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A Computational Study on Material Model Selection for Shape Memory Alloys

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ABSTRACT

Computational simulations are an essential component in today's design process. The design and fabrication of smart materials in a production environment requires analytical and computational tools that can describe smart material behavior. Of concern in this paper are the material constitutive models to be used in computational analyses. Often there are questions concerning the accuracy of constitutive models for the active components such as shape memory alloys (SMAs). These constitutive models can substantially increase computational costs in terms of both memory and time requirements. Model size limitations and use of complex constitutive models are often competing factors. Therefore whether the use of complex constitutive models for smart components actually benefit the analysis of the device is an issue of concern to those in the smart materials design community.

The current work examines the differences in computational simulations due to the choice of constitutive model for shape memory alloy. The device considered is a thick walled tube fabricated of SMA metal and subjected to torsion loading. The constitutive models examined are Tanaka's exponential model [1], Rogers-Liang cosine model [2] and Boyd-Lagoudas et al. polynomial model [3,4]. One common feature to all models is the complexity in the number of material parameters required. Experimental work used for comparison was performed independently and completed prior to initiation of the computational study [5].

INTRODUCTION

Smart materials and devices are emerging from the laboratory environment and becoming recognized as viable design options. New applications are appearing almost daily. Critical to the success of this transition are the analysis and design tools available. One important question that must be addressed is:

> Are sufficient tools available so that anyone other than a research scientist can create a practical smart material or device with assurance that its performance will be acceptable?

This is a key issue facing smart materials and devices. A build and test philosophy often dominates in the laboratory environment but is unacceptable in the manufacturing environment. What is needed in the manufacturing environment is a design methodology for smart materials and devices that parallels accepted practices for conventional materials. The designer needs tools that allow for prediction of behavior and structural integrity. The designer must have confidence that the product will perform as expected. Building prototypes of all possible design options is not a viable design methodology if smart materials and devices are to be competitive with conventional designs. In brief, analytical and computational tools are required that provide accurate simulations of smart material and device behavior.

An accepted design methodology for conventional material is finite element analysis. The versatility of finite element analysis for all aspects of design is well established. Parameter studies in which minor modifications to the design are evaluated are common practice. The basic information required for finite element analyses are component geometry and material properties. The need for accurate material properties exists for both active and conventional materials. Simple constitutive response models may be computationally efficient but may not accurately represent material performance. In this paper the performance of and the variation in calculated results due to the selection of SMA constitutive model are examined.

Many smart materials and devices have used the active response of shape memory alloys (SMAs). SMAs can provide large displacement and large strain capabilities at relatively low frequencies. Methodologies for accurately predicting performance are necessary for the designer to take advantage of SMA capabilities.

The development of SMA constitutive models is an area of much research. During the past two decades there have been many constitutive models proposed for SMAs. There are continual advancements, modifications as well as combinations of existing constitutive models. In addition new constitutive models are being presented. Many of these constitutive models are very complex and require a large number of measured constants to characterize the material. Many are cumbersome to use in the design environment. Many are one-dimensional or based on single-crystal behavior and not appropriate for use in the design of bulk material components. To date there is no consensus as to the 'best' model. The resulting situation is one where there are many competing models with little guidance on accuracy and appropriateness. This creates a frustrating situation for the designer. As stated previously the move of smart materials and devices from the laboratory to a production environment is dependent on designers having ready access to constitutive models that have a known accuracy in prediction. Accuracy and ease of use are real issues. Schroeder et al. [6] discusses the advantages and disadvantages of a select group of SMA constitutive models. Similarly, the purpose of the current work is the evaluation of two possible design simplifications and three established constitutive models for a specific design.

In this study variations in finite element calculated results that are solely due to the selection of SMA constitutive model are investigated. Five material constitutive response modeling approaches are evaluated: 100% martensite, 100% austenite, Tanaka [1], Liang-Rogers [2] and Lagoudas et al [3,4]. Computational results are compared for the different models to determine if there is a pattern of performance based on model selection.

The component modeled is a tube subjected to a constant torsion loading. The tube is a thick walled hollow cylinder fabricated from a NiTi (K-Alloy) SMA alloy with an outer radius of 0.579 cm and a wall thickness of 0.267 cm. The resulting wall thickness/diameter ratio is 0.23. The gage length of the tube is 5.84 cm. The tube is fabricated from bulk SMA material. The geometry selected is a SMA actuator design that was developed as part of the Northrop-Grumman lead Smart Wing program [7]. The purpose of the tube is to twist a wing frame raising the leading edge while lowering the trailing edge.

The tube geometry and material were chosen from a series of three tube geometries and two materials used in a series of experiments designed to examine the physical behavior of the tube under torsion and tension-torsion loading [5]. All tube geometries were similar in that all could be classified as thick walled. A single geometry and material combination was selected allowing the current work to concentrate on the variation of calculated results due to constitutive model selection. It was felt that little additional information on constitutive modeling performance could be obtained by examining additional geometries or a second material.

The usefulness of advanced constitutive models that capture SMA phenomenon is dependent on the accuracy of the model when used to evaluate performance for realistic structures. In addition to accuracy, computational requirements must also be considered when constitutive model performance is evaluated. A very accurate model that requires significantly more computer time may not be used in a design analysis due to cost or time limitations. In order to be a viable design tool constitutive models must be both accurate and require only an acceptable amount of computer resources. Acceptable run times are often based as much on corporate culture as on computer or cost considerations. Therefore it is important to provide the potential user with baseline information on run times using different constitutive models. This information is provided here for the models evaluated.

MATERIAL CONSTITUTIVE RESPONSE

As noted in the previous section numerous constitutive models have been proposed for SMAs. This paper examines differences in calculated results obtained for the SMA torque tube based on assumptions of 100% martensite, 100% austenite and on the use of three accepted constitutive models. The 100% martensite and 100% austenite cases use conventional finite element constitutive response and are evaluated to determine if these extremes provide bounds for device behavior. This modeling approach is appealing to the designer because it makes no additional demands on computational time and requires only conventional material parameters; i.e. modulus of elasticity, yield stress, Poisson's ratio and description of stress-strain response. In this approach, SMA behavior is represented in the same manner as other non-linear structural materials.

The constitutive models selected for the study are all thermodynamic based models. The three constitutive models can be considered to represent the evolution of a constitutive model. Tanaka's model as used in this work is based on 1D model describing the phase transformation of SMAs using energy balance equations and the Clausius-Duhem inequality. The internal state variable used to define the state of the material is ξ the martensite volume fraction. Details of the model are not presented here but can be found in Reference 3. In this model the transformation kinetics defined by ξ are describing using an exponential function. Tanaka's model has been extended to 3D by Boyd-Lagoudas [8].

Liang-Roger model is formulated in the same manner as Tanaka's constitutive model. A primary difference in the two models is use of a cosine function in the Liang-Rogers model to define ξ, the martensite volume fraction. The cosine function was defined empirically and agrees well with experimental data. A driving force for replacement of the exponential representation of ξ is the elimination of singularity points at 100% martensite and 100% austenite conditions. It was shown by Liang-Rogers that the cosine representation more accurately represented transformation behavior. The Liang-Rogers model evaluated can be considered to be a modification and extension of Tanaka's model.

The model of Lagoudas et al. is a thermodynamic derivation of the constitutive response of SMA materials. The model is an extension of prior work by various researchers. Details of the derivation of the model can be found in References [3] and [4]. The model uses a polynomial representation for ξ. In addition the Lagoudas et al. model accounts for 4 of the 5 phenomena of SMA material response. The five phenomena are pseudoelsaticity by transformation, pseudoelasticity by reorientation or ferroelasticity, the shape memory effect by transformation, the shape memory effect by reorientation and the two way shape memory effect. All characteristics of behavior except the two way shape memory effect are included in the model.

The three models chosen represent the evolution of concepts in the constitutive response of SMAs. Each model successful builds on its predecessors. It is not apparent whether the added complexity resulting from extensions and modifications of the original thermodynamic model is required for all geometries and design conditions. One goal of the current work is to examine the effects of model evolution on calculated results. Whether the later thermodynamic models with more complex representations of ξ provide increased accuracy is of interest. The increase in computational costs, measured in terms of run time, due to increase in representation complexity is also of concern to the designer. Unfortunately, in many cases, computational resources drive the choice of constitutive models. Comparisons such as presented here will assist the designer by providing insight into variations in accuracy based on model selection.

In all cases the constitutive models have been coded in terms of 3D stress states and defined as solution subroutines for use with ABAQUS, a commercial finite element program.

Material parameter data is based on Keefe et al. experimental results [5] and parameters defining a generic SMA alloy [9]. The martensite and austenite shear modulus values are 26.2 GPa and 48.6 GPa, respectively. Poisson's ratio is 0.33. Parameters unique to the three constitutive models are taken as equal to those for typical SMA material as defined in the User's Manual [9]. It is recognized that increased accuracy can be obtained by parameter testing for specific SMA material. In the present work, all models used general material response data. No model has more accurate material parameter than the other constitutive models. While this may not be ideal for engineering analysis of a smart material, it common for handbook values only to be available to the analyst. The issue of material parameter accuracy is important but is not addressed in this work. The approach taken of using standard values for all constitutive model parameters is considered appropriate for this comparison study of calculated results.

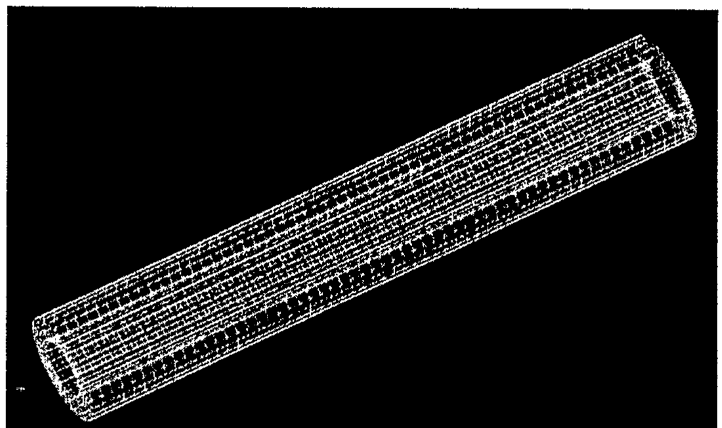
NUMERICAL SIMULATION

The commercial finite element code ABAQUS [10] is used for all analyses. The total length of tube modeled is 7.62 cm. The gage length of 5.84 cm is centered along the length of tube modeled. An exploded view of the model is shown in Figure 1. Sufficient extensions are included above and below the gage length to isolate any boundary condition end effects from the gage length. The gage section consists of 10752 elements; 6 elements in the thickness direction, 32 elements around the circumference and 56 layers in the length direction. Extension sections consist of 6 elements in the thickness direction, 32 elements around the circumference and 5 layers in the length direction. The model of end extensions and gage length of tubing consists of 12672 elements and 15010 nodes. All elements are 8 noded quadrilateral bricks. All elements are assigned the same material properties. In the case of user subroutine constitutive response, material characteristics vary from element to element as a result of the stress state in each element under load. Both stress and temperature induced transformations from one material phase to the other are included in the user subroutine.

The actuator design considered provides a moment to the wing box when the tube is installed and subjected to increased temperature. The experimental process establishes the twist response to an applied moment. This behavior is what is duplicated in the finite element simulation. In order to apply a uniform moment to the tube rigid surfaces are attached to the both ends of the cylinder. One end of the cylinder is fixed. A torsional loading is applied to the other end by means of an applied constant radial velocity. Rate effects are not included in the analysis.

100% martensite and 100% austenite cases are defined using standard ABAQUS modeling capabilities. No special elements or constitutive models are used for these runs. Two material formulations were examined; linear elastic-nearly perfectly plastic and linear elastic-plasticity slope of (1/4)E. The first formulation is nearly perfectly plastic because it was found a small slope was necessary to assistance in solution convergence near the yield point. A relationship of 6895 MPa: 1 cm/cm strain was assumed for the slope of the inelastic portion of the nearly perfectly plastic curve. In the higher plastic slope cases where the plasticity slope is defined as (1/4)E. The value of elastic modulus, E, depends on the base material assumption for the run. E_m is used for the martensite case; E_a is used for the austenite case. The resulting slope between stress and strain for the inelastic response curve are 6550 GPa: 1 cm/cm strain for martensite and 12152 GPa: 1 cm/cm strain for austenite. The yield point is estimated based on general yield information on SMAs. Yield was defined as occurring at 0.2% offset strain. This definition resulted in yield values of 52.4 MPa for austenite and 97.2 MPa for martensite. These values correspond well with reported value of 50 MPa for austenite and the reported range of 100-150 MPa for martensite [11].

Torque tube



End caps used for application of boundary conditions

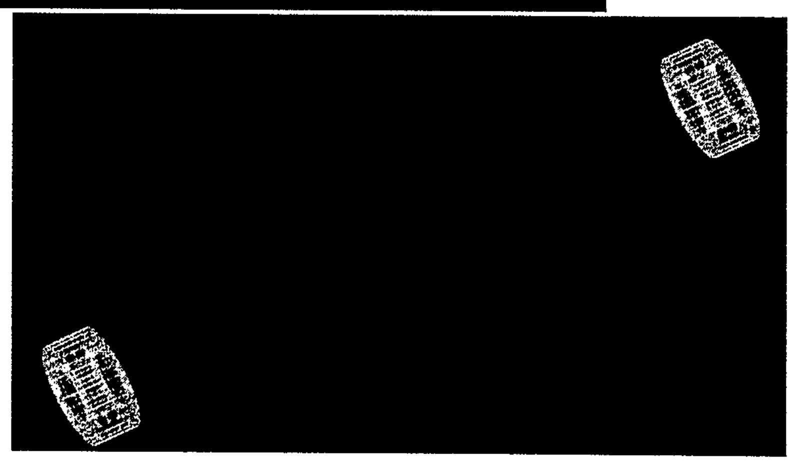


Figure 1. SMA Tube Geometry and Finite Element Model Mesh

A_s temperature is assumed to be 17°C and A_f temperature is assumed to be 34°C. These values compare favorably with reported values [11].

ABAQUS allows for users to define the material constitutive response used in the analysis. The user is responsible for accurately describing the stress-strain relationship for individual elements through use of user defined subroutines. This is the approach used to define constitutive response for Tanaka, Liang-Rogers and Lagoudas et al. models. User subroutines for all constitutive models used were provided by Lagoudas [9]. Coding as provided had been validated for use in ABAQUS. Test runs were completed to determine model stability under loading conditions.

NUMERICAL SIMULATION RESULTS

Single cases are run for each of the pure materials. There is no variation in material properties with temperature incorporated into the pure material. Standard ABAQUS solution procedures are used for these analyses.

Two series of numerical simulations were completed for the three constitutive models; the first at 34°C, the austenite finish temperature, and the second at 24°C, an intermediate temperature. In addition analyses were completed for 60°C, 80°C, 100°C, 120°C and 140°C for the Tanaka and Lagoudas et al. models. These are temperatures well above the austenite finish temperature and were of interest for possible applications. Additional temperature runs were not made for the Liang-Rogers model due to numerical difficulties encountered in the 24° and 34°C runs for the specified geometry and loading conditions. In all computational models the martensite volume fraction is set to zero at the start of the simulations. The temperature is held constant in the numerical simulation. This is equivalent to the constant temperature environment created by the heating tape on the SMA tube in the experimental procedure [5].

Comparison of Numerical Results

The result of primary interest is the applied moment vs. angle of twist loading history. Calculated results are compared for the different modeling methods for the different temperature levels.

The applied moment vs. angle of twist is shown in Figure 2 for the 100% martensite and 100% austenite cases. The increase of slope in the plastic region has a significant effect on results. Also shown in Figure 2 are moment vs. angle of twist for Tanaka, Liang-Rogers and Lagoudas et al. models at 24°C, a temperature between the austenite start and finish temperatures. At this temperature phase transformations are stress and temperature induced. In this case the martensite nearly perfectly plastic case becomes a lower bound only for higher values of angle of twist (greater than 3.5 degrees/cm). Tanaka's model is a lower bound for low to moderate angles of twist (0 to 3 degrees/cm). Liang-Rogers model become numerically unstable at a lower angle of twist than at the higher temperature case. Lagoudas et al. model again predicts a stiffer structure requiring more moment to twist at higher angles of twist. The 100% austenite nearly perfectly plastic with a slope of (1/4)E for the inelastic portion of the stress-strain curve is the upper bound for all cases considered. It is interesting to note that all curves for low to moderate angles of twist (0-2.5 degrees/cm) are bracketed by Tanaka and 100% austenite elastic-nearly perfectly plastic. This is in contrast to the 34°C case where the majority of results are bracketed by the 100% austenite elastic-perfectly plastic and (1/4)E inelastic slope cases.

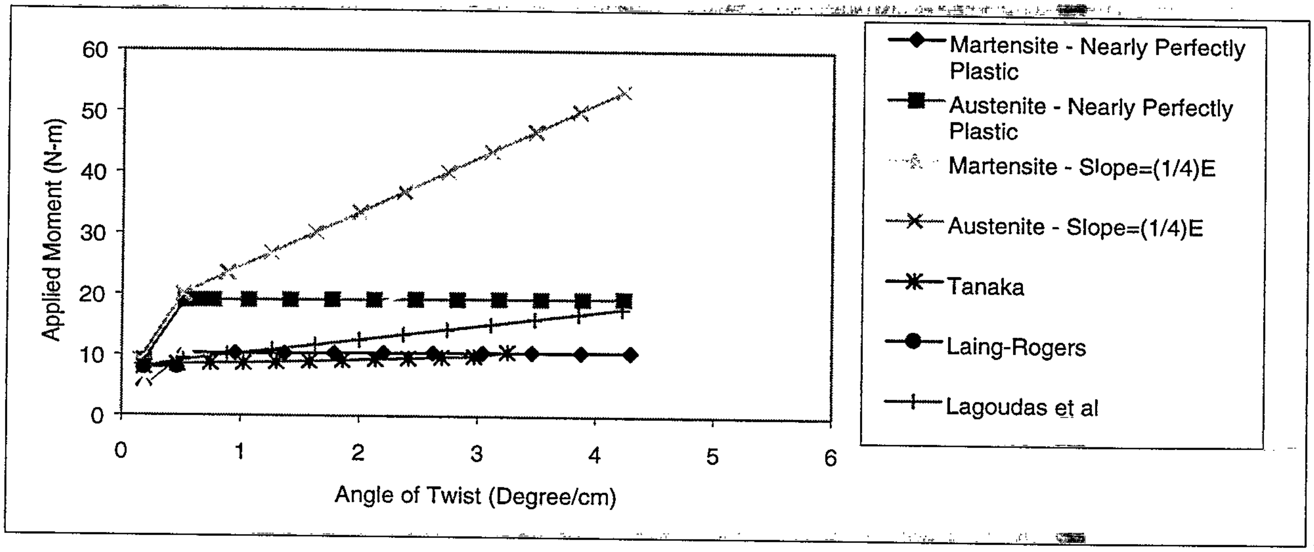


Figure 2. Applied Moment vs. Angle of Twist, Intermediate Temperature (24°C)

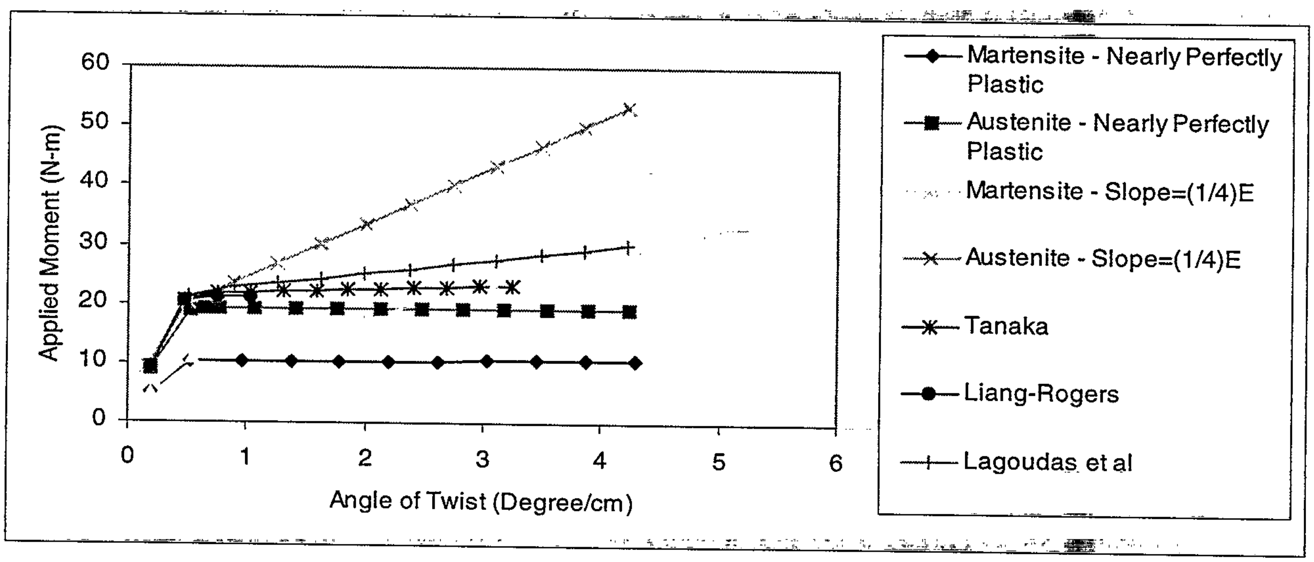


Figure 3. Applied Moment vs. Angle of Twist, Austenite Finish Temperature 34°C

Figure 3 shows the variation in calculated results at the austenite finish temperature (34°C). At this temperature transformations are stress induced. At this temperature 100% martensite elastic-nearly perfectly plastic represent a lower bound for calculated results. Austenite models with a slope of (1/4)E on the inelastic portion of the stress-strain curve serve as an upper bound. Lagoudas et al. model predicts a stiffer structure than Tanaka and Liang-Rogers. Lagoudas et al. requires more moment to twist the tube. Liang-Rogers solution exhibited severe numerical convergence problems within the ABAQUS finite element code at low levels of angle of twist (0.5 to 1.0 degrees/cm).

Figure 4 shows the applied moment vs. angle of twist for all temperatures as calculated using Tanaka's constitutive model When the temperature is at or below the austenite finish temperature, calculated results show significant reductions in response. Calculated results for temperatures at or below the austenite finish temperature start to diverge from higher temperature results at an approximate angle of twist of 0.2 degree/cm. Higher temperature responses show negligible differences until much larger angles of twist; 1 degree/cm for 60°C and larger angles for higher temperatures. As temperature increases, the region of linear moment-angle of twist response increases. Identical results are seen for all temperatures for the linear response regime. At lower temperatures smaller amounts of applied load are required to obtain a set value of angle of twist. This is consistent with the more compliant nature of the martensite phase.

All analyses complete 24 increments of loading. Greater angles of twist (4.2 degrees/cm) are obtained for temperatures at or below the austenite finish temperature. The maximum angle of twist obtained for higher temperature conditions is 3.2 degrees/cm. There is some indication in computational results that convergence is easier to obtain for Tanaka model in the lower temperature regime.

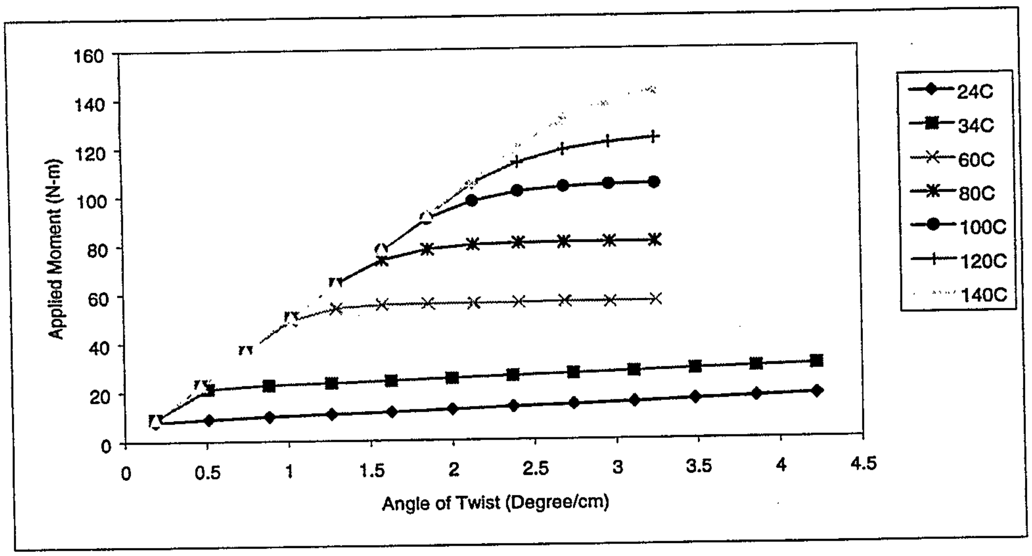
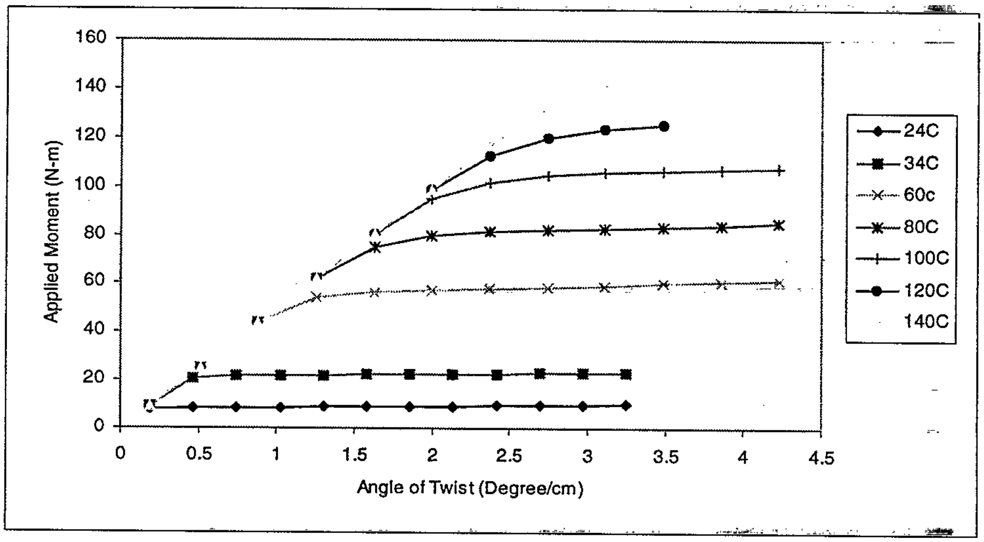


Figure 4. Applied Moment vs. Angle of Twist for Tanaka Constitutive model.

Figure 5 shows the applied moment vs. angle of twist for all temperatures as calculated using Lagoudas et al. constitutive model. As in the previous case, calculated results at and below the austenite finish temperature diverge from higher temperature results at a very low angle of twist; approximately 0.2 degree/cm. Lagoudas et al. constitutive model shows an earlier departure from linear moment-angle of twist response for higher temperatures than is seen in Tanaka's model. When the temperature is below the austenite finish temperature the calculated response shows that an only very small increase in applied moment is required for a large increase in angle of twist. Again, this is consistent with the more compliant nature of the martensite phase.

Figure 5. Applied Moment vs. Angle of Twist for Lagoudas et al. Constitutive model.



All analyses with the exception of 120°C case consist of 24 increments. The 120°C case consists of only 20 increments due to system failure during the run. Sufficient data was obtained so that it was not necessary to repeat this run. For Lagoudas et al. model greater angle of twists are obtained for temperatures above the austenite finish temperature. This is in contrast to the performance of Tanaka's model. All cases used identical convergence criteria. This is an indication of the differences in solution performance between the two constitutive models.

All analyses were run on a ring of Sun Ultras. The system used is a Department of Defense High Performance Computing Resource maintained by NRL Center for Computational Science. The system currently consists of 20 machines (32 processors) linked together. The connection between individual sun workstations is invisible to the user. Computer run times are shown in Table 1 for all conditions run. Run times reported are for similar numbers of load increments.

For the computer system used run times for Tanaka or Lagoudas et al. constitutive models are similar. Tanaka requires more time for temperatures between the austenite start and finish temperatures. Lagoudas et al. requires more time for temperatures greater than the austenite finish temperature. For the computer system used the times are not unreasonable. The only computational time determined to be unreasonable is for Liang-Rogers constitutive model and is attributable to the numerical solution problems encountered.

Table 1. Average Run Times for SMA Analyses

Condition		Average Run Time (CPU Second) 24 Increments
100% Martensite or 100% Austenite		9300
Tanaka	$T=A_f$	9340
	$A_s<T<A_f$	13450
	$T>A_f$	11302
Liang-Rogers	$T=A_f$	>13000 for 6 inc., had to abort job
	$A_s<T<A_f$	>13000 for 6 inc., had to abort job
	$T>A_f$	did not run
Lagoudas et al	$T=A_f$	9140
	$A_s<T<A_f$	9260
	$T>A_f$	13384

SUMMARY

A series of computational simulations were performed using finite element techniques to examine the differences that result from the selection of constitutive models. The device examined was a hollow tube fabricated of TiNi-Cu (K-Alloy) SMA and subjected to torsion loading. The use of 100% martensite and 100% austenite as possible bounding solutions was investigated along with the use of Tanaka [1], Liang-Rogers[2] and Lagoudas et al. [3,4] constitutive models. In the current work average generic SMA material properties were used. More accurate evaluation of constitutive parameters should increase the accuracy of computational predictions. Use of generic or handbook values is consistent with common design practices and therefore considered appropriate for this comparison study. Computer time required for the different approaches was tabulated for consideration. The work performed indicates that:

- Use of 100% austenite and 100% martensite material and conventional finite element solution techniques may or may not bound more complex constitutive responses.

- Liang-Rogers model had severe numerical difficulties once angle of twist and therefore strain reached relatively moderate values. This may be a result of the representation of ξ or stress field embedded in the model. This is an indication that the model is not as robust as either Tanaka's or Lagoudas et al.

- Tanaka and Lagoudas et al. models remained stable for high values of angle of twist. Solutions remained stable for values much higher than reported here.

- In most cases computer time requirements were similar on the cluster of Sun workstations used for the current work. The run time requirements varied for temperature regime and constitutive model used. The times were not unreasonable for the computer system and the class of problems generally run on the system by the authors.

Based on this study, complex constitutive models for SMAs are a reasonable design tool with some increases in computational resources required. However, there is still wide variation in results indicating that much work needs to be done in the field of computational model development for SMA. Additional work is required on material parameter testing in order to build a sufficient database for the accurate selection of representative material parameters for a particular SMA alloy. It is recognized that SMA material response has a strong dependence on hystersis. This will have to be addressed in future work, both computational and experimental. Creation of an experimental database of material parameters will eliminate one source of errors; i.e. generic material properties will be replaced by actual properties.

In summary there is much work that needs to be done on material constitutive response for SMAs. However, existing SMA models can be used in finite element analyses. An increased level of computer resources is needed for these analyses but the related cost is not prohibitive. The authors' opinion is that it is best to perform computational analyses with one of the complex constitutive models rather than rely on a bounding solution approach. Because there is no significant impact with respect to computer time requirements, it is recommended that the most general model be used. In the set of models evaluated in this work the most general model is that of Lagoudas et al. This model appears robust and numerically stable to high strain levels. Material parameters will be an issue but will be an issue with any model selected.

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