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AN EFFICIENT METHOD FOR THE OPTIMIZATION OF VISCOPLASTIC CONSTITUTIVE MODEL CONSTANTS

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ABSTRACT

Constitutive modeling has proven useful in providing accurate predictions of material response in components subjected to a variety of operating conditions; however, the high number of experiments necessary to determine appropriate constants for a model can be prohibitive, especially for more expensive materials. Generally, up to twenty experiments simulating a range of conditions are needed to identify the material parameters for a model. In this paper, an automated process for optimizing the material constants of the Miller constitutive model for uniaxial modeling is introduced. The use of more complex stress, strain, and temperature histories than are traditionally used allows for the effects of all material parameters to be captured using significantly fewer tests. A graphical user interface known as uSHARP was created to implement the resulting method, which determines the material constants of a viscoplastic model using a minimum amount of experimental data. By carrying out successive finite element simulations and comparing the results to simulated experimental test data, both with and without random noise, the material constants were determined from 75% fewer experiments. The optimization method introduced here reduces the cost and time necessary to determine constitutive model constants through experimentation. Thus it allows for a more widespread application of advanced constitutive models in industry and for better life prediction modeling of critical components in high-temperature applications. Keywords: constitutive modeling, optimization, viscoplastic

1 INTRODUCTION

Constitutive modeling is a field of engineering mechanics that has received considerable research attention over the past several decades, with much focus on the development of unified constitutive models. Recent advances in computer processing speed have enabled the implementation of these models into finite element analysis (FEA) software applications such as ANSYS and ABAQUS, yielding accurate and cost-effective predictions of stresses and strains in structural components under a non-generic variety of operating conditions, such as creep, fa-

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tigue, and thermal-mechanical fatigue. Under these conditions, certain alloys display inelastic behavior in the form of coupled creep and plasticity, commonly referred to as viscoplasticity. A variety of material models has been developed to correlate with mechanical test data. For this research, the Miller unified constitutive model [1] will be used to run simulations using the ANSYS general purpose FEA software. The purpose of the research is to develop a robust method of parameter determination, using a minimum number of experimental tests, which can be easily applied to many different types of viscoplastic constitutive models.

Traditional methods for step-by-step parameter determination require data from upwards of twenty experimental tests [2–4]. Often, a large amount of data is needed in order to determine only a portion of the total number of material constants. One test type used for parameter determination is a low cycle fatigue test; these tests are typically run until stress saturation occurs, sometimes approaching one hundred cycles [5]. Typically, combinations of creep, low cycle fatigue, and tensile data at various temperatures are used for material constant determination.

Numerical methods for parameter determination have been presented in previous studies, e.g., [6–8]. The optimization scheme presented here differs from these in that it is not specific to any particular constitutive model or experimental test matrix. Furthermore, it allows consideration of multiple experiments in determination of material constants, leading to broader applicability of the resulting model and drastically reducing the amount of experimental data needed to determine inelastic constitutive model parameters. For these reasons, it has the potential to reduce both monetary costs and time required to implement advanced constitutive models in industry. Thus it may allow for more accurate preliminary design of critical components, reducing the need for expensive design modifications as product development progresses.

1.1 Background

Viscoplastic constitutive modeling is an important technique used in the design of components in high temperature applications, such as in turbine engines [5]. These material models allow design engineers to predict stresses and strains in critical components using finite element analysis software. The results of such preliminary analyses allow for the optimization of shape geometry to improve factors of safety and reduce high stress concentrations. Finite element modeling can also be used to determine properties which allow for reasonable life prediction of components subject to a combination of cyclical loading and temperature cycling. The Miller model was designed for use in high temperature applications, and is capable of reasonably predicting material behavior under such conditions [1,4]. Furthermore, the Miller constitutive model was extended to a multiaxial formulation for more complex geometries and loading conditions [9]. Unfortunately, the use of advanced constitutive models is limited by the large amount of experimental data needed to determine material constants contained in the model and the often tedious step-by-step procedure used to determine these constants. This has confined the field of advanced constitutive modeling primarily to the realm of academia, rather than to widespread practical application in industry.

1.2 The Miller Unified Constitutive Model

The Miller model is most useful for predicting the behavior of materials in high temperature applications and is capable of modeling a wide range of material behavior including time-, rate-, and history-dependence. As a unified constitutive model, both creep and plastic strain are combined under the moniker of inelastic strain. The Miller model is convenient to use due to its low number of material constants and its ability to accurately simulate a range of material behavior. There are difficulties in application of the Miller model, however. The formulation of the model includes three hyperbolic sine functions, as shown in Eqs. 2. As a result, numerical simulation of the Miller model is computationally expensive [5] Furthermore, the model is only capable of reasonably predicting behavior of materials that work-harden considerably [1]. This limits its applicability to certain classes of materials, such as steels.

The theory used in the derivation of the Miller model limits its application to alloys that work-harden considerably, such as aluminum alloys and steels [1]. More specifically, the model focuses on the effects of two particular types of hardening: isotropic and kinematic. These two phenomena reflect changes in material strength with respect to deformation history. Isotropic hardening implies that material strength remains constant in all directions. For example, straining a material specimen in the tensile direction will strengthen it both in the tensile and compressive directions. Kinematic hardening, on the other hand, reflects different material strengths with respect to different orientations in a material. For example, straining a specimen in the tensile direction may strengthen it in the tensile direction but weaken it in the compressive direction [1]. These effects are accounted for in the strain rate equation. Essentially, the model predicts that the strain rate of a material under loading is a function of the difference between the applied stress (σ) and the kinematic hardening variable, divided by the isotropic hardening variable. Kinematic hardening and isotropic hardening are denoted by the scalar variables R and D, respectively, in the basic strain rate equation

$$\dot{\varepsilon} = f(\frac{\sigma - R}{D}). \tag{1}$$

In this formulation, the variables R and D take the forms of internal state variables (ISVs) which describe the internal state of

the candidate material. Even though these so-called ISVs cannot typically be measured through direct observation, they are necessary to describe the nature of the microstructure and its evolution. Since the values of R and D change during the deformation history of a material, equations are needed to model the behavior of these two factors. These equations are not solely dependent on the strain or strain rate, but rather depend on the entire previous deformation history [1]. It is through the evolution of R and D, called the back stress and drag stress respectively, that viscoplastic effects are captured by the Miller model.

In order to derive a useful function for the strain rate, steady state creep data were used as a starting point. Equations for the evolution of R and D were developed using warm working and work-hardening theory. The end result is the following set of three differential equations that are capable of predicting both steady state and transient material behavior [1]:

$$\begin{aligned}
\dot{\varepsilon} &= B\theta' \sinh^n \left[\left(\frac{|\sigma - R|}{D} \right)^{1.5} \right] \cdot sgn(\sigma - R) \\
\dot{R} &= H_1 \left(\dot{\varepsilon} - B\theta' \sinh^n (A_1 |R|) \cdot sgn(R) \right) \\
\dot{D} &= H_2 \left[|\dot{\varepsilon}| \left(C_2 + |R| - \left(\frac{A_2}{A_1} \right) D^3 \right) - C_2 B\theta' \sinh^n \left(A_2 D^3 \right) \right].
\end{aligned} \tag{2}$$

The θ' term is the only temperature-dependent factor in the Miller model. Its value depends on the current temperature of the material T and the melting temperature T_m of the material. It can be expressed as

$$\theta'(T) = \begin{cases} \exp\left(-\frac{Q}{k(0.6T_m)} \cdot \left[\ln\left(\frac{0.6T_m}{T} \right) + 1 \right] \right) & , T \leq 0.6T_m \\ \exp\left(-\frac{Q}{kT} \right) & , T \geq 0.6T_m \end{cases} \tag{3}$$

where k is the ideal gas constant. Within Eqs. (1) and (3) there are eight viscoplasticity constants which must be determined. Table 1 gives ranges for the constants available in the literature [4, 5, 9]. None of these parameters are temperature-dependent; temperature affects only the θ' term. The testing procedure that has historically been used to determine these constants is outlined in [1].

The Miller unified constitutive model satisfies several important criteria that make it appropriate for testing an optimization procedure such as this one. Since the verification of the optimization procedure depends heavily on simulations conducted by ANSYS, it is important that the model be suitable for implementation into a finite element analysis program. The Miller model has been implemented into ANSYS as a user-programmable feature (UPF). This is a custom feature that allows for a user to define a constitutive model that will be used by ANSYS to predict material behavior. Another important factor is the dependence of material constants on temperature. If several of the constants changed with temperature, an attempt at optimization would be further complicated by the need for more isothermal tests at various temperatures. This is clearly in opposition with the overall goal of reducing the number of tests required. In the Miller model, none of the material constants are temperature-dependent [1], meaning fewer tests will be required. A third consideration that makes the Miller model suitable is that only cyclical and creep (or stress relaxation) data are needed to determine the constants. Both of these tests are relatively simple and can be conducted with equipment that is readily available.

Table 1. Typical values of material constants for the Miller model.

Material Constant	Units	Typical Values
A_1	ksi^{-1}	0.8-0.93
A_2	ksi^{-3}	$7.4\text{x}10^{-5}$-$5.94\text{x}10^{-3}$
B	s^{-1}	1.03×10^{14}-1.0×10^{15}
C_2	ksi	0.1-50
H_1	ksi	280-10,000
H_2	(unitless)	100
n	(unitless)	1.60-5.8
Q	cal/mol	91,000-104,600

1.3 Type 304 Stainless Steel

Application of the Miller model will be limited to type 304 stainless steel in this research. The chemical composition of this alloy is shown in Table 2. Type 304 stainless steel is frequently used in high temperature applications due to its corrosion resistance properties, which result from the inclusion of chromium and nickel in the chemical composition [11]. The dependence of ultimate tensile strength (UTS) and 0.2% yield strength on temperature is shown in Fig. 2. Both of the material properties decrease in value as temperature increases. Similarly, the elastic modulus decreases as temperature increases, as shown in Fig. 1. The ultimate tensile strength must be considered in the design of experimental tests for parameter determination; the Miller model does not include failure criteria, so the experimental tests designed for parameter determination must avoid approaching the UTS. Likewise, the fatigue life of type 304 stainless steel, shown in Fig. 3, must be considered during experimental design. If the necessary data is not collected before fatigue fracture occurs, the experimental data will be useless. These existing data for

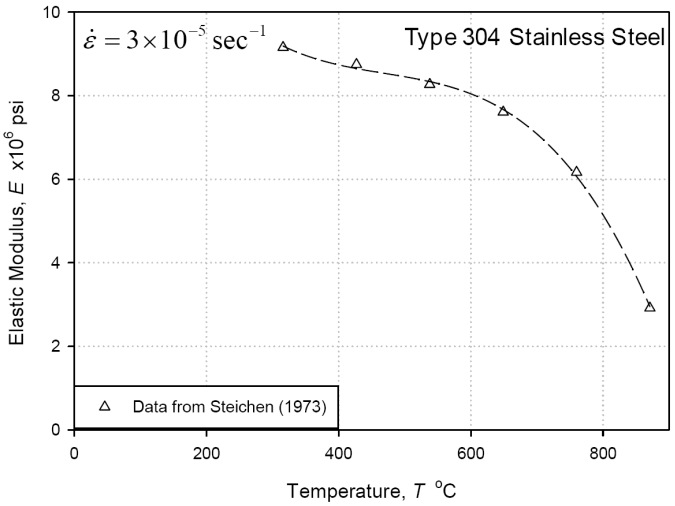

Figure 1. TEMPERATURE DEPENDENCE OF ELASTIC MODULUS FOR TYPE 304 STAINLESS STEEL

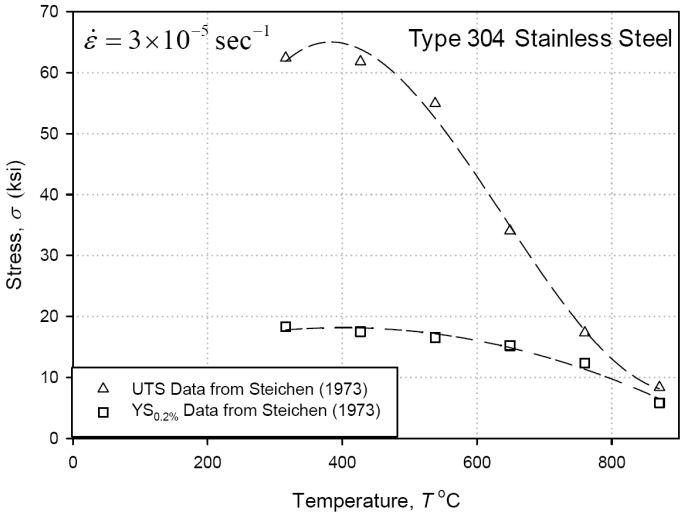

Figure 2. TEMPERATURE DEPENDENCE OF ULTIMATE TENSILE STRENGTH AND 0.2%-OFFSET YIELD STRENGTH FOR TYPE 304 STAINLESS STEEL

type 304 stainless steel will be kept under consideration while developing simulated experiments for material parameter determination to ensure that excessive damage or premature failure will not occur in material specimens.

2 MODELING APPROACH

In order to compare theoretical results with experimental test data, the Miller model was implemented into a finite element program known as ANSYS. Since the tests conducted for parameter estimation are typically uniaxial the most appropriate model of an experimental test specimen is a single three dimensional SOLID185 element consisting of eight nodes. All loads or displacements were applied to the top four nodes, while the bottom of the element had fixed displacement in the z-direction. The element cross sectional area was allowed to deform to account for the effects of Poisson's ratio. In this manner, uniaxial experimental tests were simulated.

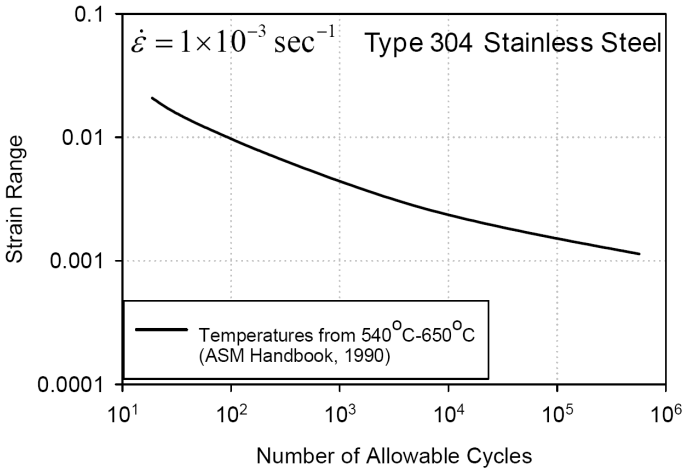

Figure 3. FATIGUE LIFE OF TYPE 304 STAINLESS STEEL AT ELEVATED TEMPERATURES

Table 2. Chemical composition of type 304 stainless steel [10]

Carbon	Chromium	Nickel	Manganese	Silicon
0.052 (wt %)	18.92	9.52	1.1	0.52
Phosphorus	Sulfur	Molybdenum	Nitrogen	Iron
0.011	0.01	0.12	0.052	Balance

Since the research objective was to develop a procedure for automatically determining the material constants of the Miller unified constitutive model with a minimum number of experiments, an automated optimization routine was needed that could compare simulations with experimental data to determine the parameters. For this purpose, a program called uSHARP was written. It is capable of determining constitutive model parameters requiring only a single initial guess, which can be obtained from previously determined constants existing in literature. Any type of data can be used in the optimization process, including stress, strain, or even stress and strain rates. Before further discussion of the optimization procedure executed by uSHARP, it is pertinent to discuss the limitations of the software package.

First, uSHARP was written for constitutive models which are well understood, such as the Miller model. The program

Table 3. Objective function parameters

Symbol	Meaning
n	number of time steps in the simulation
$w(t_i)$	weight at time t_i
$y_{exp}(t_i)$	interpolated value at time t_i
$y_{sim}(t_i)$	simulated value at time t_i
$(y_{exp})_{max}$	$y_{exp}(t_{i^*})$, where $\lvert y_{exp}(t_{i^*})\rvert = \max\lvert y_{exp}(t_i)\rvert$

should only be used when the appropriate orders of magnitude for the material parameters are known. The routine has demonstrated an inability to converge when the initial guess is not close to the proper order of magnitude. As such, the best initial starting point will be values that have previously been determined through the standard means for another material. This limitation, however, is a result of the optimization algorithm implemented into the current version of uSHARP, and not a problem with uSHARP itself. The application of a more robust optimization algorithm could mitigate this problem. Additionally, the constitutive model must accurately represent the behavior of the material for which it is being used. For example, the Miller model does not incorporate damage evolution; therefore it would not be appropriate for predicting tertiary creep damage in a material.

In order to use the uSHARP routine to optimize material constants, it is imperative that the time steps in test histories of the experimental and simulated data match closely. It is easy to simulate complicated test histories; it is difficult, however, to carry these out experimentally due to errors in equipment and natural imprecision present in the current usage of PID controllers. Emerging research into more advanced control systems indicates that in the near future these complicated test histories will be accurately replicated [12].

The uSHARP optimization routine makes use of an iterative procedure to determine the material constants through successive simulations. Simulations are conducted which match the test history of the experimental data and the material parameters are varied until a "best fit" is achieved. An objective function is constructed which provides a measure of the discrepancy between the experimental and simulated data. When the objective function is minimized over the set of material constants, the simulated data is considered to be a best fit to the experimental data, and the material constants determined by the program are considered to accurately reflect the behavior of the experimental data. The model and constants can then be used to simulate more complex service histories.

Since the uSHARP routine was designed so that multiple test types could be used simultaneously, a simple least squares function was not adequate. Different orders of magnitude present in different data types would naturally skew the value of the objective function towards higher orders of magnitude. Additionally, different data sets contain different numbers of data points, which would lead to skewing in the objective function by weighting tests with higher numbers of data points higher than tests with fewer data points. To account for these phenomena, a standard weighted least squares function was developed to allow for the simultaneous use of different experimental test types without unintended skewing. The form of this objective function is

$$S = \frac{1}{n}\sum_{i=1}^{n} w(t_i)\left(\frac{y_{exp}(t_i) - y_{sim}(t_i)}{(y_{exp})_{max}}\right)^2. \tag{4}$$

This equation contains several different parameters, which are described in Table 3. For convenience, quantities computed at time t_i will henceforth be denoted by a subscript, i.e., $y_i = y(t_i)$. The objective function accounts for the differences between the experimental and simulated data at each time index as a percentage of the maximum value of the experimental data set. This has the effect of scaling all test types to the same order of magnitude. Additionally, the total least squares value is normalized to the number of data points used in its calculation. This prevents test data containing more time indices from being weighted higher than data with fewer time indices. uSHARP can use multiple tests simultaneously in the determination of material parameters. This is done by adding the individual objective function values from each test type together, and minimizing the value of the combined objective function:

$$S_{tot} = \sum_{j=1}^{m} S_j \tag{5}$$

where m is the total number tests being combined.

It is important to note that the uSHARP objective function requires experimental and simulated data at the same time value. Finite element simulations and experimental data often have different time increments, so the experimental data points are linearly interpolated to the same times as the finite element simulation. Time is the independent variable in the uSHARP objective function because each time is unique within the dataset.

The uSHARP objective function is a weighted least squares function. Depending on the test type being used, a different weighting function will be employed. Currently, weighting functions have been developed for two different test types: low cycle fatigue and stress relaxation. Each weighting function is designed to emphasize the more dynamic regions of material behavior, where the Miller model parameters influence the material behavior most prominently. The simplest of the weighting functions is used for low cycle fatigue tests. All data points above a certain stress magnitude in tension and compression are weighted with a value of 2.5, while all points below this value are weighted

as 1.0. This range of values was determined from practical experience and its utility was verified in the experimental results. The effect of the weighting scheme is an emphasis on the inelastic regions of material response where the Miller model, and not simple elastic theory, predicts the behavior.

The weighting function developed for the stress relaxation is more complicated, using both the stress rate and the derivative of the stress rate. It takes the form

$$w_i = \frac{C_0 + C_1 |\dot{\sigma}_i| + C_2 |\ddot{\sigma}_i|}{|C_0 - C_1 |\dot{\sigma}_i| - C_2 |\ddot{\sigma}_i||}, \tag{6}$$

where

$$C_o = \frac{7}{3} \left(C_1 |\dot{\sigma}_{i^*}| + C_2 |\ddot{\sigma}_{i^*}| \right) \tag{7}$$

and i^* satisfies

$$|\dot{\sigma}_{i^*}| = \max |\dot{\sigma}_i| . \tag{8}$$

Here, C_1 and C_2 are equal to unity and serve to eliminate nonequivalent units. The weighting function in Eq. 6 is designed to keep all values of w_i between 1.0 and 2.5. The lower value of 1.0 is set automatically as the stress relaxation approaches a steady state value. The definition of C_0 ensures that the weighting function reaches a maximum of 2.5 at the time at which the maximum stress relaxation rate occurs. This is desirable in order to determine the hardening parameters present in the Miller model more accurately. The effects of the hardening parameters are greatest at times when relaxation is occurring most rapidly. Since continuous experimental data are not available, finite difference approximations were used to calculate the stress rate and derivative of the stress rate as

$$\dot{\sigma}_i = \frac{\sigma_{i+1} - \sigma_i}{t_{i+1} - t_i} \tag{9}$$

$$\ddot{\sigma}_i = \frac{\sigma_{i+1} - 2\sigma_i + \sigma_{i-1}}{(t_{i+1} - t_i)(t_i - t_{i-1})} \tag{10}$$

Several criteria were used in the selection of the optimization algorithm. First, it was desired that no derivatives or gradients be required for minimization. The complex nature of the Miller model would make such calculations difficult and would limit the robustness of the uSHARP routine by requiring modification for use with any other constitutive model. To this effect, an optimization algorithm requiring only objective function evaluations was strongly desired. Second, due to the length of time required to carry out a single finite element simulation, an efficient optimization algorithm requiring a minimum number of iterations was desired. While this would almost certainly constrain the uSHARP routine to the use of a local optimizer, the length of time required for an optimization run would be practical and not too costly in terms of computation time. Lastly, an optimization algorithm requiring only a single initial guess was desired, since usually a set of material constants for a particular constitutive model can be found in the literature. All of these desired characteristics are met by the Hooke-Jeeves direct search algorithm [13], a robust local optimization algorithm. The optimization procedure utilized in uSHARP is outlined in Fig. 4.

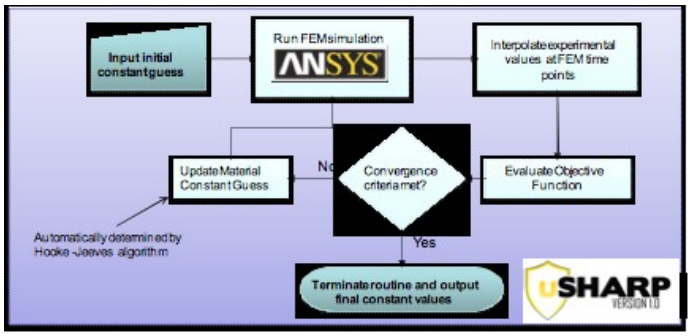

Figure 4. OPTIMIZATION PROCESS

Table 4. Miller constants for "experimental" test data, type 304 stainless steel

Inelastic Constant	Value	Strongly influences
A_1 (ksi^{-1})	0.8	Cyclic behavior at high strain ranges
A_2 (ksi^{-1})	7.42×10^{-5}	Cyclic behavior at high strain ranges
B sec^{-1}	1.0×10^{15}	Secondary creep
C_2 ksi	1.0×10^{-1}	Cyclic behavior at low strain ranges
H_1 ksi	2.8×10^{2}	Cyclic behavior at intermediate strain ranges
H_2	1.0×10^{2}	Cyclic and isotropic hardening, primary creep
n	5.8	Secondary creep

3 EXPERIMENTAL PROCEDURE

3.1 Advanced Candidate Experiments

The focus of the research was determining a small number of candidate experiments that would allow for the determination

of the material parameters with a minimum amount of experimental data. These experiments take the form of numerically simulated mechanical test data generated from the UPF with the published Miller constants for type 304 stainless steel, shown in Table 4 [4]. These simulated experiments are useful in designing the actual mechanical experiments that will be performed with future research. After an analysis of the material parameters was performed based on Miller [1] the necessary test conditions were determined for the parameter determination.

The experimental behavior affected by each of the constants is shown in Table 4. The absence of the Q parameter must be noted. The determination of this parameter requires data at different temperatures. To maintain simplicity for the preliminary stages of the research, isothermal test conditions were used, eliminating the ability to determine Q. Future research will include non-isothermal test histories to enable the identification of this parameter.

Two candidate experiments were identified for use with the aforementioned uSHARP optimization routine. In order to run the uSHARP routine, "experimental" tests were simulated using the ANSYS finite element program. The material constants from [4] for type 304 stainless steel were used for these simulations. The value for Q was set at 91,000 cal/mole, as defined by Miller. In this way, the material constants of the "experimental" test data were already known, allowing for verification of the optimization routine once uSHARP had determined values for material parameters. Once the key simulated experiments have been identified and the parameter optimization process has been fully developed, experimental specimens will be used to obtain actual data. The uSHARP optimization routine can then be verified under real conditions.

One simulated "experimental" test that was used was a strain-controlled low cycle fatigue test with ramping strain amplitude, as shown in Fig. 5(a). The strain amplitude for the first cycle was 0.05%, and the amplitude of the last cycle was 0.5%. The time per quarter cycle was held at a constant 10 seconds, and the simulated temperature was 593°C. The strain rates experienced during the test ranged from $5.0\text{x}10^{-3}$ % sec^{-1} to $5.0\text{x}10^{-2}$ % sec^{-1}. This was done in order to provide material behavior at different strain rates, an important consideration with a strain rate sensitive model such as the Miller model [1]. Additionally, different strain amplitudes in a single test provide a broad spectrum of material behavior using only one test specimen. This low cycle fatigue test was used to simulate the non-hardening and cyclic material behavior so the corresponding constants could be determined. Six cycles were simulated in order to allow for reasonable simulation times.

The second "experimental" test type used to determine the material parameters was a strain-controlled stress relaxation test, also at 593°C. Two different strain amplitudes were applied in one test, as depicted in Fig. 5(b). The first strain amplitude was 0.075%, followed by a ramping up to a level of 0.1%. Each of

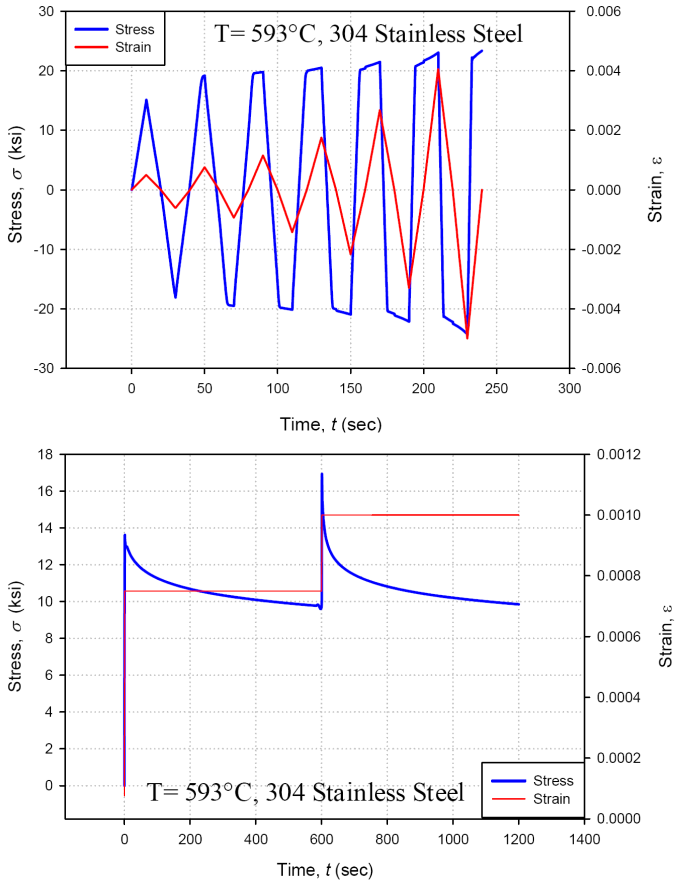

Figure 5. EXPERIMENTAL (A) LOW-CYCLE FATIGUE TEST AT 593°C AND (B) STRESS RELAXATION TEST AT 593°C USED FOR PARAMETER DETERMINATION

the amplitudes was held for 600 seconds. One second was used as the strain ramping time. The two different strain amplitudes were used in order to gather material information under different conditions using only one test.

In addition to the previous two candidate experiments, a third test was designed to be used along with the low cycle fatigue and stress relaxation tests. A strain-controlled ratcheting test was simulated at 593°C for fifteen cycles. The strain for the test was increased 0.05% under loading and decreased 0.025% during unloading, as depicted in Fig. 6. This process was repeated fifteen times for a maximum amplitude of 0.4%. The time between successive peaks was held at a constant 40 seconds so that the strain rates varied. A high number of cycles was simulated in the ratcheting test to account for any shortcomings resulting from the low number of cycles present in the "experimental" low cycle fatigue test. This resulted in a significantly longer computation time; the compromise, it was hoped, would come in the form of more accurate constants. All three tests would be used

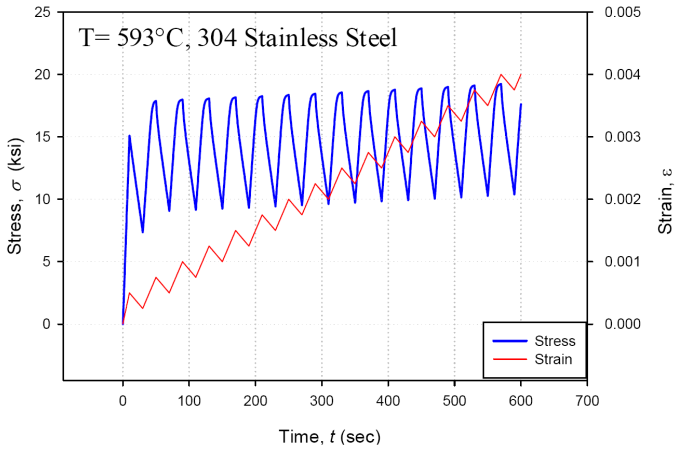

Figure 6. RATCHETING TEST USED FOR PARAMETER DETERMINATION

simultaneously during the parameter determination process.

All of the simulated "experimental" tests were designed so that they could be conducted by the available hardware, thus allowing for actual experimental validation following the preliminary trial runs using the aforementioned synthetic data. None of the "experimental" tests feature instantaneous changes in strain level; there are no strain rates which are not achievable mechanically. While it was assumed that more complex control systems will enable more complicated experimental tests to be conducted, the experimental tests that would be conducted for validation would be controlled by a PID controller. Correspondingly, none of the tests designed here should present too great a challenge in mechanical testing; they are slightly more complex versions of standard experiments which are routinely conducted and are all isothermal. Furthermore, to ensure that the designed experiments could be conducted on specimens without premature failure, all of the strain rates and maximum strain amplitudes were kept to levels at or below those of the data found in [4].

3.2 Parameter Determination using uSHARP

The "experimental" data that were used to validate the uSHARP optimization routine were created by finite element simulation of the previously outlined strain controlled experiments, using the constants for type 304 stainless steel determined by [4]. As mentioned previously, the uSHARP routine performs best when the appropriate orders of magnitude for the constants are already known. It is assumed that for any future parameter determination runs using a different alloy the constants developed for stainless steel will be used as a starting guess. This assumption is provided as justification for choosing an initial guess which is on the proper order of magnitude. During every optimization run, the evolution of the constants and the objective function value were recorded after each iteration. This enabled for real time updates of these values as the parameter determination progressed, and created a comprehensive log of these values for analysis following an optimization run.

Table 5. Initial parameters for optimization procedure. "Experimental" data constants are repeated here for convenience.

Inelastic Constant	"Experimental" Value	Initial Guess
$A_1\ (ksi^{-1})$	0.8	1.0
$A_2\ (ksi^{-1})$	7.42×10^{-5}	1.0×10^{-5}
$B\ sec^{-1}$	1.0×10^{15}	1.0×10^{15}
$C_2\ ksi$	1.0×10^{-1}	1.0×10^{-1}
$H_1\ ksi$	2.8×10^{2}	1.0×10^{2}
H_2	1.0×10^{2}	1.0×10^{2}
n	5.8	1.0

3.3 Addition of Random Noise

In order to better simulate actual experimental testing and the inevitable associated measurement errors, the three simulated "experimental" datasets were modified by adding random noise. The resolution of the load cell available on the in-house testing rig was used as a guideline to develop a realistic range for the random noise. While this method of adding error does not account for any systematic bias that may be present during actual mechanical testing, it does add in an element of statistical sampling error. This allows for verification of the uSHARP routine under less-than-ideal circumstances. For the purposes of this research it is assumed that under careful experimental consideration, systematic error can be minimized, leaving primarily a statistical noise error.

Random noise was also added to verify the technique of using simulated data to match experimental tests. If the results for noisy experimental data match the results for ideal experimental data, it is more likely that the technique of using simulated data is sound. To this end, the uSHARP optimization routine was used to determine material constants for the "experimental" data both with and without the added noise.

4 RESULTS AND DISCUSSION

4.1 Material Parameter Determination

The uSHARP routine was used twice to determine the Miller model material parameters. In addition to the "ideal" simulated experiments, data with random noise was also used with the optimization routine. In each case the initial guess, presented in Table 5, was the same to allow for a comparison of the converged

Table 6. Converged values of material constants

Inelastic Constant	"Experimental" Value	Converged Values (no noise)	Converged Values (with noise)
A_1 (ksi^{-1})	0.8	0.1959	1.524
A_2 (ksi^{-1})	7.42×10^{-5}	2.616×10^{-5}	2.754×10^{-5}
B sec^{-1}	1.0×10^{15}	1.005×10^{15}	8.963×10^{14}
C_2 ksi	1.0×10^{-1}	1.521×10^{-1}	3.811×10^{-2}
H_1 ksi	2.8×10^{2}	2.796×10^{2}	3.051×10^{2}
H_2	1.0×10^{2}	1.024×10^{2}	8.062×10^{1}
n	5.8	5.801	5.723

solutions for each data set. Note that the initial guesses are on the same order of magnitude as the actual values for the constants, and for some parameters, the initial guess is the same as the experimental value. However, due to the high nonlinearity of the Miller model equations, the initial guess generates a simulated test history that diverges significantly from the "experimental" data, even when some of the parameter values match.

The final converged values determined by uSHARP for each case can be seen in Table 6. It is evident from the results that the same solution was not obtained in both cases for each parameter. Only the values for A_2, B, H_1, H_2, and n were reasonably close in the final converged solutions for the data with and without noise. The values for A_1 and C_2, however, differ by nearly an order of magnitude. Furthermore, a comparison of the optimized values for the material constants with the values used to generate the "experimental" data indicates that the optimization routine did not resolve the "correct" value for all of the parameters. While the values for B, H_1, H_2, and n converge reasonably to the experimental set values, the values for A_1, A_2, and C_2 do not. This appears to imply that the uSHARP routine did not determine usable values for these material parameters. However, the simulated test histories using optimized constants are visibly close fits to the experimental test histories, as can be seen in Figs. 7 and 8.

In each case, the material parameters determined by the uSHARP optimization routine have provided excellent fits across the entire range of data, despite being distinct from the experimental data parameters. This suggests that for a given set of experimental data, a unique solution for material parameters might not exist. If the discrepancies were due to the candidate experiments not fully capturing the effects of each material parameter, then the non-uniqueness of the material constants could be explained by the under-determination of the optimization problem. At any rate, the discrepancies demonstrate that any attempt to determine constitutive model parameters must involve a careful

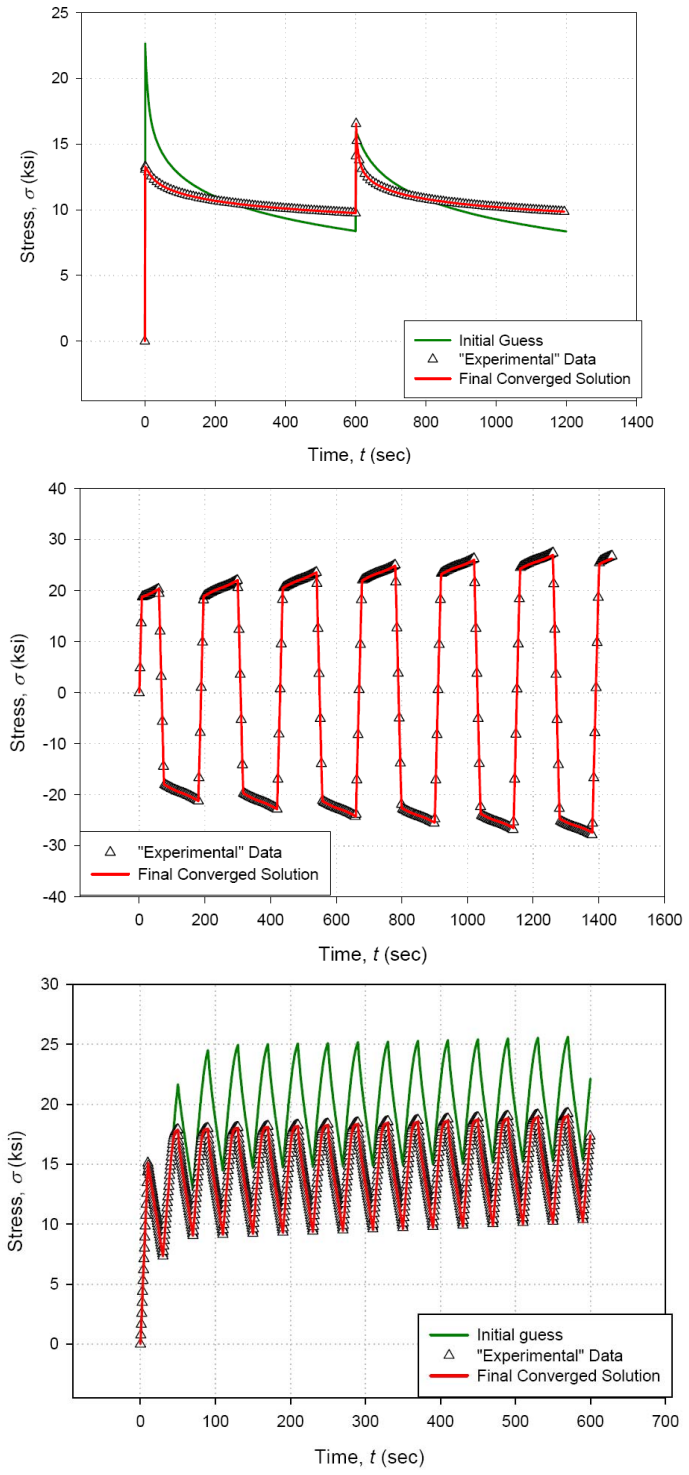

Figure 7. USHARP CONVERGENCE RESULTS FOR (A) STRESS RELAXATION, (B) LOW-CYCLE FATIGUE, AND (C) RATCHETING STRAIN AMPLITUDE FOR NOISELESS DATA

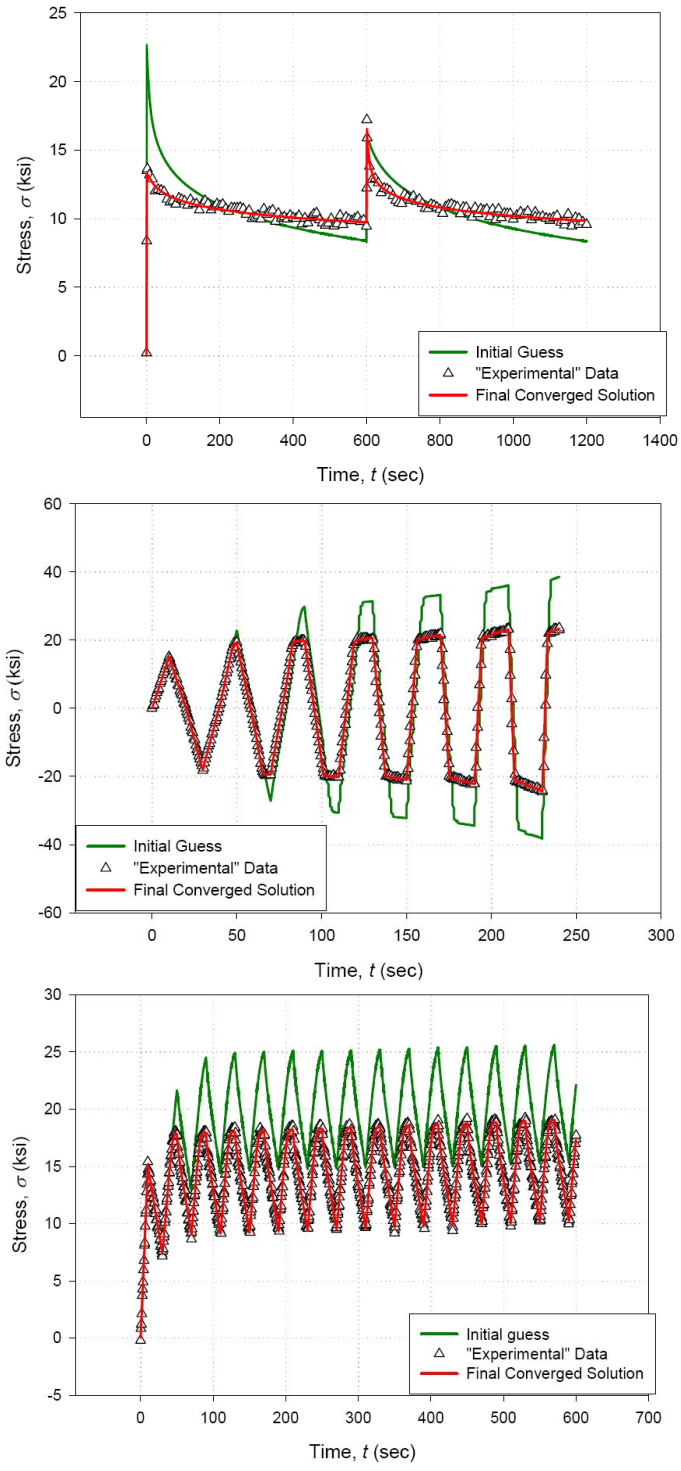

Figure 8. USHARP CONVERGENCE RESULTS FOR (A) STRESS RELAXATION, (B) LOW-CYCLE FATIGUE, AND (C) RATCHETING STRAIN AMPLITUDE FOR DATA WITH RANDOM NOISE

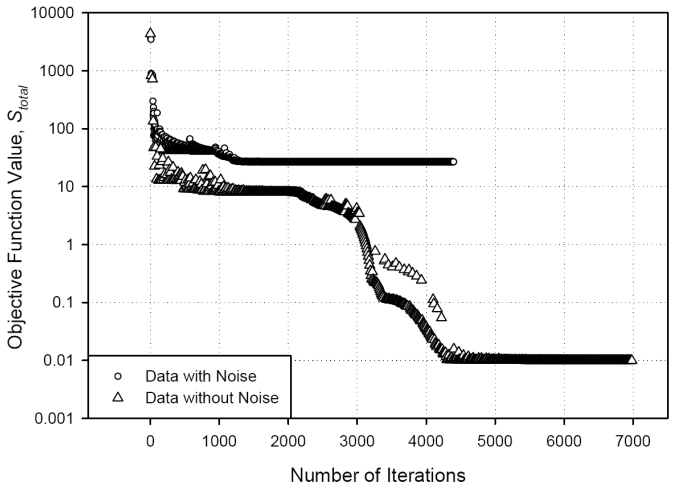

Figure 9. OBJECTIVE FUNCTION CONVERGENCE FOR DATA WITH AND WITHOUT RANDOM NOISE

consideration of the experimental test matrix to be used. While the converged values for the material constants have accurately reproduced the "experimental" test history in this case, there is no guarantee that the same correlation will occur under more complex or longer-duration test histories.

Comparing the number of iterations required for convergence indicates that the noiseless data took nearly 2500 more iterations to converge than the data with noise. Additionally, the final objective function value for the data without noise was nearly three orders of magnitude lower than that of the data with the added noise. Both of these trends can be explained by the fact that without any random errors, the model can perfectly reproduce simulated data, meaning that the differences between the optimized-constant simulated data and the experimental data may be extremely small. On the other hand, when noise is added, there is a limit to how well the model can fit the data, so that the minimum of the objective function is much higher. Comparing the evolution of objective function values in both cases shows that for both data sets the initial objective function value was approximately equal. Because the objective function value at convergence is much lower for the noiseless data, many more iterations are required.

The method employed by the uSHARP routine has proven successful at determining viscoplastic constitutive model parameters. Furthermore, the program has been constructed in such a way as to be applicable to a wide class of constitutive models with little modification. Similar results have recently been obtained applying uSHARP to other constitutive models. The only optimization criterion available in the determination of constitutive model parameters is the evaluation of an objective function indicating the caliber of fit between a current guess and experi-

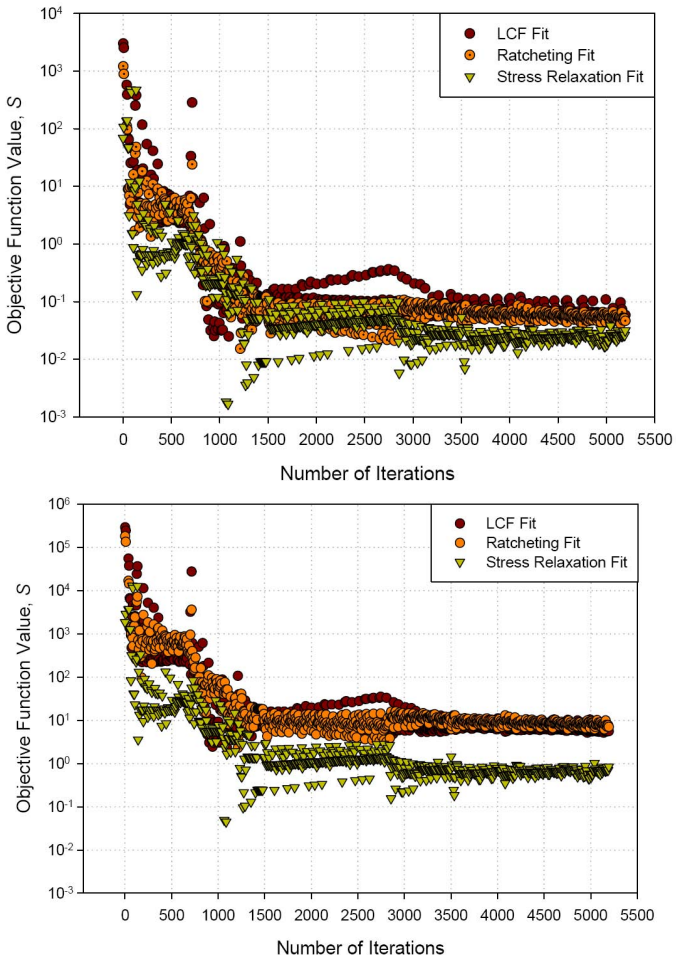

Figure 10. INDIVIDUAL FUNCTION VALUES FOR THREE EXPERIMENTAL TESTS USING (A) THE USHARP OBJECTIVE FUNCTION (EQ. 4) AND (B) STANDARD OBJECTIVE FUNCTION FROM LITERATURE (EQ. 11)

mental data. In this regard, uSHARP has performed well, generating a nearly perfect fit in both cases and minimizing the objective function, as seen in Fig. 9. However, it has been demonstrated that an objective function minimum, corresponding to an excellent fit, does not necessarily indicate a unique solution for the material parameters. This problem may, in fact, be unavoidable when an inadequate test matrix is used to determine constitutive model parameters. It is thought, however, that with more careful consideration of candidate experiments, the uSHARP optimization routine may be used to successfully determine material parameters with a greater level of accuracy. This will be left for validation in future work.

4.2 Objective Function Analysis

The objective function featured in the uSHARP routine was designed to enable the use of different test types and data sets simultaneously for parameter determination. It is pertinent to perform an analysis as to whether or not this goal has been achieved. The standard objective function commonly used for automated parameter determination is a simple, weighted least squares function [14, 15]. This is typically expressed as

$$S = \sum_{i=1}^{n} w_i (y_{exp,i} - y_{sim,i})^2 \tag{11}$$

where n is the number of data points, w_i is a weighting factor, $y_{exp,i}$ is the experimental data point, and $y_{sim,i}$ is the simulated data point. Multiple datasets are then combined in the form of Eq. 5. To provide an indication of the utility of Eq. 4, the uSHARP objective function, the individual S-values of each of the three tests were recorded during the optimization process for the data without noise. By comparing these results with S-values calculated using Eq. 11 during the same optimization run, the proposed objective function can be compared with the standard from current literature. For both equations, the uSHARP weighting functions were used. The evolution of S throughout the optimization process for both cases is shown in Fig. 10. The results show that the use of the standard least squares error function would have been insufficient for the simultaneous use of the experimental data used during the parameter determination runs. Equal consideration would not have been given to each test. Use of the uSHARP objective function, however, eliminates this problem.

The use of Eq. 11 would have been sufficient for the combination low-cycle fatigue / ratcheting test. The least-squares values for both tests are approximately on the same order of magnitude, meaning that neither of the curves would receive more weight than the other during the optimization process. However, the inclusion of the stress relaxation test creates a problem when using Eq. 11. For the duration of the optimization process, the value of S for the stress relaxation test is at least an order of magnitude lower than the values for the two other tests. This creates a natural bias during optimization, providing more consideration to the ratcheting and low-cycle fatigue tests. This trend is not evident with use of the uSHARP objective function. The individual S values remain on the same order of magnitude for the duration of the optimization process. This is proof that uSHARP allows for the use of several different test types without undue consideration of any single test over the others. Clearly, the proposed objective function represents an improvement over the standard objective function commonly used for automated constitutive model parameter determination.

5 CONCLUSIONS

The uSHARP optimization routine was successful in determining values for the material constants which created excellent fits with the "experimental" data. While the final converged constants were not close to the "experimental" values in all cases, this merely indicates an experimental test matrix which is not adequate for capturing the effects of all of the material constants. Thus, there is a need to verify the adequacy of the experimental test matrix used in an automated parameter determination routine before the results can be trusted. A procedure using synthetic data where the "experimental" constants are already known, similar to the method used here, would be a good initial step to verify the adequacy of any test matrix before making the commitment to actual experiments using test specimens. Use of the uSHARP routine shows great promise in simplifying the procedure of parameter determination. Since the uSHARP optimization process is completely contained, calling on an external program (ANSYS) to provide the necessary finite element simulations, it is expected to be adaptable to any constitutive model or finite element software package. In this way, the developed parameter determination method was designed to be broadly applicable to suit the needs of many different users, as its procedure is not specific to the Miller model. The form of the objective function used in the uSHARP routine demonstrated superiority over the traditional form commonly found in literature. The goal of enabling the use of multiple test types simultaneously with minimal user input was satisfied, ensuring that every "experimental" test used had equal consideration during the parameter determination process. While the weighting functions were determined through a trial and error process, they have performed favorably. In each case, the set of constants that minimized the objective function produced a close fit to simulated experimental data.

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