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COMPARISON OF MATERIAL MODELS OF SHAPE MEMORY ALLOYS APPLIED TO MESO-SCALE INTERACTIVE FIBRE RUBBER COMPOSITES

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Abstract: Shape memory alloys (SMAs) are prominent members in the smart material family with a diversified field of applications. They are playing a major role in medical and automotive industries with applications ranging from dental braces, stents to thermal valves, body frames, wipers etc. The diversified applications of SMAs have created a need to develop and implement material models for the analysis of SMA driven elements for better understanding of their structural behaviour. Many models have been developed to capture the prolific properties of SMAs. One such model is the Souza & Auricchio SMA material model incorporated in ANSYS with the ability to solve with the option of choosing superelastic and SME properties. However, this model has a limitation in terms of the one-way SME that cannot be useful for meso-macro scale applications with curved or irregular shaped SMAs. This paper compares a user-defined material model (Woodworth & Kaliske SMA material model) and the Souza & Auricchio model using a meso-scale approach of interactive fibre rubber composites in ANSYS Workbench. This model has the ability to simulate the one-way SME with applied pre-stretch, which subsides the problem of modelling and solving curved or irregular shaped SMAs, and is verified using a U-shape SMA profile. As the model is under development, this paper also highlights the advantages and limitations of the user-defined model.

Key words: Souza & Auricchio model, Interactive fibre rubber composites, Shape memory alloys, Woodworth & Kaliske model

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1 INTRODUCTION

Shape memory alloys (SMAs) can convert electrical energy into mechanical energy in terms of the Shape Memory Effect (SME). SMAs are a class of smart materials with wide applications ranging from medical industry to the automotive-aircraft industry. They possess high energy density corresponding to high reaction forces, making them suitable for various industrial applications. SMAs are capable of recovering their original shape due to martensite-austenite and austenite-martensite phase transformations triggered by temperature difference and also by the applied stress field [1]. The phase transformations due to difference in temperature are known as SME, and those triggered by an applied stress field correspond to superelasticity or pseudo-elasticity. The structural changes during phase transformations happen due to diffusionless transformation and shear lattice distortions. Austenite is stable in terms of atomic structures at high temperatures and is considered as the parent phase, whereas martensite is stable at lower temperatures. Martensitic crystals contribute to many martensitic variants and are further classified into twinned and de-twinned martensite structures. Detwinned martensite leads to the generation of transformation strain while twinned martensite is associated with no transformation strain.

Predicting the structural integrity of SMA driven applications is of utmost importance to use their prolific properties at full potential. Many mathematical models were developed to enable a systematic understanding of the SMA behaviour. Fremond [2] proposed mathematical models on the thermomechanical evolution of SMAs at a macroscopic scale based on solid-solid phase transformations in terms of free energy and dissipation potential combining with the laws of thermodynamics. The model couples the balance equations to the partial differential inclusion of martensite and austenite phase variables, with temperature and displacements as unknown variables. Based on this model, Colli et al. [3] discussed the asymptotic stability for dynamical systems considering a one-dimensional case. This material model has received higher considerations pertaining to qualitative behaviour of systems, along with the Falk-Konopka model [4], in which the free energy of the crystal structure depends on the full-strain tensor and temperature. There are many other models (some are referred in [5],[6],[7],[8]) explaining the thermo-mechanical behaviour of SMAs in terms of martensitic deformations and their applications to finite element analysis. The most prominent model implemented in the finite element software is the Souza & Auricchio model [9], which is available in the commercial FEM software ANSYS. They introduced the model in its original isothermal setting by considering the energy and dissipation mechanisms with a tensor variable representing the inelastic strain. This allowed for direct extensions and additions to incorporate new features and phenomena.

One of the limitations to this model in ANSYS is that the SMA needs to be pre-stretched in order to develop pre-strain to utilize the contraction force exerted. It is relatively impractical to pre-stretch an SMA wire in the model, which has different profiles with curved bends and turns. Thus, the model is limited to using straight SMA wires, which is not reasonable for predicting more general applications.

Woodworth et al. [10], [11] proposed an SMA model incorporating the functional fatigue

(FF), transformation induced plasticity (TRIP) and pre-stretch in the SMA wires. The pre-stretch in the model allows modelling of the one-way SME for wires which were previously stretched and is the basis for the current work. Although, it is worth mentioning that the effect of having varied SMA profiles in a composite is not focused in here, rather the complexity and advantages of modelling different profiles is discussed, and the cross-section of the SMA profile is always a wire.

2 Material Models

2.1 Souza & Auricchio SMA Model

The Souza & Auricchio SMA model is a constitutive model developed to describe the behaviour of SMAs based on the thermodynamics of irreversible processes and the theory of small strains. This model takes the effects of both thermal and mechanical loading into account, and the material state is evaluated based on the corresponding energy and the dissipation mechanism. The model includes a set of constitutive equations relating state variables to stress and strain of the material. The material phase structure in this model is described by a tensor variable representing the inelastic strain [9]. A unique feature of the Souza & Auricchio SMA model is that it considers the evolution of transformation strain during deformation and is used to account for material's microstructural changes along with temperature.

The SME model implemented in the finite element software ANSYS is based on the 3-D thermomechanical model for stress-induced solid transformations [12], [13] and is as follows

$$\Psi(\varepsilon, T, \varepsilon_{tr}) = \frac{1}{2}(\varepsilon - \varepsilon_{tr}) : D : (\varepsilon - \varepsilon_{tr}) + \tau_M(T)||\varepsilon_{tr}|| + \frac{1}{2}h||\varepsilon_{tr}||^2 + I_{\varepsilon_{tr}}(\varepsilon_{tr}) \tag{1}$$

with D as the material elastic stiffness tensor, ε is total strain, ε_{tr} is transformation strain, $\tau_M(T)$ is a positively monotonic increasing function of temperature, T is temperature, h is a hardening parameter and $I_{\varepsilon_{tr}}(\varepsilon_{tr})$ is an indicator function to satisfy constraints on the transformation norm.

For the finite element analysis, the stress and consistent tangent stiffness matrix are updated with the help of a backward Euler integration scheme.

2.2 Woodworth & Kaliske SMA Model

The Woodworth & Kaliske model (WK) [10] is a phenomenological mathematical model used to describe the behaviour of SMAs under mechanical loading. This model was developed considering the FF and TRIP in the SMAs which can affect their long term behaviour. The model was extended further in [11] by considering the reorientation, which is dependent on the FF behaviour, a logarithmic evolution of saturation is considered and also a pre-stretch is accounted for SMA wires, which are used for actuation mechanisms. In this model, the mechanical behaviour of SMAs is governed by a set of internal state variables, which evolve with time as a function of applied strain and temperature. These internal state variables are usually a set of functions, which are driven by the history of deformation and temperature. The WK model also describes the stress-strain behaviour of SMAs under different loading conditions by a set of constitutive equations, which relate stress-strain and temperature to the internal state variables.

The constitutive equations include terms that describe the effect of deformation behaviour such as martensitic transformation. The total strain in the model is decomposed into

$$\varepsilon = \varepsilon_e + \varepsilon_\theta + \varepsilon_t + \varepsilon_r - \varepsilon_0, \tag{2}$$

where ε_e is the elastic strain, ε_θ is thermal strain, ε_t is transformation strain, ε_r is residual or transformation induced plasticity strain and ε_0 is initial strain due to pre-stretch. The initial pre-stretch in the manuscript is defined by

$$\varepsilon_0 = \varepsilon_L \chi_0^S N_{t,0}, \tag{3}$$

where ε_L is the maximum transformation strain; χ_0^S is the initial-oriented martensite volume fraction; $N_{t,0}$ is the pre-stretch direction.
The total Helmholtz free energy $\psi = \psi(\varepsilon, \theta, \chi^S, N_t, \chi_r, \chi_d, \varepsilon_r, \mathbf{B})$ is defined as

$$\psi = elastic + thermal + interaction + constraint + residual\, stress, \tag{4}$$

where

$$\textbf{elastic} \;\; = \tfrac{1}{2} K tr(\varepsilon)^2 + \mu ||e_e||^2 - 3\alpha K tr(\varepsilon)(\theta - \theta_0), \tag{5}$$

$$\textbf{thermal} \;\; = e_0^A - \eta_0^A \langle \theta - \theta_0 \rangle + c_v[(\theta - \theta_0) - \theta \ln(\tfrac{\theta}{\theta_0})] + \triangle\eta_t \chi^S \langle \theta - \theta_0 \rangle, \tag{6}$$

$$\textbf{interaction} \;\; = g^t(\chi^S, \chi_r, \chi_d) + \tfrac{1}{2}\mu_t ||\varepsilon_t||^2, \tag{7}$$

$$\textbf{constraint} \;\; = -\zeta^{S0}(\chi^S - \chi_r) - \zeta^{S1}(1 - \chi^S - \chi_d) + \tfrac{1}{2}\zeta^{cd}||N_t||^2, \tag{8}$$

$$\textbf{residual stress} \;\; = -\mathbf{B} : \varepsilon_t - \tfrac{1}{2}\varepsilon_L ||\mathbf{B}||^2, \tag{9}$$

where K is bulk modulus; μ is shear modulus; α is the coefficient of thermal expansion; e_e is deviatoric elstic strain; e_0^A is the reference internal energy; η_0^A is the reference internal entropy; c_v is the specific heat; $\triangle\eta_t$ is entropy difference during transformation; g^t is interaction energy due to hardening; μ_t is hardening modulus for transformation; $\zeta^{S0}, \zeta^{S1}, \zeta^{cd}$ are Lagrange multipliers and **B** is the residual stress. The constitutive equations and the discrete SMA model are elaborated in the original manuscript, and it is referred to [11].

3 Materials and Methods

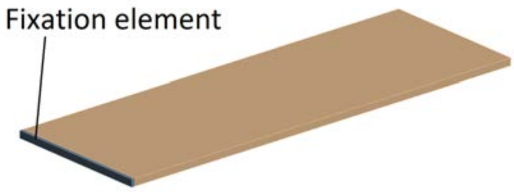
3.1 Simulation

In this section, the modelling of the SMA integrated fibre rubber composites is discussed. Two SMA integrated fibre rubber composite models are used and compared based on the Souza & Aurrichio model and the user-defined Woodworth & Kaliske model. This comparison is made to verify the user-defined model based on the deformations obtained in the IFRC structures. This verification is considered to be the reference for future models in the line of work with different SMA profile structures. It is worth noting that the functional property of superelasticity or pseudoelasticity is not focused in this work, as the SME precedes the importance in the functionality of the interactive fibre rubber composites. A polyethylene (PTFE) body is replaced here in place of the sheath around the SMA wire to reduce the contact of SMA with the elastomer.

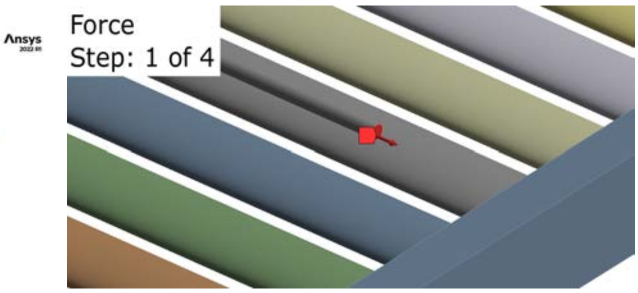
Souza & Auricchio Model

The Souza & Auricchio model implemented in ANSYS accommodates both superelastic and SMEs. The principle of the SME is that the SMA in twinned martensite state is changed to detwinned martensite state by applied load and unload. Upon heating, the SMA transforms into its parent phase austenite, and when cooled, again returns to the twinned martensite state without any noticeable structural change. This can also be termed as one-way SME. When the material is typically deformed into a temporary state at low temperature, it undergoes an elastic deformation and tries to return to its original shape, but is prevented from doing so by the applied load. Phase transformation occurs, when the material is heated above the martensitic transformation temperature and returns to its original shape by recovering the strain, which was induced during the elastic deformation.

In ANSYS, the force is applied in the first load step, followed by an elastic set back, contacting the SMA to a fixation element and increase in temperature in the SMA. The cooling and cyclic effects are not discussed in order to reduce the computational effort and are considered in future work. A fixation element is bonded to one end of the composite in order to fix the SMA after elongation. When heated, the SMA attempts to deform into austenite by pulling the fixation element and creating the bending deformation in the composite structure. The geometrical representation is shown in Figure 1.



(a) IFRC with fixation element at one end



(b) Image showing force applied on the SMA

Figure 1: IFRC simulation model

Woodworth & Kaliske Model

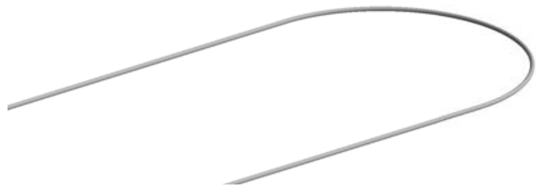


Figure 2: U-shape SMA profile

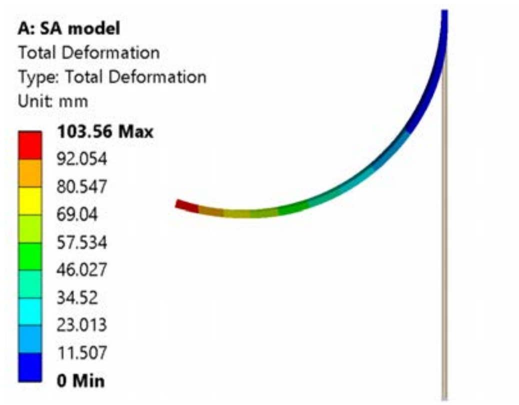
The Woodworth & Kaliske model is implemented in ANSYS Workbench as a user-defined-function. This model is developed to determine the behaviour of SMAs and is able to consider the FF and TRIP of the SMAs. Additionally, the pre-stretch Eq. (3) is included in the model to simplify the modelling of the one-way SME, which enables to assign a strain in the SMA before integrating into the composite model. This helps in modelling different profiles of the SMA and also reduces the number of load steps in the analysis, thus reducing the modelling effort. By modelling different profiles of SMA, the deformations based on various arrangements of SMA can be predicted in the composite, paving a way to obtain three-dimensional deformations in the composite. In this model, temperature is the only load step to be given to the SMA to obtain phase transformations. The fixation element is directly bonded from the beginning to the SMA and the composite. The modelling structure is the same for both the models and the modelling images are shown in Figure 1. Initially, straight wires are modelled to compare the results. A ”U” shape SMA profile (Figure 2) is also tested, and the simulation results are documented. One of the major considerations for both the models is that, weft yarns are neglected as they have negligible influence on the bending deformations, and only warp yarns are modelled.

4 Results

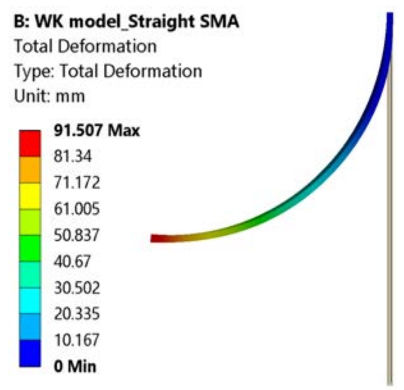
The simulation results are compared based on the total deformations of the composite, volume fractions of the SMA, deformation angle and the computation time. The IFRC simulation based on the Souza & Auricchio model showed a total bending deformation of 103.56 mm (Figure 3a), with a deformation angle of 108.7°. Whereas, the Woodworth & Kaliske model showed a maximum deformation of 91.5 mm (Figure 3b), with a deformation angle of 91.7°. Both the models had the same boundary conditions and mesh considerations. Also, the two models did not converge on the whole, but the martensite to austenite transformation was complete in Souza & Aurrichio model (Figure 3c), whereas, the solution stopped with an incomplete martensite to austenite transformation in the Woodworth & Kaliske model (Figure 3d). Although, the same properties were applied to SMA in both the models, the Souza & Auricchio model was able to solve better for the unsymmetrical conditions. However, the Woodworth & Kaliske model showed full convergence for the ”U” profile shape of the SMA. A maximum deformation of 95.8 mm (Figure 4a) with the deformation angle of 104.2° and a complete transformation from martensite to austenite was observed (Figure 4b). Upon observations for the straight SMA profiles, there are few contact adversities between the fixation element to the other contact bodies, resulting in penetration and small sliding between the faces. These discrepancies might have led to the high force convergence values, making the computation more difficult. The results are tabulated according to the models and are shown in Table 1.

Table 1: Result comparisons for Souza & Aurricchio (SA), Woodworth & Kaliske (WK) models

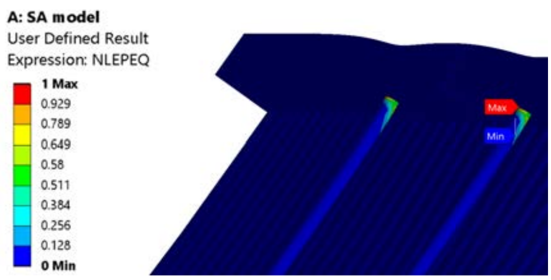
Model	SMA profile	Total deformation	Deformation angle	Computation time
SA	straight SMAs	103.56 mm	108.7°	$\approx 39h$
WK	straight SMAs	91.5 mm	91.7°	$\approx 14h$
WK	U SMA	95.8 mm	104.2°	$\approx 40h$



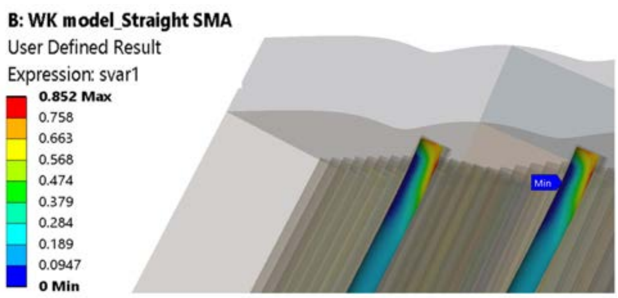
(a) Total deformation in the Souza & Auricchio model for straight SMAs



(b) Total deformation in the Woodworth & Kaliske model for straight SMAs

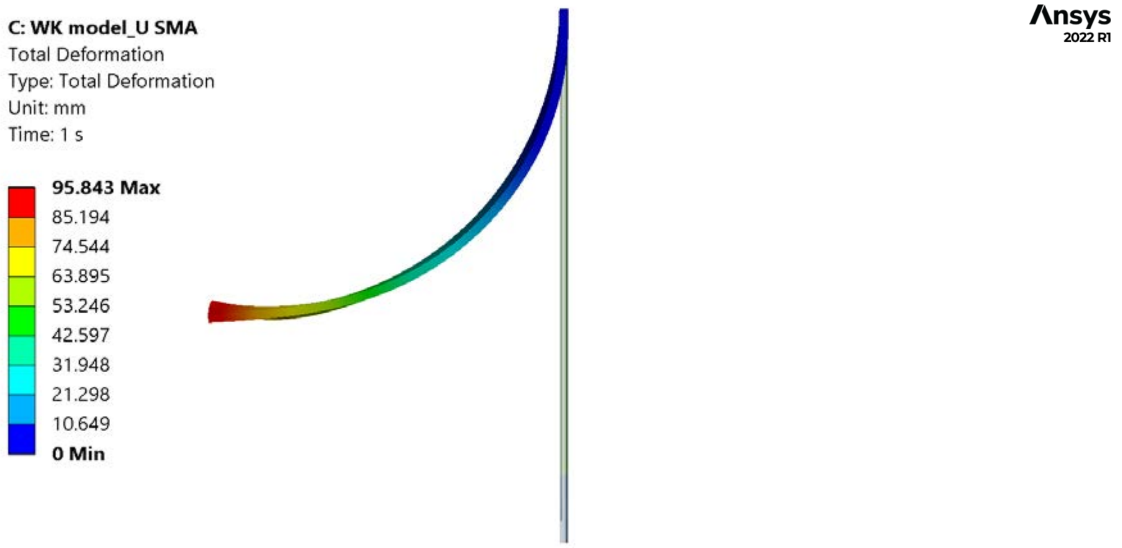


(c) Volume fraction - martensite to austenite (descending order) - Souza & Auricchio model

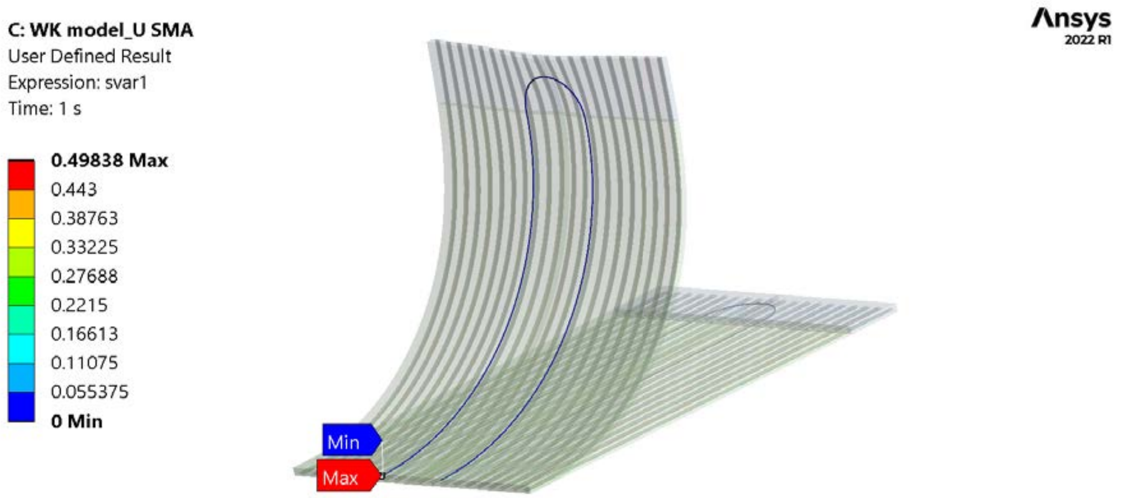


(d) Volume fraction - martensite to austenite (descending order) - Woodworth & Kaliske model

Figure 3: Total deformations and volume fractions in both models with straight SMAs



(a) Total deformation in the Woodworth & Kaliske model for U shape SMA



(b) Volume fraction - martensite to austenite (descending order) - Woodworth & Kaliske model

Figure 4: Total deformation and volume fraction in the Woodworth & Kaliske model for U shape SMA

5 Conclusion

A comparison of an existing material model for straight SMA wires in ANSYS with that of the user-defined developed model was performed in order to verify the latter. The results have shown a comparable difference based on the deformations obtained for the two models with the former producing higher deformations leading to a 10% difference between the two models. This difference is observed due to the fact that the wire was not transformed completely to austenite for the Woodworth & Kaliske model. It is also observed that the fixing of SMA at the free end of the structure with the fixation element could reduce the total amount of force transmitted on to the composite structure due to contact penetration and small sliding. An alternative is to tie the nodes at the edge of the free end of the SMA to the inner edge of the PTFE tube. Experience has shown that, due to large bending deformations, the same problem related to sliding pertains, thus decreasing the efficiency of deformation potential in the composite. In the other case with "U" SMA profile, a full convergence is observed with the Woodworth & Kaliske model, with comparable results with the straight SMAs. This can be termed as a successful implementation of the Woodworth & Kaliske SMA model, with a defined prestretch value to model the different SMA profiles. However, care should be taken as the irregular shapes of SMA in the composite may lead to difficulties in meshing the composite structure, thus increasing the computation time. Overall, it can be concluded that the Woodworth & Kaliske SMA model is verified with the Souza & Auricchio model and is potentially efficient to model and simulate various SMA profiles. In the future work, both the models are validated based on the activation experiments of the IFRC.

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