as that of A_0 . Although this is strictly not a requirement for obtaining physically meaningful constants, it allows for a much more efficient exploration of the design space. If needed, the analyst can relax this constraint provided efficiency and run time are not an issue. Equation 6 shows the orders of magnitudes (in superscript) of each coefficient required to enforce this constraint, for a hypothetical initial estimate of A_0 at 1.E11.

$$h_0 = A_0^{O(11)} + A_1^{O(9)}T^{O(2)} + A_2^{O(7)}T^2^{O(4)} + A_3^{O(12)}\dot{\epsilon}_{cr}^{O(-1)} + A_4^{O(13)}\dot{\epsilon}_{cr}^2^{O(-2)} \quad (6)$$

The penalty on efficiency is for two reasons: 1) very large values of the material constants leads to a high number of failed FE analyses, which creates too many discontinuities in the feasible design space for the optimization algorithm to navigate it efficiently, and 2) We have already obtained a good estimate for A_0 and it would be inefficient to explore larger values for A_1 , A_2 , A_3 and A_4 which essentially provide a temperature and strain rate correction to the constant term A_0 .

3: Establish the minimum number of experimental data sets required

Since the Modified Anand model expresses h_0 as a bivariate polynomial with 5 coefficients (Equation 5), a total of 5 temperatures and strain rates would be the minimum number of variables required for calibrating these constants. Thus, we choose three experimental data sets at $(0.02s^{-1}, 233K)$, $(0.1s^{-1}, 398K)$ and $(0.02s^{-1}, 253K)$; and use them for the calibration. Given that we intend to capture the entire operating range of temperatures and strain rates with just five points, it is vital to include at least two extreme data sets, and one in between.

Alternatively, we may visualize h_0 as a surface, as shown in Figure 4 and calculate the minimum number of points needed to fit this surface in the strain rate–temperature space.

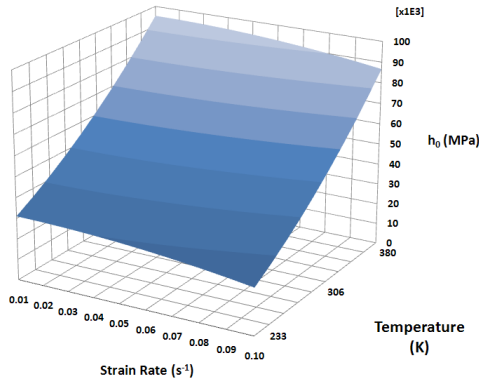


Figure 4: h_0 visualized as a surface in the temperature–strain rate space

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4: Choose a suitable optimization algorithm

We choose the Hooke–Jeeves (HJ) algorithm [11] for the initial estimation and the NCGA [12], for the subsequent calibration. HJ is a relatively cheap direct penalty method that is well suited for both linear and non-linear design spaces and does not require the calculation of gradients. It works quite well when the initial feasible design is undetermined, as is the case with this optimization problem. NCGA is a well established multi-objective exploratory technique chosen for its ability to treat individual objectives separately. By a crossover process typical of genetic algorithms [12], it generates a pareto set, wherein all solutions are equally good in terms of the overall objective and improving one objective is impossible without sacrificing one or more of the other objectives. The optimum is picked from among the pareto points.

5: Calibrate the material model

Having settled on a robust starting point, a constrained design space and appropriate algorithms, we calibrate the Modified Anand model using our basic approach and workflow (See Figure 3). We choose two objective functions to minimize:

1. Absolute area difference between simulation and experiment stress–strain curves
2. Maximum difference between the simulation and experiment curves.

Minimizing the “absolute area difference” objective function brings all the simulation data points in proximity to the experimental data points, while minimizing the “maximum difference” objective function focuses on reducing the local maximum differences between the two data sets. When used in combination, these objective functions provide a robust solution to the data matching problem.

Finally, we normalize each design variable by its range to ensure that the overall objective is not dominated by design variables with high orders of magnitude. Similarly, when multiple objectives are used, we weight the objectives so that each receives the same relative importance in the overall objective.

6: Verify the validity of the material constants

We use the calibrated material model constants to generate simulation data at unfitted experimental data sets and verify the accuracy of the fit.

7: Additional experimental data sets

In general, if an *average* response of the material model over a range of temperatures and strain rates is desired, we include more experimental data covering the entire range over which the average is desired.

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5: RESULTS

1: Estimation of A_0

A_0 is estimated by fitting the material model to the experimental stress-strain curve measured at $T=398$ K and $\dot{\epsilon}_{cr}=0.1s^{-1}$. The Hooke-Jeeves optimization technique is used for obtaining this initial estimate for A_0 . See Table 3 for the estimated value for A_0 . We choose to explore only the physically meaningful values of A_0 and therefore constrain the space to positive values of A_0 .

Parameter	Lower Bound	Initial Value	Upper Bound	Final Value	Number of Opt. Iterations	Number of Abaqus runs
A_0	0	0.1	1E14	5.40771E10	45	45

Table 3.Initial value of A_0 , the upper and lower bounds placed on A_0 and final A_0 .

2: Calibration

Using the initial estimate of A_0 , the upper and lower bounds are determined for the other four constants A_1 , A_2 , A_3 and A_4 . Note that only minor variations are allowed for A_0 . The NCGA optimization technique is used for determining the optimum solutions for the constants. The design space and the optimization calibrated values for the material constants are shown in Table 4. Each optimization iteration involves running three Abaqus simulations (in parallel) to generate the stress-strain data sets to compare against the chosen three experimental curves. Hence the number of Abaqus runs is three times the number of optimization iterations.

Design variable	Lower Bound	Initial value	Upper bound	Calibrated values	Number of Opt. Iterations	Number of Abaqus runs
A_0	1E10	1E10	7E10	1.22102E10	200	600
A_1	-1E8	0	1E8	-9.98487E7		
A_2	-1E6	0	1E6	7.7510E5		
A_3	-1E11	0	1E11	6.20213E9		
A_4	-1E12	0	1E12	-9.18945E11		

Table 4. Design space for calibration and solution

3: Verification

The calibrated constants for the Modified Anand material model in Table 4 are obtained from the three experimental stress-strain data sets. The calibrated material constants are verified against the remaining five experimental data sets. Figure 5 shows the comparison between the experiments and predictions of Modified Anand model with calibrated values for different temperature and strain rates. The plots show a good match between the experimental and simulation data sets and the material constants are able to predict the material behaviour at all the data points well.

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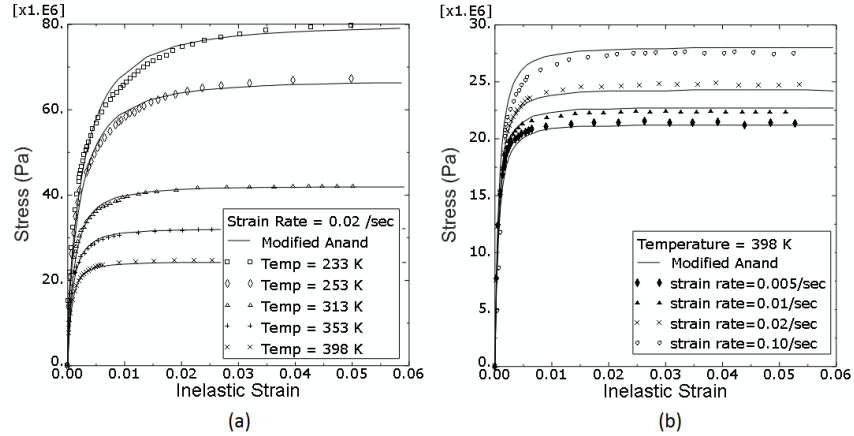


Figure 5: Comparison of experiments and predictions of calibrated Modified Anand model: (a) stress-strain curves with different temperatures at strain rate 0.02/s, (b) stress-strain curves with different strain rates at temperature 398K

6: COMPARATIVE STUDY

The calibration workflow is run with different optimization techniques to study the convergence behaviour and the effectiveness of the optimization techniques in minimizing the objectives. Four different classes of optimization techniques are chosen in this study: NCGA- a multi-objective genetic algorithm, Pointer [13] – a combination of numerical and exploratory techniques, Downhill Simplex [14] - a direct exploratory technique and MMFD [15] - a gradient based numerical technique. A population size of 10 and 20 generations are specified for NCGA while the Pointer is set to run for 3 hours to find the optimum solution. A maximum of 40 design iterations are specified for Downhill Simplex and MMFD techniques. The values calibrated by each of these techniques and the number of iterations for convergence is tabulated in Table 5. For comparison, the values calibrated by Chen at al. are also included in the table.

Opt. Technique	Classification	Calibrated Values					Number of Opt. Iterations	Number of Abaqus Runs
		A0	A1	A2	A3	A4		
Chen et al		-9.093E10	9.600E8	-0.956E6	-3.260E12	2.497E13		
NCGA	Multi-objective Exploratory	1.221E10	-9.984E7	.775E6	6.200E9	-9.18945E11	200	600
Pointer	Combination Numerical and Exploratory	1.358E10	-9.889E7	.755E6	-9.890E10	-8.455E11	218	654
Downhill Simplex	Direct Exploratory	1.600E10	1.914E7	.213E6	-2.150E10	-5.5309E10	80	240
MMFD	Direct Gradient	1.425E10	1.072E7	.275E6	1.070E9	7.76E9	82	246

Table 5. Comparison of material constant values calibrated by optimization techniques

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The non-uniqueness of the calibrated values obtained from each of the optimization techniques is evident from Table 5.

One of the optimization objectives in this study is to minimize the absolute area difference between the simulation and experiment stress-strain curves. Table 6 compares this objective for the different optimization techniques at the optimum solution and lists them along with the solution from Chen et al. From Table 6, it is evident that NCGA and Pointer have been able to calibrate constants for the Modified Anand model more accurately when compared to MMFD and Downhill Simplex techniques. On the other hand, the MMFD and Downhill Simplex methods converge to a solution with lesser number of iterations (Table 5). However, we note that MMFD and Downhill Simplex techniques are easily trapped in local optima, while NCGA and Pointer techniques are more successful in seeking out the global optimum.

Opt. Technique	Sum of the absolute area difference between experiment and simulation curves at optimum solution ($\times 1E06$)								
	T=233K $\dot{\epsilon}_{cr}=.02s^{-1}$	T=253K $\dot{\epsilon}_{cr}=.02s^{-1}$	T=313K $\dot{\epsilon}_{cr}=.02s^{-1}$	T=353K $\dot{\epsilon}_{cr}=.02s^{-1}$	T=398K $\dot{\epsilon}_{cr}=.005s^{-1}$	T=398K $\dot{\epsilon}_{cr}=.01s^{-1}$	T=398K $\dot{\epsilon}_{cr}=.02s^{-1}$	T=398K $\dot{\epsilon}_{cr}=.1s^{-1}$	Sum over all the curves
Chen et al.	.06085	.06339	.02265	.01364	.01021	.01925	.02816	.02498	.2431
NCGA	.05973	.05780	.01506	.02337	.01827	.01914	.02487	.04108	.2591
Pointer	.05823	.05973	.02446	.01232	.01838	.01860	.02677	.03317	.2516
Downhill Simplex	.06075	.06083	.05322	.02663	.03791	.02473	.04925	.02014	.3332
MMFD	.06057	.06073	.04671	.02174	.03423	.02224	.04449	.02272	.3131

Table 6. Comparison of the sum of the absolute area differences between experiment and simulation curves for optimization techniques at the optimum solution

It can also be seen from Table 5 that the constants obtained from the pure curve-fit approach employed by Chen et al. achieves a slightly better fit with experiments when compared with optimization techniques like NCGA and Pointer. This can be explained by the fact that while Chen et al. allowed a negative A_0 , we imposed a physically-motivated positive value constraint on A_0 . Also, Chen et al. used a total of 20 experimental data sets to fit the coefficients while we are using only three data sets to get these results

7: CONCLUSIONS

We present a general methodology for the calibration of temperature and strain rate sensitive creep material models. With this method and an Isight optimization workflow, we calibrate the nonlinear scaling of the dynamic strain hardening of the Modified Anand model, defined by material constants A_0 , A_1 , A_2 , A_3 and A_4 .

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Our method produces material constants that are both physically meaningful and also give a good fit to all our experimental data sets. We minimize the number of experimental data sets and the computational cost required for this calibration effort. We show that a total of five temperatures and strain rates are sufficient to calibrate five material constants in the Modified Anand model. We verify that we get a good fit at the remaining experimental data sets and emphasise the need to include more data when a good fit is not obtained.

Further, we compare solutions from selected optimization algorithms available in Isight and the computational effort required for each solution. We note that while gradient-based and direct exploratory techniques require a smaller computational effort, they are more likely to be trapped in local optima. Conversely multi-objective exploratory techniques and combinatorial methods may require a significantly larger effort, but are able to find the global optimum. When the “terrain” of the design space is not known we recommend a combinatorial method.

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