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Optimization of Residual Stresses in MMC's Through the Variation of Interfacial Layer Architectures and Processing Parameters

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PREFACE

This report summarizes the work performed under the contract **NAS3-26571**. The objective of this work was the development of efficient, user-friendly computer codes for optimizing fabrication-induced residual stresses in metal matrix composites through the use of homogeneous and heterogeneous interfacial layer architectures and processing parameter variation. To satisfy this objective, three major computer codes have been developed and delivered to the NASA-Lewis Research Center, namely **MCCM**, **OPTCOMP**, and **OPTCOMP2**. **MCCM** is a general research-oriented code for investigating the effects of microstructural details, such as layered morphology of SCS-6 SiC fibers and multiple homogeneous interfacial layers, on the inelastic response of unidirectional metal matrix composites under axisymmetric thermomechanical loading. **OPTCOMP** and **OPTCOMP2** combine the major analysis module resident in **MCCM** with a commercially-available optimization algorithm and are driven by user-friendly interfaces which facilitate input data construction and program execution. **OPTCOMP** enables the user to identify those dimensions, geometric arrangements and thermoelastoplastic properties of homogeneous interfacial layers that minimize thermal residual stresses for the specified set of constraints. **OPTCOMP2** provides additional flexibility in the residual stress optimization through variation of the processing parameters (time, temperature, external pressure and axial load) as well as the microstructure of the interfacial region which is treated as a heterogeneous two-phase composite. Overviews of the capabilities of these codes are provided together with a summary of results that address the effects of various microstructural details of the fiber, interfacial layers and matrix region on the optimization of fabrication-induced residual stresses in metal matrix composites.

Notice: The **MCCM**, **OPTCOMP**, and **OPTCOMP2** codes are being made available strictly as research tools. Neither the authors of the codes nor NASA-Lewis Research Center assume liability for application of the codes beyond research needs. Any questions or related items concerning these computer codes can be directed to either Professor Marek-Jerzy Pindera at the Civil Engineering & Applied Mechanics Department, University of Virginia, Charlottesville, VA 22903 (Tel: 804-924-1040, e-mail: marek@virginia.edu), Dr. Robert S. Salzar, an NRC Fellow, at the Structural Fatigue Branch, NASA-Lewis Research Center, Cleveland, OH 44135 (Tel: 216-433-3262), or Dr. Todd O. Williams at the Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545 (Tel: 505-665-9190).

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1.0 INTRODUCTION

This final report summarizes the work funded under the contract **NAS3-26571**. The objective of this work was the development of efficient, computer-based algorithms for optimizing fabrication-induced residual thermal stresses in metal matrix composites (MMCs). The development of these algorithms was motivated by the need to reduce the high residual stresses, and thus the potential for cracking, in advanced MMCs such as SiC/Ti that arise due to large mismatch in the thermal expansion coefficients of the fiber and matrix phases, lack of matrix ductility, and the high processing temperature [1]. The approach used in developing the residual stress optimization algorithms was based on the introduction of multiple, inelastic layers at the fiber/matrix interface with either homogeneous or heterogeneous microstructures, and subsequent tailoring of the geometry, thermal and elastoplastic properties of the interfacial region in a way that "smooths out" or reduces the apparent thermal expansion mismatch between the fiber and matrix phases. This is a generalization of the compliant/compensating layer concept proposed by Arnold et al. [2,3,4] who have established rules for the optimum design of a single, homogeneous interfacial layer in terms of the layer's dimensions and thermoelastoplastic properties using extensive finite-element calculations.

Three major computer codes have been developed and delivered to satisfy the objectives of this contract, namely **MCCM**, **OPTCOMP**, and **OPTCOMP2**. These computer codes facilitate the identification of optimum fiber/matrix interfacial region designs through the marriage of an efficient analytical approach for the residual stress field determination in unidirectional MMCs and an optimization algorithm, both residing within a user-friendly, menu-driven interface. This design-oriented interface provides an automated data construction and subsequent program execution procedure for identifying optimum fiber/matrix interfacial region architectures, as well as processing histories, that will minimize (or maximize) the desired stress or strain components (or their combinations). Detailed description of these computer codes, instructions for their use and illustrative examples have been provided in the corresponding user's guides [5,6,7]. Herein, we provide a brief overview of the capabilities of these codes together with a summary of results generated using these codes and the appropriate references.

MCCM is a general research-oriented code for investigating the effect of microstructural details, such as the layered morphology of SCS-6 SiC fibers and multiple interfacial layers, on the inelastic response of unidirectional MMCs under axisymmetric thermomechanical loading. It was developed primarily as a research tool with several built-in inelastic constitutive models for the individual constituent response, and therefore does not have a menu-driven interface for data file construction and subsequent program execution. Both **OPCOMP** and **OPTCOMP2** combine the major analysis module resident in **MCCM** with the commercially-available

optimization package **DOT**¹ [8], and are driven by user-friendly interfaces which facilitate input data construction and program execution. The computer program **OPTCOMP** enables the user to identify those dimensions, geometric arrangements and thermoelastoplastic properties of the interfacial layers that minimize or maximize stresses, strains, or a user-constructed function based on these field quantities, induced by thermomechanical loading (including processing) for the specified set of constraints. The interfacial layers are treated as homogeneous, and the inelastic response of the interfacial layers and the matrix is modeled using the classical incremental plasticity theory. The computer program **OPTCOMP2** provides additional flexibility in the stress, strain or a user-constructed function optimization through variation of the processing parameters (time, temperature, external pressure and axial load) as well as the microstructure of the interfacial region which is treated as a two-phase composite. The inelastic response of the constituent phases can be modeled using either the classical incremental plasticity theory, Bodner-Partom viscoplasticity theory or a user-defined, rate-dependent inelastic model, thereby allowing either time-independent or time-dependent processing history optimization. Despite apparent similarities between **OPTCOMP** and **OPTCOMP2**, the differences in the data file structure necessitated by the different optimization features made it impractical to combine these two programs into a single optimization package containing all the features of both.

Two additional programs have also been developed with the same analysis capabilities as **OPTCOMP** and **OPTCOMP2** but without the optimization capability. They are called **RTSHELL** and **RTSHELL2** and are subsets of **OPTCOMP** and **OPTCOMP2**, respectively, with the corresponding menu-driven, user-friendly interfaces modified to exclude the optimization option. These programs facilitate efficient characterization and evaluation of different unidirectional MMCs subjected to combined axisymmetric thermomechanical loading in the presence of different fiber and interfacial layer microstructures.

¹License for the **DOT** source code must be purchased separately from VMA Engineering (Vanderplaats, Miura & Associates, Inc.), 5960 Mandarin Ave., Suite F, Goleta, CA 93117. Phone: (805) 967-0058.

2.0 ANALYTICAL FOUNDATIONS

The approach employed in each computer program for determining the response of uni-directional metal matrix composites subjected to the specified loading (including residual stress calculation) is based on a micromechanics multiple concentric cylinder model, Figure 1, and utilizes a novel analytical technique for the solution of axisymmetric, elastoplastic boundary-value problems developed by Pindera et al. [9,10]. This solution technique combines elements of the **local/global stiffness matrix formulation** originally developed for efficient analysis of elastic multilayered media (Bufler [11], Pindera [12]), and Mendelson's method of successive elastic solutions for elastoplastic boundary-value problems [13]. The response of heterogeneous interfacial layers is calculated using Aboudi's method of cells micromechanics model for discontinuously-reinforced composites [14]. The optimization algorithm is based on the **method of feasible directions** available in the commercial package **DOT**. A brief outline of the analytical solution and the optimization algorithm employed in the above computer codes is briefly sketched out below to facilitate clear understanding of the computer code capabilities described in the following sections. A more detailed presentation can be found in the cited references.

2.1 Analytical Model

The multiple concentric cylinder model shown in Figure 1 consists of a fiber, an interfacial layer region and a surrounding matrix region. The fiber and interface regions may exhibit layered morphologies, with the individual sublayers possessing either homogeneous, Figure 1a, or heterogeneous, Figure 1b, microstructures. The matrix region also admits a heterogeneous morphology, Figure 1b. The heterogeneous regions are two-phase regions, consisting of an inclusion phase embedded in a matrix phase. The inclusion phase forms a triply-periodic array in the $x-r-\theta$ coordinate system centered at the origin of the concentric cylinder, and is assumed to be sufficiently small relative to a heterogeneous layer's thickness so that the layer's macroscopic response can be calculated using a micromechanics model. The shape of the inclusion phase has a square cross section in the $r-\theta$ plane and an arbitrary length along the x -axis. The fiber, interface and matrix layers exhibit temperature-dependent elastic or inelastic behavior. The elastic layers may be (transversely) isotropic, or (radially or circumferentially) orthotropic, while the inelastic layers are initially isotropic and are modeled using either the incremental plasticity theory with isotropic hardening, Bodner-Partom or Robinson (available only in **MCCM**) unified viscoplasticity theory [5], or a user-defined rate-dependent model. To simulate actual processing conditions, the multiple concentric cylinder is subjected to an axisymmetric thermomechanical loading, consisting of a spatially uniform temperature change, external pressure and axial stress or strain, applied simultaneously or individually in a monotonic or cyclic manner.

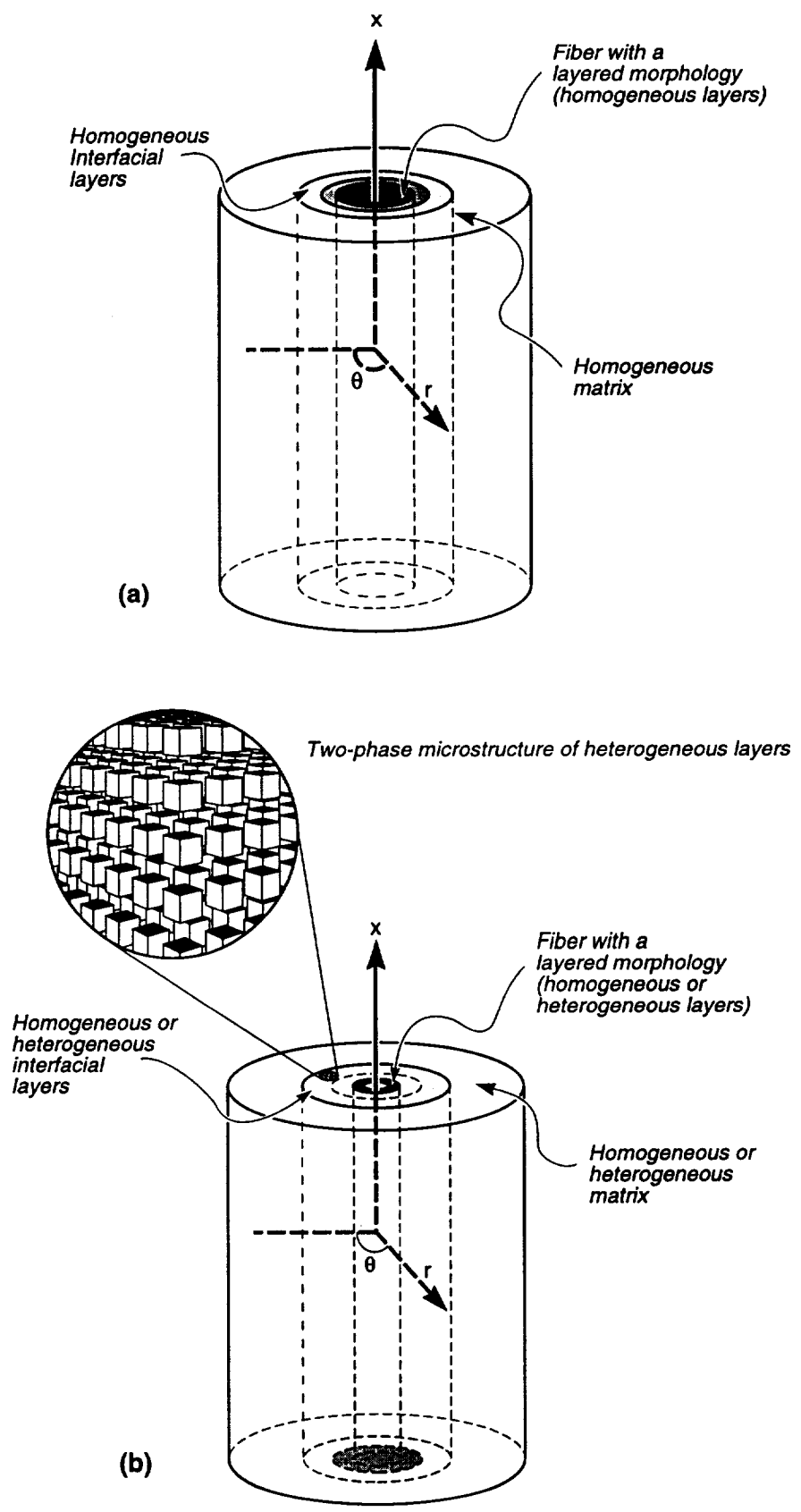


Figure 1. Multiple concentric cylinder model with homogeneous and heterogeneous microstructures.

The solution to the multiple concentric cylinder assemblage subjected to the specified loading is obtained using the displacement formulation under the assumption of generalized plane strain. For the prescribed axisymmetric loading, the longitudinal, tangential and radial displacement components u , v and w , referred to the cylindrical coordinate system x - r - θ have the form: $u = u(x) = \epsilon_0 x$; $v = 0$; and $w = w(r)$, where ϵ_0 is the uniform longitudinal strain for all layers. The solution for the radial displacement $w(r)$ in each layer is obtained from the single surviving Navier's equation using standard techniques. For orthotropic, elastic layers we get:

$$w(r) = A_1 r^\lambda + \frac{A_2}{r^{-\lambda}} + \frac{(C_{\theta x} - C_{rx})}{(C_{rr} - C_{\theta\theta})} r \epsilon_0 + \sum_{i=x,\theta,r} \frac{(C_{ri} - C_{\theta i})}{(C_{rr} - C_{\theta\theta})} \alpha_{ii} r (T - T_0) \quad (1)$$

where $\lambda = (C_{\theta\theta}/C_{rr})^{1/2}$ and $r_{k-1} \leq r \leq r_k$ (where r_{k-1} and r_k are the inner and outer radii of the k th layer, respectively). For isotropic, inelastic layers we get:

$$w(r) = A_1 r + \frac{A_2}{r} + \frac{1}{2r} \int_{r_{k-1}}^r \sum_{i=x,\theta,r} \frac{(C_{ri} + C_{\theta i})}{C_{rr}} \epsilon_{ii}^{in}(r') r' dr' + \frac{r}{2} \int_{r_{k-1}}^r \sum_{i=x,\theta,r} \frac{(C_{ri} - C_{\theta i})}{C_{rr}} \epsilon_{ii}^{in}(r') \frac{dr'}{r'} \quad (2)$$

where C_{ij} 's ($i, j = x, r, \theta$) are the elastic stiffness elements, and the distribution of the inelastic strains, $\epsilon_{ii}^{in}(r)$, appearing in the solution for the radial displacement in an isotropic, inelastic layer, is assumed to be known at the beginning of each thermal load increment.

Rather than developing a system of equations for the unknown coefficients A_1 , A_2 and the uniform axial strain ϵ_0 appearing in the solution for each layer from the boundary conditions, interfacial traction and displacement continuity conditions, and the longitudinal force equilibrium condition, the problem is reformulated in terms of the interfacial radial displacements as the basic unknowns using the concept of a **local stiffness matrix**. This reformulation provides an efficient and automated solution procedure for arbitrarily layered concentric cylinder configurations in the presence of inelastic effects, facilitating investigation of various microstructural details on the response of MMCs (cf. Pindera et al. [9,10]). The local stiffness matrix relates the interfacial tractions at the inner and outer radii of the k th layer to the corresponding interfacial radial displacements. To construct the local stiffness matrix for the k th layer, the coefficients A_1^k and A_2^k are first expressed in terms of the layer's interfacial radial displacements, and then substituted into the equation for the radial stress component given in terms of the known radial displacement field. The final step entails an evaluation of the radial stress in the k th layer at the inner and outer radii in order to generate the radial tractions at those locations.

The form of the local stiffness matrix equation for the k th layer in the state of generalized plane strain and in the presence of thermal and inelastic effects is given in equation (3) below,

$$\begin{Bmatrix} -\sigma_{rr}^- \\ \sigma_{rr}^+ \end{Bmatrix}_k = \begin{bmatrix} k_{11} & k_{12} \\ k_{21} & k_{22} \end{bmatrix}^k \begin{Bmatrix} w^- \\ w^+ \end{Bmatrix}_k + \begin{Bmatrix} k_{13} \\ k_{23} \end{Bmatrix}^k \epsilon_0 + \begin{Bmatrix} f_1 \\ f_2 \end{Bmatrix}^k \Delta T + \begin{Bmatrix} g_1 \\ g_2 \end{Bmatrix}^k \quad (3)$$

where the superscripts "-" and "+" designate quantities at the layer's inner and the outer radii. The elements $k_{11}^k, \dots, k_{23}^k$ are functions of the geometry and elastic material properties of the k th layer (which may vary with temperature). The thermal terms f_1^k and f_2^k are functions of the thermal expansion coefficients, and the plastic terms g_1^k and g_2^k are given in terms of the integrals of the plastic strain distribution in the k th layer. Expressions for the above quantities have been reported by Pindera et al. [9,10] for transversely isotropic and orthotropic, elastic layers, and isotropic, inelastic layers. When the individual layers are treated as homogeneous, as is the case in the computer programs **MCCM** and **OPTCOMP**, the elastic, thermal and plastic properties of each layer necessary to calculate the various terms in equation (3) are provided by the user. When the individual layers are treated as heterogeneous, which is an option in the computer program **OPTCOMP2**, the various terms in equation (3) are calculated using the three-dimensional version of the method of cells micromechanics model once the user specifies the constituent properties and microstructure of the layers.

The interfacial displacements are determined by constructing a system of equations that satisfies the continuity of tractions and displacements across each interface within the concentric cylinder assemblage, the external boundary conditions and the longitudinal force equilibrium. This system of equations is represented in terms of a global stiffness matrix which is assembled by superposing the local stiffness matrices of each layer given in equation (3) along the main diagonal in the manner shown below in equation (4) when the axial loading is specified in terms of the external axial load L_x ,

$$\begin{bmatrix} k_{22}^1 + k_{11}^2 & k_{12}^2 & 0 & \cdot & k_{23}^1 + k_{13}^2 \\ k_{21}^2 & k_{22}^2 + k_{11}^3 & \cdot & \cdot & \cdot \\ 0 & k_{21}^3 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & k_{22}^n & k_{23}^n \\ \phi_{22}^1 + \phi_{11}^2 & \cdot & \cdot & \phi_{22}^n & \sum \psi_k \end{bmatrix} \begin{Bmatrix} w_1 \\ w_2 \\ \cdot \\ w_n \\ \epsilon_0 \end{Bmatrix} = \begin{Bmatrix} 0 \\ \cdot \\ \cdot \\ T_r \\ L_x \end{Bmatrix} - \begin{Bmatrix} f_2^1 + f_1^2 \\ \cdot \\ \cdot \\ f_2^n \\ \sum \Omega_k \end{Bmatrix} \Delta T - \begin{Bmatrix} g_2^1 + g_1^2 \\ \cdot \\ \cdot \\ g_2^n \\ \sum \Pi_k \end{Bmatrix} \quad (4)$$

where w_k is the common interfacial displacement between the k th and $k+1$ layers. The first n equations are obtained by enforcing the continuity of interfacial tractions and displacements (starting from the core denoted by the superscript 1 and progressing outward), and the external boundary condition on the radial traction T_r . The $n+1$ equation is obtained by imposing the longitudinal equilibrium condition. Explicit expressions for the elements of the last row, ϕ_{11}^k , ϕ_{22}^k , ψ_k , Ω_k , and Π_k have also been provided by Pindera et al. [9,10]. As in the case of the elements g_1^k and g_2^k , Π_k is also given in terms of the integrals of the inelastic strain distribution. A similar system of equations is obtained when the axial loading is specified in terms of the uniform axial strain ϵ_0 .

The elements g_1^k , g_2^k and Π_k of the inelastic force vector on the right hand side of equation (4) depend implicitly on the interfacial displacements. Thus an incremental solution technique is employed within an iterative framework in solving for the interfacial displacements. This is carried out using the iterative scheme outlined by Mendelson [13] as follows. For the given thermomechanical load increment, the current inelastic strain at any point in each layer is expressed in terms of the strain from the preceding loading state plus an increment that results from the imposed load increment.

$$\epsilon_{ij}^{in}(r) |_{\text{current}} = \epsilon_{ij}^{in}(r) |_{\text{previous}} + d\epsilon_{ij}^{in}(r) \quad (5)$$

Calculation of the current inelastic strains at a sufficiently large number of radial locations in each layer allows accurate determination of the integrals of the plastic strain distributions necessary to determine the elements g_1^k , g_2^k and Π_k of the inelastic force vector in equation (4). Updated values of the interfacial displacements are then obtained from these equations. With a knowledge of the current interfacial displacements and the axial strain ϵ_{xx}^0 , solutions for the radial displacement $w_k(r)$ at any point within the given layer are obtained, from which radial and tangential total strains, and their corresponding stresses, are calculated. These are then used to obtain new approximations for the inelastic strain increments using the chosen constitutive model. The iterative process is terminated when the differences between two successive sets of inelastic strain increments are less than some prescribed value. Then, the next load increment is applied and the iterative solution procedure repeated. As discussed by Williams and Pindera [15], the above solution procedure is very robust and its convergence is quite fast. Its accuracy has been verified using finite-element analysis by Pindera et al. [16,17] for a number of different configurations comprised of materials with a wide range of thermoelastoplastic properties.

The converged stress distributions in the individual regions of the concentric cylinder assemblage are then used to determine the user-specified objective function that is subsequently employed in the optimization procedure executed by DOT described next.

2.2 Optimization Scheme

The solution procedure for the inelastic response of the multiple concentric cylinder assemblage described in the preceding section provides a mechanism for extracting the magnitudes of residual stresses in the matrix phase for the prescribed values of the interfacial layers' geometric and material parameters. In order to efficiently select those geometries and properties that yield a desirable or optimal residual stress pattern, it is necessary to incorporate the outlined solution procedure into an optimization algorithm. This is readily accomplished since closed-form expressions, equation (4), are available that describe the response of the multiple concentric cylinder to the specified loading in terms of the assemblage's geometric parameters and the constituent materials' properties. By varying these parameters (including the loading parameters) or *design variables* in an optimization scheme, optimal interfacial layer properties, microstructures and dimensions, as well as processing histories can be determined that minimize or maximize the chosen objective function. The optimization algorithm to be described in this section, together with the analysis algorithm described earlier, constitute two of the three major modules in the computational packages **OPTCOMP** and **OPTCOMP2** developed under the terms of the contract.

The optimization problem is, in general, formulated as follows,

Minimize or maximize the user-defined objective function $F(\mathbf{X})$, where \mathbf{X} is a set of design variables, subject to the constraints $g_j(\mathbf{X}) \leq 0$ where $j = 1, \dots, M$, with the following side constraints, $X_i^l \leq X_i \leq X_i^u$ where $i = 1, \dots, N$, with u and l denoting upper and lower limits for each design variable X_i .

The objective function $F(\mathbf{X})$ can be selected from a number of objective functions available in **OPTCOMP** and **OPTCOMP2** that characterize an optimum "design" of the interfacial layers. These objective functions provide a rational measure of the residual stress pattern in the model, such as the maximum value of the hoop stress at the fiber/matrix interface. A user-defined objective function option is also available. The design variables employed in **OPTCOMP** are those parameters that describe the interfacial layers' geometry and properties, namely the layer thickness, coefficient of thermal expansion, elastic modulus, yield stress and hardening modulus. The design variables employed in **OPTCOMP2** are those parameters that either describe the microstructure of the interfacial region, namely the inclusion volume content, or the processing history, namely temperature, pressure, average axial stress or uniform axial strain, and time. A number of constraint functions $g_j(\mathbf{X})$ which can be imposed on the residual stress pattern are available, such as a maximum allowable axial stress at the fiber/matrix

interface. A user-defined constraint function option is also available. Finally, the side constraints (i.e., lower and upper bounds) that can be imposed on the design variables are commensurate with the physical problem at hand, such as maximum interfacial layer thickness.

The optimization algorithm incorporated in the software package **DOT** is based on the method of feasible directions, Vanderplaats [18]. This method, briefly outlined here, essentially searches the n-dimensional design variable space in an iterative manner along the constraint boundaries for the "global optimum". Once an initial set of design variables, \mathbf{X}_0 is specified by the user, the search procedure is carried out according to the following algorithm,

$$\mathbf{X}^q = \mathbf{X}^{q-1} + \alpha^* \mathbf{S}^q \quad (6)$$

where q is the iteration number, \mathbf{X}^q is the vector of design variables at the q -th iteration, \mathbf{S}^q is the current direction in the n-dimensional design variable space, and α^* is the distance travelled along the search direction specified by \mathbf{S} . In this method, the **usable sector** is defined as any direction \mathbf{S} in the design space that improves the objective function. This is defined mathematically in terms of the inequality,

$$\nabla F(\mathbf{X}_0) \cdot \mathbf{S} \leq 0 \quad (7)$$

where $\nabla F(\mathbf{X}_0)$ is the gradient of the objective function at the given design point. The **feasible sector** is defined in any direction \mathbf{S} in the design space which does not violate the design constraints. This is defined mathematically by the following inequality,

$$\nabla g_1(\mathbf{X}_0) \cdot \mathbf{S} < 0 \quad (8)$$

where $\nabla g_1(\mathbf{X}_0)$ is the gradient of the constraint function at the present design point. The intersection of the two sectors is called **usable-feasible sector**. These sectors are indicated in Figure 2. Any search direction \mathbf{S} in this sector will improve the design, and at the same time, will not violate any of the design constraints. Once a suitable search direction is found, a one-dimensional search is performed to locate the distance α^* to the minimum (or maximum) in that direction. The newly located design is then defined as the next design point. This process is repeated at each design point until the convergence criteria is reached (in this case the Kuhn-Tucker conditions).

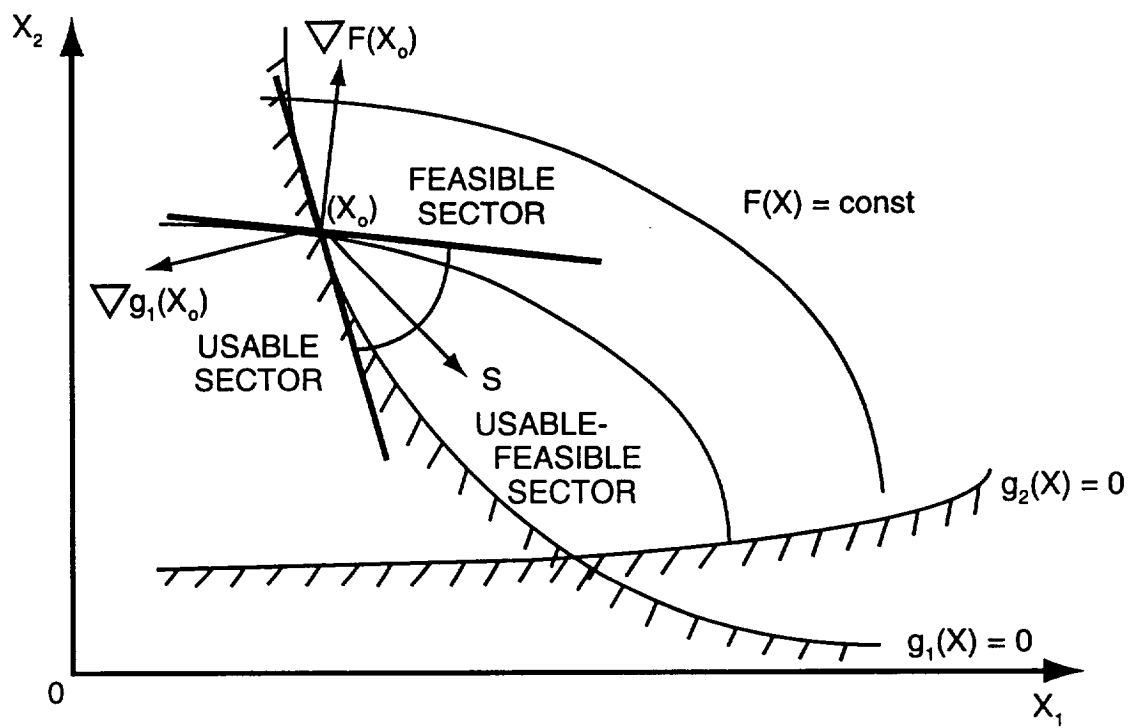


Figure 2. Schematic illustrating the method of feasible directions for two design variables (after Vanderplaats [18]).

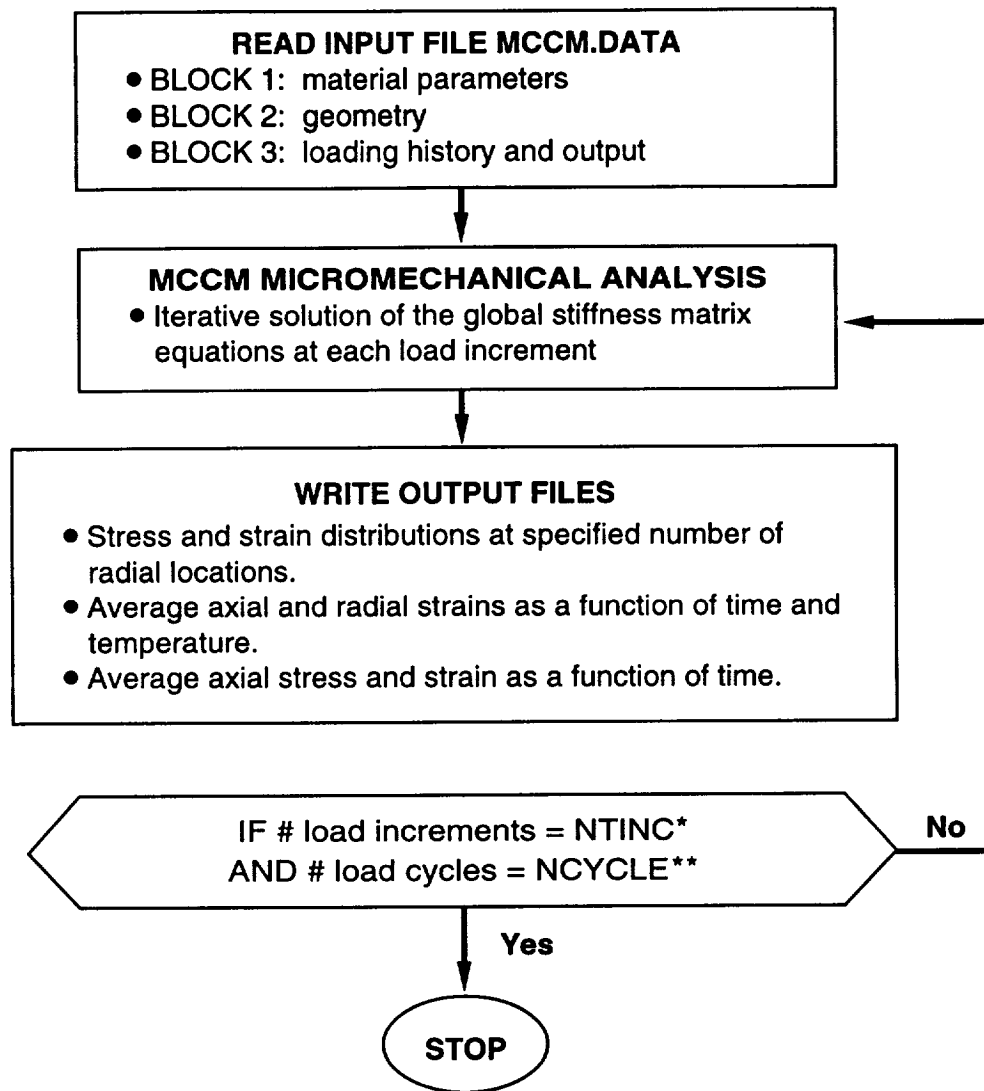
3.0 DELIVERABLES

Brief descriptions of the structure, features and capabilities of the computer codes **MCCM**, **OPTCOMP/RTSHELL** and **OPTCOMP2/RTSHELL2** delivered to the NASA-Lewis Research Center in fulfillment of the terms of the contract **NAS3-26571** are provided in the following sections. More detailed information about the use of these computer codes, illustrated by step-by-step examples, is provided in the corresponding user guides [5,6,7].

3.1 MCCM (MULTIPLE CONCENTRIC CYLINDER MODEL)

MCCM is an executable file developed to investigate the effect of microstructural details on the inelastic response of unidirectional metal matrix composites under axisymmetric thermomechanical loading. The microstructural details include the layered morphology of such ceramic fibers as the SCS-6 SiC fiber used in titanium matrix composites (DiCarlo [19], Lerch et al. [20], Wawner [21], Ning and Pirouz [22]), as well as the presence of interfacial layers between the fiber and the matrix. The interfacial layers often arise naturally due to chemical reactions between the fiber and the matrix (Wawner and Gundel [23]). Alternatively, they can be introduced deliberately in order to minimize residual fabrication stresses in advanced metal matrix composites such as SiC/Ti (Arnold et al. [2,3,4]) which can be sufficiently large so as to produce different types of micro-cracks in the fiber or at the fiber/matrix interface (Larsen et al. [1], Brindley et al. [24,25], McKay et al. [26]). By introducing compliant or compensating layers (those with a higher thermal expansion coefficient than the matrix) between the fiber and matrix phases, Arnold and co-workers have demonstrated that the circumferential stress at the fiber/matrix interface can be reduced at the expense of increasing the axial stress, thereby decreasing or eliminating the possibility of radial microcracking.

The flow chart outlining the logical organization of the computer code is given in Figure 3. **MCCM** may be employed to generate the effective behavior of a unidirectional composite under arbitrary axisymmetric thermomechanical loading in terms of macroscopic stresses and strains from which the appropriate instantaneous properties can be calculated. In addition, pointwise distributions of the stress, strain, and displacements fields within each layer of the multiple concentric cylinder assemblage can be determined. Since the solution methodology employed to generate these quantities is analytical rather than numerical (e.g., finite-element or finite-difference schemes), as outlined in Section 2.1, there is no need to generate meshes or grids every time the geometrical details or morphology of the fiber or the interfacial region are changed. Different configurations are efficiently handled by changing a few lines in the input file of **MCCM** that can be executed on a personal computer/work station. This feature makes the computer program attractive for use by a material scientist, designer and/or analyst alike. The



*NTINC = total number of load increments
 **NCYCLE = total number of load cycles

Figure 3. Flow chart of the computer code **MCCM**.

construction of an input data file, while not fully automated through a menu-driven interface as in **OPTCOMP** and **OPTCOMP2**, is nevertheless simple. As illustrated in Figure 3, it consists of three distinct blocks. Block 1 is designated for the specification of the constituent properties of the individual layers within the concentric cylinder. Each of the layers is homogeneous and can be either elastic or inelastic. The elastic layers may be isotropic, transversely isotropic, or orthotropic (radially or circumferentially), while the inelastic layers are taken as initially

isotropic and are modeled using either time-independent incremental plasticity with the Prandtl-Reuss flow rule and isotropic hardening or one of two unified viscoplasticity theories. These include the Bodner-Partom and the Robinson viscoplasticity models. In addition, a user-defined inelastic constitutive model is available. Temperature-dependence of the material parameters is incorporated in all the constitutive models. Block 2 is designated for the specification of the concentric cylinder configuration and geometry (which can be arbitrary). Finally, Block 3 is designated for the specification of the loading history, which can involve the simultaneous application of temperature, average axial stress or uniform axial strain, and external pressure (or any combination of these) in a monotonic or cyclic manner. The capabilities and options available within MCCM are summarized in Table I.

Table I. Capabilities available within MCCM.

Type	Description
Multiple concentric cylinder geometry	Fiber: layered morphology (homogeneous layers) Interfacial region: layered morphology (homogeneous layers) Matrix: layered morphology (homogeneous layers)
Constitutive models	Elastic: isotropic, transversely isotropic, orthotropic materials Plastic: incremental plasticity (Prandtl-Reuss relations) with isotropic hardening Viscoplastic: Bodner-Partom (with isotropic hardening) and Robinson (with kinematic hardening) unified theories for isotropic materials Inelastic: user-defined, rate-dependent inelastic relations for isotropic materials
Integration schemes	Spatial: successive elastic solutions (incremental plasticity) Time: forward Euler integration technique (viscoplastic models)
Loading capabilities	Thermal: monotonic or cyclic, spatially uniform ΔT Mechanical: monotonic or cyclic external pressure + axial tension or compression Combined: monotonic or cyclic ΔT + external pressure + axial tension or compression
Predictive capabilities	Effective thermal expansion response Effective inelastic stress-strain response Internal stress and strain distributions within each layer

3.2 OPTCOMP/RTSHELL

OPTCOMP is an executable file developed to identify those optimum architectures and properties of the interfacial region in unidirectional metal matrix composites that minimize (or maximize) stresses, strains, or a user-constructed function based on these quantities, induced by axisymmetric thermomechanical loading (including processing). As indicated in Section 2.2, this is accomplished through variation of the interfacial layers' thickness, coefficient of thermal expansion, elastic modulus, yield stress, and hardening modulus.

In essence, **OPTCOMP** is based on three modules, namely: a user interface which provides a menu-driven, user-friendly environment for defining the optimization problem and executing the program; an analysis code which, in addition to generating the elastoplastic solution to the concentric cylinder assemblage subjected to specified loading, also controls the execution of the optimization procedure; and the optimization package **DOT**. The data provided during the problem definition stage through the user interface is subsequently used to generate a solution to the defined inelastic boundary-value problem which, in turn, is used as input in the optimization algorithm. The capabilities of the analysis module employed in **OPTCOMP** are very similar to **MCCM**. The exception is the number of available inelastic constitutive theories for the response of the individual regions within the multiple concentric assemblage, which is limited to incremental plasticity, in contrast with **MCCM** which also includes two unified viscoplasticity theories and a user-defined model. Table II summarizes the features and capabilities of **OPTCOMP**.

The program is executed by typing the command *optcomp* at the unix prompt. This initiates the menu-driven, user-friendly interface, providing the user with the main menu comprised of the following four options: create new data file; run existing data file; enter new materials into databank; and exit shell. The choice of a given option initiates the sequence of events outlined in Figure 4. Specifically, the choice of the first option allows the user to create a new data file that defines a given optimization problem. Selection of this option initiates a sequence of input commands that define the given optimization problem in terms of: the concentric cylinder geometry and material properties corresponding to each region (fiber, interfacial layer(s) and surrounding matrix); the choice of design variables, objective function and associated constraints; and the applied loading. The sequence of input commands is logically divided into the three distinct data input blocks that describe the geometry, optimization parameters and loading for a given problem.

After the data file that defines the optimization problem has been created, the program returns to the main menu. This file can then be executed immediately by selecting the second

Table II. Capabilities available within OPTCOMP.

Type	Description
Multiple concentric cylinder geometry	Fiber: layered morphology (homogeneous layers) Interfacial region: layered morphology (homogeneous layers) Matrix: layered morphology (homogeneous layers)
Constitutive models	Elastic: isotropic, transversely isotropic, orthotropic materials Plastic: incremental plasticity (Prandtl-Reuss relations) with isotropic hardening
Integration scheme	Spatial: successive elastic solutions (Mendelson)
Loading capabilities	Thermal: monotonic or cyclic, spatially uniform ΔT Mechanical: monotonic or cyclic external pressure + axial tension or compression Combined: monotonic or cyclic ΔT + external pressure + axial tension or compression
Optimization features	Design variables: interfacial layers' CTE, elastic moduli, yield stress, hardening modulus, thickness Objective functions: fiber radial stress; interfacial layer axial, hoop, radial and hydrostatic stress; matrix axial, hoop, radial and hydrostatic stress, and radial strain; composite axial strain; user-defined function Constraints: interfacial layer axial, hoop and radial stress; matrix axial, hoop, radial and hydrostatic stress; composite axial strain; user-defined function

option, or stored for later use. If a file defining the optimization problem already exists (i.e., it has been constructed at an earlier time), then the user can execute it by bypassing the first option and directly choosing the second option. During execution of the optimization procedure, the current values of the design variables, their lower and upper bounds, and the current values of the objective function and constraints are written to a data file at every iteration on the design variables. This information is also written to the screen, if so specified, thus allowing the user to both record and monitor the optimization process.

Choosing the third option allows the user to enter new fiber, interface and matrix material properties into the appropriate material databanks for use at some later time in an optimization problem. Through a sequence of interactive commands similar to those that are initiated when

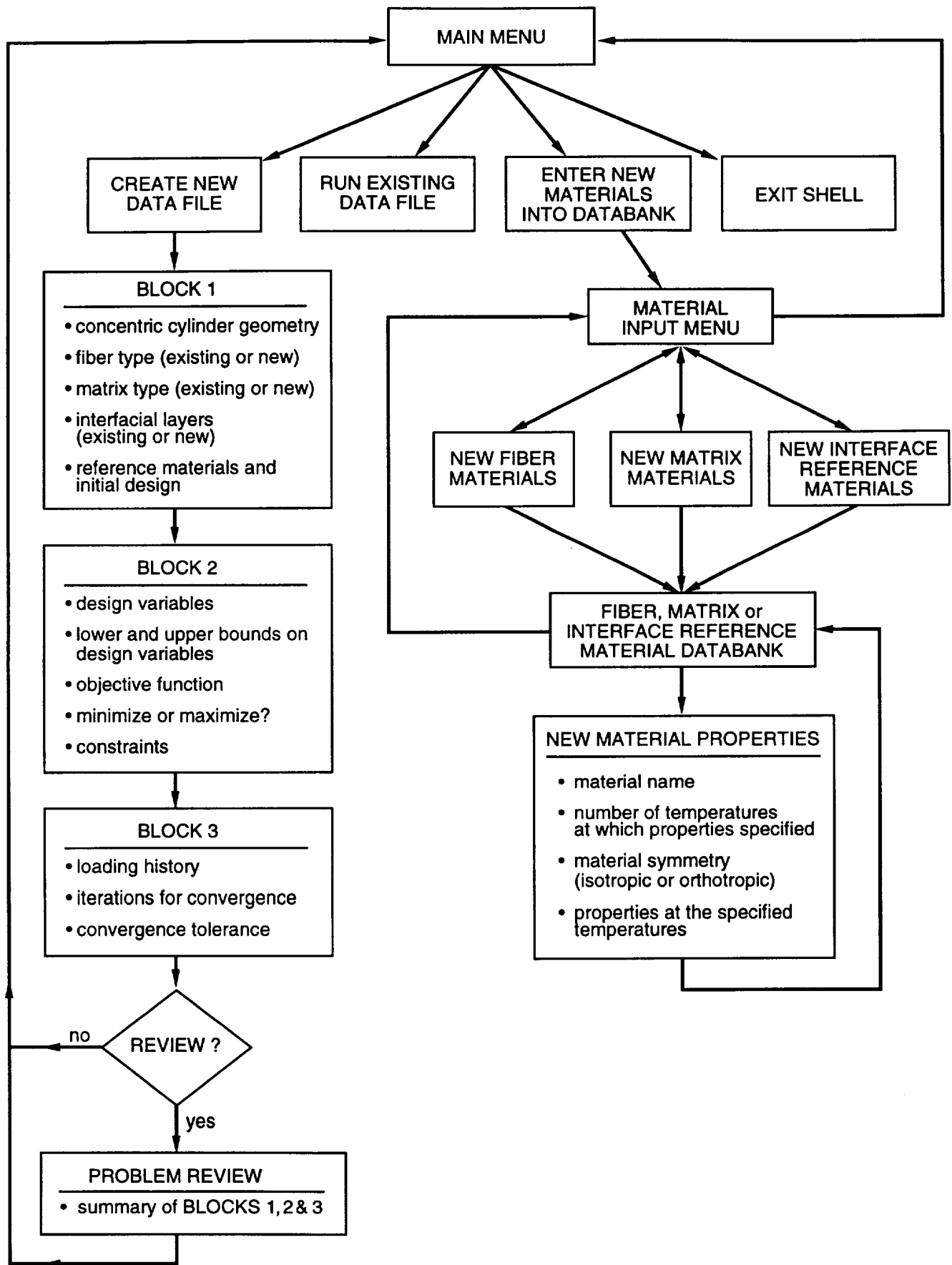


Figure 4. Flow chart for the menu-driven user interface of **OPTCOMP**.

the first option is chosen, the user is prompted to supply the following information for either a fiber, an interfacial layer or a matrix material: the name of the new material; number of temperatures at which properties of this material will be specified; material symmetry type (i.e., whether the material is isotropic, transversely isotropic or orthotropic); and finally the temperatures and the corresponding material properties. The material properties supplied by the user include the Young's modulus, Poisson's ratio, instantaneous (tangential) thermal expansion coefficient, yield stress, and hardening slope (based on a bilinear stress-strain representation of the elastoplastic behavior).

Finally, the execution of **OPTCOMP** is terminated when the fourth option is selected.

RTSHELL, a subset of **OPTCOMP**, is an executable file with the same analytical capabilities but without the optimization option. This program facilitates efficient characterization and evaluation of different metal matrix unidirectional composites subjected to rate-independent, combined axisymmetric thermomechanical loading in the presence of different fiber and interfacial layer architectures characterized by homogeneous sub-layers. The program employs the same material property data banks as **OPTCOMP**, and is driven by the same user-friendly interface, with **Block 2** (see Figure 4) that defines the optimization problem deleted.

3.3 OPTCOMP2/RTSHELL2

OPTCOMP2 is an executable file developed to identify either an optimal processing history or an optimal microstructure of the interfacial region in unidirectional metal matrix composites that minimizes (or maximizes) fabrication-induced stresses, strains, or a user-constructed function based on these field quantities. As indicated in Section 2.2, the processing history optimization is accomplished through variation of temperature, pressure, average axial stress or uniform axial strain, and time. The optimization of the interfacial region's microstructure is accomplished through variation of the inclusion volume fraction of the heterogeneous two-phase interface.

The basic make-up of **OPTCOMP2** is essentially the same as that of **OPTCOMP**, consisting of the menu-driven user interface, the analysis code and the optimization package **DOT**. The user interface has been modified to accommodate the different optimization capabilities provided by **OPTCOMP2**, including optimization problems explicitly involving time which require the use of rate-dependent constitutive theories for the individual constituents' response. The capabilities of the analysis module employed in **OPTCOMP2** are almost identical to **MCCM**. The only difference is the absence of the Robinson unified viscoplasticity theory for modeling the response of the individual constituents. Table III summarizes the features and capabilities of **OPTCOMP2**.

The program is executed by typing the command *optcomp2* at the unix prompt. As in the case of **OPTCOMP** described in the preceding section, this initiates the menu-driven, user-friendly interface with the main menu comprised of the same four options as before. The choice of a given option initiates the sequence of events outlined in Figure 5, which have essentially the same structure as those in **OPTCOMP** and thus will not be discussed in detail. The major differences to be noted include the reversed order of defining the optimization problem and the loading history during the data creation sequence of commands when the first option on the main menu is chosen, and the new material property entry format when the third option on the main menu is chosen. In the first instance, the reversed order is due to the dual optimization capability of **OPTCOMP2** which requires that both the interfacial region's microstructure and processing history be defined prior to defining the optimization problem. In the second instance, the new material property entry format is due to the new manner of storing material properties by constitutive model type rather than constituent type.

RTSHELL2, a subset of **OPTCOMP2**, is an executable file with the same analytical capabilities but without the optimization option. This program facilitates efficient characterization and evaluation of different metal matrix unidirectional composites subjected to rate-dependent

or rate-independent, combined axisymmetric thermomechanical loading in the presence of different fiber and interfacial layer architectures characterized by homogeneous or heterogeneous sub-layers. The program employs the same material property data banks as **OPTCOMP2**, and is driven by the same user-friendly interface, with **Block 3** (see Figure 5) that defines the optimization problem deleted.

Table III. Capabilities available within **OPTCOMP2**.

Type	Description
Multiple concentric cylinder geometry	Fiber: layered morphology (homogeneous or heterogeneous) Interfacial region: layered morphology (homogeneous or heterogeneous) Matrix: homogeneous or heterogeneous
Constitutive models	Elastic: isotropic, transversely isotropic, orthotropic materials Plastic: incremental plasticity (Prandtl-Reuss relations) with isotropic hardening Viscoplastic: Bodner-Partom unified viscoplasticity theory with isotropic hardening Inelastic: user-defined, rate-dependent inelastic relations for isotropic materials
Integration scheme	Spatial: successive elastic solutions (Mendelson) Time: predictor-corrector (forward Euler + Runge-Kutta)
Loading capabilities	Thermal: monotonic or cyclic, spatially uniform ΔT Mechanical: monotonic or cyclic external pressure + axial tension or compression Combined: monotonic or cyclic ΔT + external pressure + axial tension or compression
Optimization features	Design variables: interfacial layers' inclusion volume fraction; temperature, external pressure, axial stress/strain and time histories Objective functions: fiber radial stress; interfacial layer axial, hoop, radial and hydrostatic stress; matrix axial, hoop, radial and hydrostatic stress, and radial strain; composite axial strain; user-defined function Constraints: interfacial layer axial, hoop and radial stress; matrix axial, hoop, radial and hydrostatic stress; composite axial strain; user-defined function

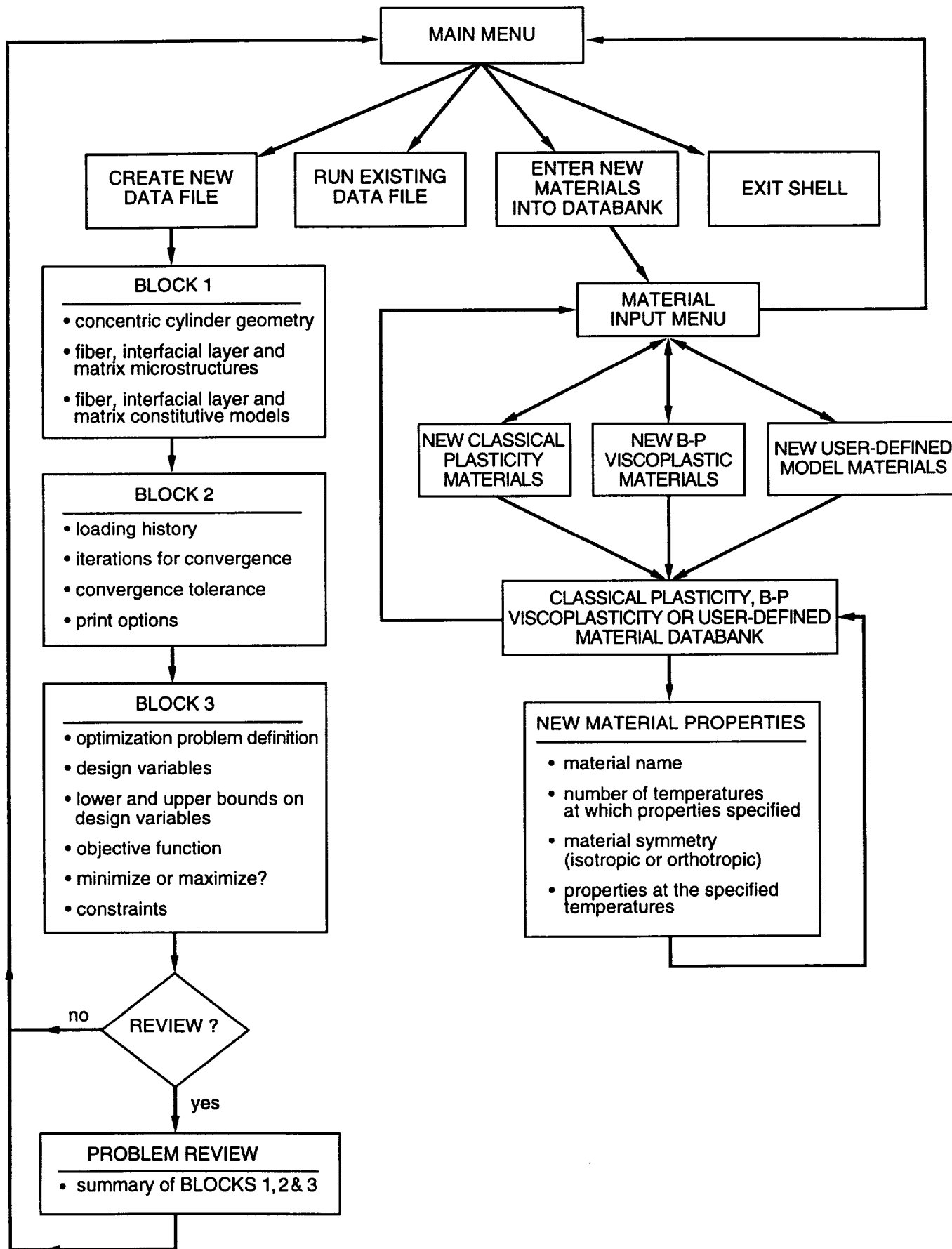


Figure 5. Flow chart for the menu-driven user interface of OPTCOMP2.

4.0 SUMMARY OF RESEARCH ACTIVITIES AND RESULTS

4.1 Metal Matrix Composites

The development of the aforementioned computer codes was accompanied by the following investigations:

- Effect of fiber morphology on residual stresses
- Effect of multiple compliant/compensating layers on residual stresses
- Effectiveness of graded interfacial layers in reducing residual stresses
- Residual stress optimization using functionally graded interfaces with homogeneous and heterogeneous microstructures
- Effect of matrix microstructure on residual stresses

The results of these investigations have been summarized in the references listed in Table IV. A brief summary of these investigations, along with their major conclusions, is provided below.

The effect of the SCS-6 SiC fiber's microstructure, consisting of five distinct regions, on the residual stresses in SiC/Ti₃Al composites was investigated by Pindera and Freed [27]. While the fiber's layered microstructure did not significantly affect the residual stresses in the matrix phase of the composite relative to those in a composite containing homogenous SiC fibers with equivalent homogenized properties, the stresses in the fiber itself were affected substantially by the fiber's microstructure. The effect of the SCS-6 SiC fiber's microstructure on potential failure modes during the fabrication cool down was subsequently discussed by Pindera et al. [9,10] and correlated with experimental observations. In this investigation, the authors also considered the presence of multiple compliant/compensating layers at the fiber/matrix interface in order to study the potential benefit of this approach in reducing the thermally-induced residual stresses relative to the single interfacial layer concept investigated by Arnold et al. [2,3,4]. The effect of grading the thermal expansion coefficient of the interfacial region through the use of multiple interfacial layers with different thermal expansion characteristics but otherwise the same elastoplastic properties was subsequently studied. The results indicated that grading the thermal expansion coefficient in the interfacial region using multiple layers provides no significant advantage over the use of a single interfacial layer with an equivalent or averaged thermal expansion coefficient in reducing the residual hoop and axial stresses in the matrix phase at the fiber/matrix interface. However, the results suggested that the use of multiple interfacial layers could have a potentially beneficial effect on the stress distribution in the interfacial region itself, particularly if both the thermal expansion properties, together with the elastic and inelastic

Table IV. Summary of published results addressing the effects of fiber, interfacial layer and matrix microstructural details on the response of MMCs.

Reference	Investigated effect
Pindera and Freed [27]	Effect of SCS-6 SiC fiber microstructure on fabrication-induced residual stresses
Pindera et al. [9,10]	Relationship between SCS-6 SiC fiber microstructure and subsequent fiber-initiated failure modes during processing. Effect of interfacial region's layered morphology on fabrication-induced residual stresses
Williams et al. [28]	Effectiveness of layered and graded interfacial layers in reducing residual stresses
Salzar and Barton [29]	Optimization of fabrication-induced stress and plastic strain fields using layered and functionally graded interfaces
Salzar et al. [30]	Parametric study of the effect of fiber and interfacial layer properties on fabrication-induced residual stresses in two MMC systems. Verification of the optimization algorithm.
Pindera et al. [31]	Effect of the morphology of heterogeneous, two-phase interfacial layers on fabrication-induced residual stresses
Pindera and Freed [32]	Effect of the morphology of heterogeneous, two-phase aluminide matrix on fabrication-induced residual stresses and radial microcracking
Williams and Pindera [33]	Effect of the morphology of layered SiC-6 SiC fibers and heterogeneous, two-phase aluminide matrix on TMF-induced residual stress and plastic strain fields

properties, were graded. Grading in this case could potentially reduce the generally high stresses in the interfacial region when compensating layers are used, thereby avoiding failure in the interfacial region itself. Such an investigation was subsequently conducted by Williams et al. [28]. In particular, grading both the thermoelastic and plastic properties of the interfacial region produced an engineered interface with a nearly uniform plastic strain distribution which resulted in acceptable hoop stress in both the matrix and the interfacial region after cool down as well as after thermal cycling up to the stress-free temperature. Salzar and Barton [29] subsequently verified this result upon combining the multiple concentric cylinder model with the optimization

algorithm DOT. Further verification of the optimization algorithm was provided by Salzar et al. [30] who also investigated the effect of fiber and interface layer properties on fabrication-induced residual stresses in a parametric study aimed at confirming the design rules for single interfacial layers established by Arnold and co-workers.

In the investigations discussed above, the grading of the interfacial region using multiple compliant/compensating layers was accomplished with homogeneous layers. This was subsequently extended by Pindera et al. [31] to allow the possibility of grading using homogenized interfacial layers composed of an inclusion phase embedded in a matrix phase. By selecting appropriate combinations of the inclusion and matrix phases, and by varying the inclusion volume fraction, interfacial layers with specific and physically realizable properties can be produced using this approach. The results revealed that homogenizing the interfacial region with different proportions of materials having the same properties as those of the fiber and the matrix is not an effective approach in reducing the residual stresses in the matrix phase. However, in the case of highly ductile (i.e., compliant) compensating layers, homogenization with elastic inclusions can be successfully employed to lower both the fabrication-induced hoop stress in the matrix phase and the level of plasticity in the interface, thereby reducing the potential for ratchetting during subsequent cyclic loading. By appropriately varying the concentration of the inclusion phase, nearly uniform plastic strain distributions in the interfacial region can be obtained, thereby increasing the potential for shakedown during thermomechanical fatigue applications.

In addition to the above investigations addressing the effects of fiber and interfacial layer morphologies on the evolution of residual stresses in MMCs, Pindera and Freed [32] also investigated the effect of the microstructure of the $\alpha_2 + \beta$ titanium aluminide matrix on the fabrication-induced radial microcracking in SiC/Ti₃Al composites. It was illustrated that the temperature-activated depletion of the ductile β phase at the fiber/matrix interface gave rise to sufficiently high hoop stress in the brittle α_2 -rich region upon cool down to cause radial microcracking. Further results addressing the importance of the fiber and matrix microstructural details on accurate prediction of the evolution of stresses and plastic strains in SiC/Ti₃Al composites during thermomechanical fatigue loading were provided by Williams and Pindera [33].

4.2 Metal Matrix Composite Tubes

The work funded through this contract resulted in a spin-off technology that has also been made available to the NASA-Lewis Research Center, in addition to the deliverables outlined in Section 3.0. In particular, the solution methodology for arbitrarily layered concentric cylinders subjected to axisymmetric thermomechanical loading outlined in Section 2.1 was extended by Salzar et al. [34,35] to enable investigation of axisymmetric and torsional thermomechanical loading of MMC tubes laminated with arbitrarily oriented layers. This was accomplished by developing a solution for the inelastic response of a monoclinic layer situated within an arbitrarily laminated MMC tube, and subsequently constructing the layer's local stiffness matrix for assembly into the global stiffness matrix. The instantaneous inelastic response of transversely isotropic, orthotropic or monoclinic layers that comprise the tube was determined using the continuous reinforcement version of Aboudi's method of cells, in contrast with **OPTCOMP2**, since the individual layers were assumed to be reinforced by continuous fibers. The solution's utility was subsequently demonstrated in applications involving the use of functionally graded layer architectures to optimize the tube's response to internal pressure through plastic strain suppression. The functional grading was accomplished by varying the fiber volume content in the individual layers. Additional examples of the use of functionally graded layer architectures in optimizing the response of MMC tubes have been provided by Salzar [36]. This solution methodology for arbitrarily laminated MMC tubes is currently being further generalized by Dr. Salzar, presently an NRC Fellow at the NASA-Lewis Research Center, through the incorporation of rotational effects in order to enable investigation of the behavior of rotating MMC shafts for applications in propulsion and drive systems.

5.0 GRADUATE AND POST-GRADUATE STUDENT TRAINING

In addition to the deliverables and results generated in the course of this investigation, this contract also provided support for two PhD candidates, namely R. S. Salzar and T. O. Williams, whose dissertations were based in large measure on the performed work. As mentioned in the preceding section, Dr. Salzar is presently involved in the optimization of MMC composite tubes at the NASA-Lewis Research Center, which is a continuation of his doctoral and post-doctoral work at the University of Virginia [37]. Dr. Williams is currently employed at the Los Alamos National Laboratory where he is working in the area of microstructural characterization of composite materials, which was the main thrust of his dissertation [38].

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