Probabilistic Ceramic Matrix Composite Behavior

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SUMMARY: In this paper an overview of in-house activities pertaining to Ceramic Matrix Composite (CMC) modeling and probabilistic CMC material behavior simulation are presented. The approach consists of a synergistic combination of two in-house developed methodologies. The first methodology is concerned with modeling of CMC behavior using micromechanics and macromechanics. The second one consists of a FPI (Fast Probability Integration) technique that takes into account the uncertainties occurring on various scales in a composite and computes the cumulative probabilistic distribution functions of composite global behavior. The methodology is applied to two CMC material systems including a woven CMC system. Results are presented in terms of cumulative probabilistic distribution functions of composite stiffnesses, thermal properties and strengths. In addition to cumulative distribution functions (CDFs) of response, the FPI technique provides additional information regarding the sensitivity of the response with respect to the primitive variables. The sensitivity information is very useful from the design point of view and can be used to rank the various input variables in the order of their importance in controlling the output response and scatter.

KEYWORDS: micromechanics, macromechanics, fiber substructuring, unit cell, cumulative distribution function, probability density function, and sensitivities

INTRODUCTION

Recent growing interest in advanced ceramic matrix composites (CMCs) for high temperature applications has generated considerable research activity in analytical modeling and testing of these composites. These are the materials of the future and are actively pursued for use in propulsion system components at NASA. Advanced CMCs offer superior thermal stability, higher stiffness/weight ratio, and structural tailoring capabilities. Analytical modeling and experimental characterization of their behavior is fundamental to their reliable use. The analysis of fiber reinforced CMCs presents many modeling challenges due to heterogeneity of these materials. Unlike their homogeneous isotropic counterparts, the anisotropic construction of laminated composites results in many unique phenomena that occur at different geometrical scales - at the global (laminate) level, the lamina (ply) level as well as at the fiber-matrix (constituent) level. To account for these phenomena in a more accurate manner, a unique micromechanics based fiber sub-structuring technique has been developed. Although, the technique is applicable to any kind of composite material behavior simulation, it is particularly well suited for simulating aspects unique to ceramic matrix composite behavior. Furthermore, the brittle nature of CMCs manifests in an increase in scatter in the observed behavior of these materials necessitating the development of formal probabilistic methods for these composites. All of these must be formally accounted for if CMC behavior is to be predicted with assurance that the component will have the required reliability during its operating life. Consequently, there is need for analytical tools that quantify the uncertainty in the "response" variables while taking into account the inherent scatter in the basic or "primitive" variables. Primitive variables are the constituent properties/parameters that participate at the lowest level (e.g., the micromechanics level) in defining a global property. The fiber volume ratio and the individual constituent properties such as fiber modulus, matrix thermal expansion coefficient, and fiber tensile strength are some of the primitive variables. These are assumed to be independent and have their own statistical distributions. Response variables are those that characterize the composite behavior, such as the moduli, thermal conductivities, composite strengths, etc.

In the current practice of deterministic approaches, uncertainties are usually accounted for by using safety factors. This approach can often yield overly conservative designs thereby reducing the potential of many advanced composite materials. Currently, work is underway at NASA-Glenn Research Center (formerly NASA Lewis Research Center) to incorporate probabilistic distribution of the material behavior and fabrication related parameters into micromechanics and the macromechanics of ceramic matrix composites. The primary objective of this work is to develop an efficient computational design tool that could account for all of the uncertainties in the constituent properties in a more rigorous manner and also provide the overall composite properties and their probabilistic distributions. Such information could then be used to design the structural component to meet the necessary life requirements. In addition to providing more rigor to the analysis as than the so called "safety factor approach" does, such procedures would enhance interpretation of the experimentally measured CMC properties with a wide range of scatter. Furthermore, the procedure will help in identifying the dominant variables those that most influence a specific response, thereby providing the guidelines for quality control during the fabrication process of these materials. Thus, the methodology could be applied not only to the design but also to the development of a better material.

The approach taken in the present effort is to combine ceramic matrix composite analysis embedded in the computer code CEMCAN (Ceramic Matrix Composite Analyzer) [1-2] and fast probability integration techniques (FPI) available in NESSUS (Numerical Evaluation of Stochastic Structures Under Stress) [3]. The results are in the form of cumulative probability distribution functions (CDF's) for ply/laminate properties of ceramic matrix composites. A CDF is a relationship defined by the value of a property (response variable) with respect to its cumulative probability of occurrence. In addition, the probabilistic sensitivities of response variable to inherent scatter in primitive variables are obtained as by-products of the FPI technique. In the present paper, this methodology will be demonstrated for different CMC systems including woven and plain architectures with typical results. The results will be presented in terms of probabilistic density and cumulative distribution functions for stiffness related, thermal and heat transfer related properties. Also, comparison of predicted probabilistic strengths versus experimentally obtained distributions will be presented. Due to space limitations many details are omitted, however, the appropriate references are cited.

PROBABILISTIC CERAMIC MATRIX COMPOSITE ANALYSIS

As mentioned above, the present work adopts an integrated approach, which is a synergistic combination of two in-house developed methodologies. The first methodology is concerned with CMC micromechanics and macromechanics. The second one consists of an FPI (Fast Probability Integration) technique that takes into account the uncertainties occurring on various scales in a composite and computes the cumulative probabilistic distribution of composite global behavior. A schematic of the integrated approach is shown in figure 1.

The computer code CEMCAN utilizes a novel and unique fiber sub-structuring technique in conjunction with conventional micromechanics that is based on a mechanics-of-materials approach [1-2]. As shown in parts of Figure 1, CEMCAN's methodology consists of

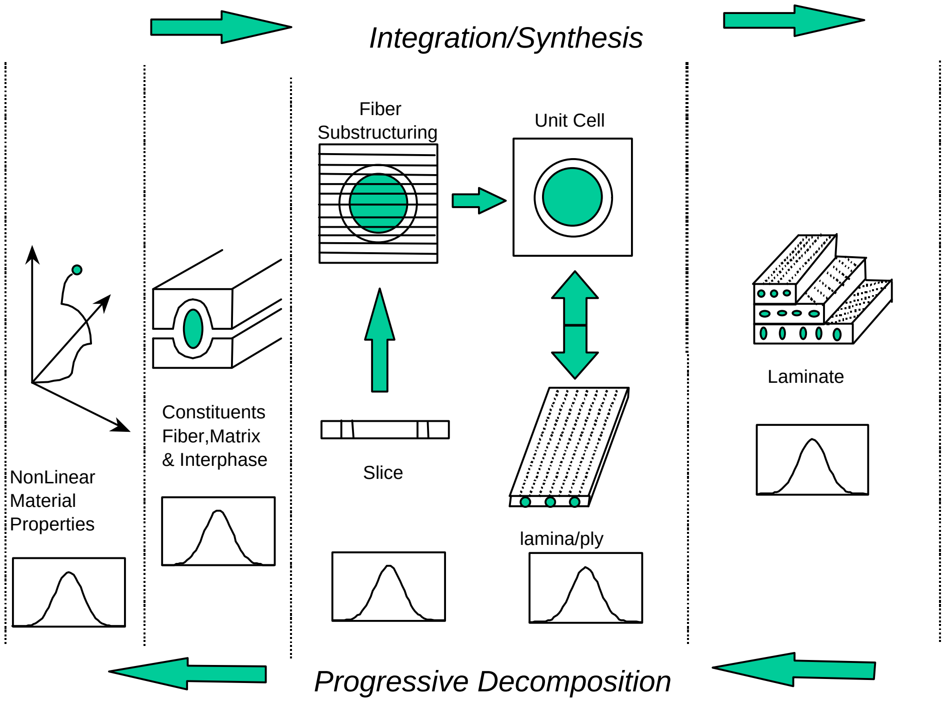

Figure 1. Integrated probabilistic ceramic matrix composite mechanics approach

incremental synthesis of the properties starting from constituents – namely, the fiber, the matrix, and the interphase-- to form a slice. The slice-level properties are obtained using composite micromechanics equations, which are represented by simplified closed-form equations. The slice level properties are in general equivalent elastic properties such as moduli, Poisson's ratios, thermal expansion coefficients and heat conductivities. From slice level to a single lamina level and, subsequently, to laminate level, the code repeatedly applies classical laminate theory to obtain composite-level properties and response. Given a specific set of loads, the code can progressively decompose, as indicated in the Figure 1, retracing the steps followed during the upward synthesis to yield laminate-, ply-, and slice-level responses and constituent microstresses. The code can predict ply- and laminate-level thermal and mechanical properties as well as detailed description of resulting microstresses due to an applied load. It also accounts for non-linear effects due to material nonlinearities as well as due to the local stress redistribution resulting from progressive fracture. By analyzing the response of CMC's, one can account for fabrication-related parameters. A more detailed description of this methodology can be found in reference 4.

There are a number of approaches available for obtaining probabilistic response from a set of independent variables and the expressions describing the response behavior. Monte-Carlo simulation technique is one such fairly common approach to obtain CDF's of composite properties, given the probability distributions of constituent properties, which are considered as independent variables. In this technique, randomly selected values of the input variables, which based on their known probabilistic distributions, are used to deterministically compute the value of the response variable. This is repeated, usually several hundreds of times, to build the response probabilistic characteristics. In essence, this technique requires a large number of simulations to generate CDF's of output variables. Although inherently simple, a large number of output sets that must be generated to obtain a reasonably accurate CDF of output variables becomes its obvious disadvantage. Furthermore, if the deterministic computation of the response is complicated and time-consuming the computational costs could become prohibitive. Obviously, to circumvent this computationally very expensive and time-consuming procedure, more efficient approaches and algorithms are needed.

For more than a decade NASA Glenn Research Center has been engaged in developing efficient probabilistic methods. As a result of this intensive program, an FPI (ref. 3) was developed as a part of the in-house computer code NESSUS (Numerical Evaluation of Stochastic Structures Under Stress) to solve a large class of engineering problems. FPI is a probabilistic analysis tool that implements a variety of methods for probabilistic engineering analysis and design. A schematic of the integration of FPI and CEMCAN is shown in Figure 2. The integrated computer code is called PCEMCAN (Probabilistic Ceramic Matrix Composite Analyzer). The role of CEMCAN was to provide the functional relationships (micromechanics and macromechanics) that tie the constituent properties to the equivalent composite behavior. The role of FPI was to perform probabilistic analyses by utilizing the properties generated by CEMCAN. In general FPI requires the following:

(1) The independent and uncorrelated input (design) variables and their probability distributions must be defined. Constituent properties, FVR (Fiber Volume Ratio), VVR (Void Volume Ratio), ply thickness, ply alignment, etc. are independent variables that determine the composite properties.
(2) There must be a function (called the performance function) that defines the relationship between the response variable and independent variables. Ply or laminate properties are response variables in this paper. As shown in the figure 2. (middle box in the top line) variable Z, is a dependent variable whose uncertainties are required to be computed. Variables X_1, X_2, and X_3 are independent variables.

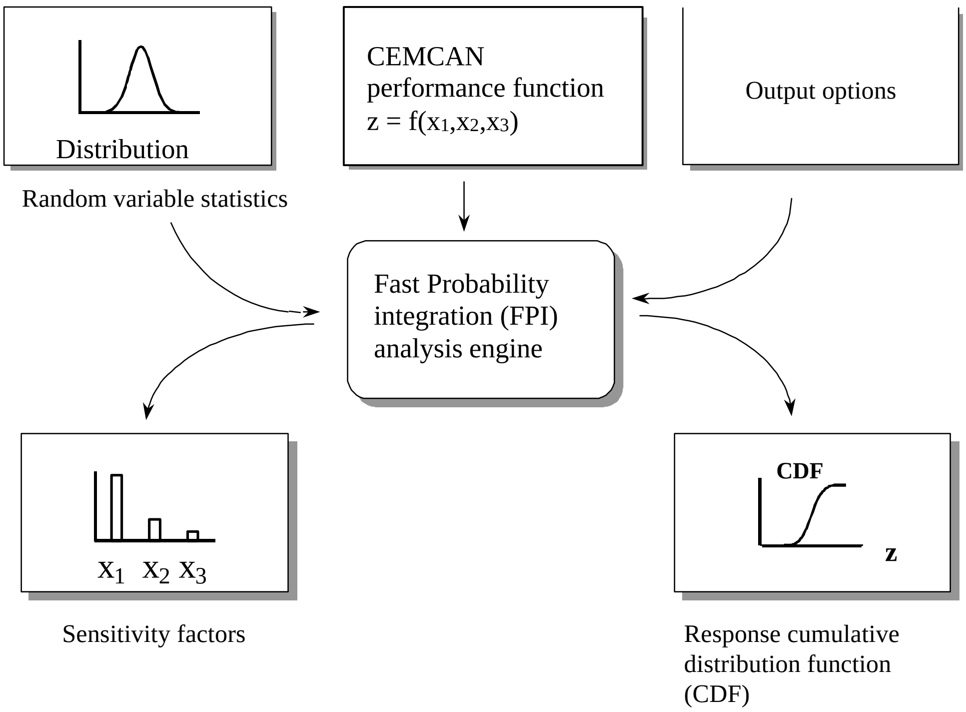

Figure 2. Fast probability integration input-output schematic

The variables that are uncertain in nature are identified as independent in step (1). Their probability distributions can be obtained from the available measured data or can be assumed based on experience and judgment. For most problems, it is difficult to determine analytical expressions representing relationship between independent and dependent variables. In case of ceramic matrix composites, it is very complicated to build relationships for the ply or laminate properties as a function of constituent properties, fabrication parameters, etc. CEMCAN code has such relationship built in using micromechanics and macromechanics theory. A performance function is developed by using a numerical approach. In this approach an explicit response function is developed by perturbing the independent random variables about their magnitude and using CEMCAN to compute response. Discrete evaluations of response variables for perturbed values of independent variables are used to fit into a function using regression analysis. The uncertainties of a response variable are quantified in the form of a CDF by the following procedure:

(1) The primitive variables and the corresponding probabilistic distributions are selected. (For example, to generate the CDF of the composite longitudinal modulus, the primitive variables could be the fiber modulus, matrix modulus, fiber volume ratio, and so forth.) For a given set of values of primitive variables, the micromechanics and macromechanics in CEMCAN computer code is used to compute the desired response variable.
(2) The whole process is repeated to generate a table of response variable values that correspond to perturbed values of the primitive variables.
(3) The FPI analysis then uses the previously generated table to compute the CDF and the corresponding sensitivities of the response at user defined probability levels.

Sensitivity information is very useful for studying the probabilistic variation of the response. Note that the sensitivity obtained here should not be confused with the conventional deterministic sensitivities of the response. Sensitivity in probabilistic analysis consists of a product of two parts. The first part has the usual meaning, akin to the deterministic sensitivity. The second part is the result of the scatter in a primitive variable and it accentuates the deterministic sensitivity. The magnitude of the sensitivity factor provides a way of ranking the importance of the individual physical variables. The sign of the sensitivity factor indicates how a specific random variable influences the failure probability. For example, a positive value of sensitivity indicates increase in failure probability with the increase in random variable. Thus, the sensitivity information obtained from FPI is very useful from the design point of view. The significant variables' scatter can be controlled to improve the reliability. Thus weak physical variables with large uncertainties may have probabilistic sensitivity factors more important than strong physical variables with small standard deviations. Variables with no scatter (deterministic) will obviously result in zero values for the sensitivity implying the response scatter is unaffected by such variables.

RESULTS AND DISCUSSION

Two different CMC material systems were considered in this work. The first system was SiC/RBSN (silicon carbide SCS-6 fiber in a reaction-bonded silicon nitride matrix). The second material system was a 5-harness 0/90 Sylramic Fiber/CVI-SiC/MI-SiC woven composite. The probabilistic material behavior simulation methodology embedded in PCEMCAN was applied to these two CMC systems. Results were obtained in terms of CDF's of the composite stiffness, strength, and thermal related properties.

<u>Probabilistic behavior simulation of SiC/RBSN CMC material system:</u>

This composite system is known to have a very compliant and weak interphase. The mean values of the constituent properties are shown in Table 1, which is taken from reference 5. As was mentioned before, the uncertainties in the composite system occur at various levels both due to the inherent scatter in the material properties as well as uncertainties associated with manufacturing processes. They may occur at constituent (fiber, matrix or interphase) level, at the ply level (fiber volume ratio, void volume ratio, thickness of interfacial region etc.) and the composite level (ply angle, lay-up etc.). Specifically, in this work, fiber volume ratio (FVR), fiber modulus (E_f), matrix modulus (E_m), interphase modulus (E_i), interphase thickness (t_i), coefficients of the thermal expansion of the fiber, matrix and the interphase (α_f , α_m and α_i), thermal conductivities of the fiber, matrix and the interphase (K_f, K_m, and K_i), room temperature tensile strengths of the fiber, matrix and the interphase (S_f, S_m and S_i) were considered random; other parameters were assumed to be deterministic. The interphase is a distinct region with a finite thickness, that arises as a result of fiber coatings or as a "reaction-zone" arising due to chemical reaction between the fiber and the matrix material as these composites are processed at very high temperature. In any case, interphase material is assumed to have its own properties that are different from both fiber or matrix properties. For illustrative purposes the assumed distribution types and parameters for the selected random variables are as shown in Table 2. However, the actual distributions for primitive variables based on experimentally measured values whenever available. The micromechanics and macromechanics embedded in CEMCAN computer code are used to compute composite properties. The micromechanics equations are not shown here for the sake of brevity but are readily available elsewhere (Ref. 2). The Fast Probability Integration (FPI) technique is used to obtain cumulative distribution functions (CDF) of the required properties. As mentioned before, FPI offers very valuable additional information in the form of sensitivity factors, which represents sensitivity of output variable uncertainty to the uncertainty in the selected primitive random variables.

Selected results from this effort are shown in Figures 3-4. A more detailed set of results can be found in Ref. 6. The CDF of composite longitudinal modulus, E_{c11} and its probabilistic sensitivity to the various primitive variables are shown in Figures 3 and 4. The computed mean value of E_{c11} for this particular composite is 183 GPa with a scatter range of 155 to 224 GPa. In other words, if one were to experimentally determine the longitudinal modulus of such a composite system, one can expect values anywhere in the range indicated by the scatter. Such information obviously gives one useful insight with which to design and plan test setup and the number of tests for a particular material study. Sensitivity factors provide information regarding the ranking of importance of various input variables in controlling the output response/scatter. For example, E_{c11} is most sensitive to the fiber volume ratio (Figure 4). This should be expected because the longitudinal modulus is essentially controlled by the fiber-dominated behavior. Also important are the matrix modulus, fiber modulus and the interface thickness. If one wishes to control the scatter in the longitudinal modulus of this particular composite, the biggest payoffs will result from controlling the scatter in the fiber volume ratio (FVR). On the other hand, the modulus of the interphase material has no effect on the scatter of ply longitudinal modulus. In this situation, any effort in the processing or elsewhere that will change the modulus of the interphase will not help control the scatter in longitudinal modulus. Another point of interest is that the sensitivities remain constant throughout the probability range considered. In order to verify these results

Table 1: Constituent Properties of SiC/RBSN Composite [a]

Property	SiC Fiber	RBSN Matrix	Interphase
Modulus, GPa (Msi)	390 (56.6)	110 (15.95)	3.5 (0.5)
Poisson's ratio	0.17	0.22	0.22
Shear modulus, GPa (Msi)	117 (17)	45 (6.5)	1.4 (0.2)
Coef. of thermal expansion,ppm/^{0}F)	4.1 (2.3)	2.9 (1.6)	2.0 (1.1)
Thermal conductivity, W/m-K (Btu/ft-hr-^{0}F)	22 (12.7)	5 (2.9)	2.0 (1.2)

[a] Fiber and matrix properties are taken from reference 5 and interphase properties are based on calibration explained in reference 4

Table 2. Primitive Input Variables Distribution Parameters

Variable	Units	Distribution Type	Parameter 1 Mean Value	Parameter 2 C.O.V.
Fiber modulus, E_f	GPa (Msi)	Normal	390 (56.6)	0.05
Fiber coeff. of thermal exp. α_f	Ppm / ^{0}K(^{0}F)	Normal	4.4 (2.4)	0.05
Fiber thermal conductivity, K_f	W/m-K(Btu/ft-	Normal	22 (13)	0.05
Fiber tensile strength, S_f	hr/^{0}F)	Weibull	2 (285)	0.05
Matrix modulus, E_m	GPa (ksi)	Normal	110 (15.95)	0.1
Matrix coeff. of thermal exp., α_m	GPa (Msi)	Normal	2.1 (1.2)	0.1
Matrix thermal conductivity, K_m	Ppm/ ^{0}K(^{0}F)	Normal	4.2 (2.4)	0.1
Matrix tensile strength, S_m	W/m-K(Btu/ft-	Weibull	93 (13.5)	0.15
Interphase modulus, E_i	hr/^{0}F)	Normal	3.5 (0.5)	0.15
Interphase coeff. of thermal exp.,α_i	MPa (ksi)	Normal	2.1 (1.2)	0.1
Interphase thermal cond, K_i	GPa (Msi)	Normal	2.4 (1.4)	0.1
Interphase tensile strength, S_i	Ppm/^{0}K (^{0}F)	Weibull	80 (11.6)	0.15
Fiber vol. ratio, fvr	W/m-K(Btu/ft-	Normal	0.36	0.1
Thickness of interphase, t_i	hr/^{0}F)	Normal	4.2 (.17)	0.2
	GPa (ksi)			
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	μm (mils)			

a limited number of Monte-Carlo simulation studies were also undertaken. The CDF for the longitudinal modulus obtained from 10000 samples is also shown along in Figure 3. As seen from the figure, Monte-Carlo results agree very well with those from FPI. Sensitivity information based on Monte-Carlo simulation was not obtained because doing so would have involved a substantial additional effort with little added value, and is beyond the scope of the activity. Results similar to the above were obtained for other moduli, thermal expansion coefficients, conductivities as well and were reported in Reference 6.

The next set of results shown are for $[0]_8$ laminate probabilistic first matrix cracking strength (FMCS) in Figures 5 and 6. The details of analytical modeling approach for the stress strain behavior can be found in Reference 7. The approach accounts for processing induced residual stresses, and stress redistribution due to continuous matrix cracking. The deterministic stress strain behavior for this material exhibits a bilinear behavior with a sharp "knee" that signifies the first matrix cracking strength (FMCS). Beyond this point, essentially the fibers carry the load till they break in a brittle manner in the end. Laboratory tests were conducted on 60 samples and based on the observed results cumulative distribution functions were constructed [7]. Figure 5 shows a comparison of predicted CDF versus experimental CDF for the first matrix cracking strength. Figure 6 shows the sensitivities of various primitive variables on the observed FMCS behavior.

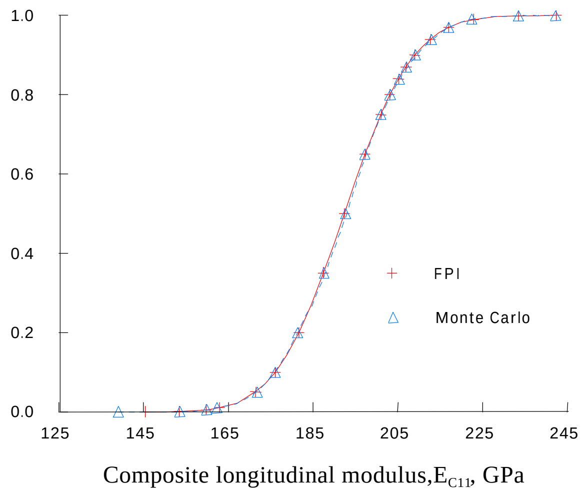

Figure 3. Cumulative distribution function of Longitudinal modulus E_{c11} of $[0]_8$ SiC/RBSN Composite

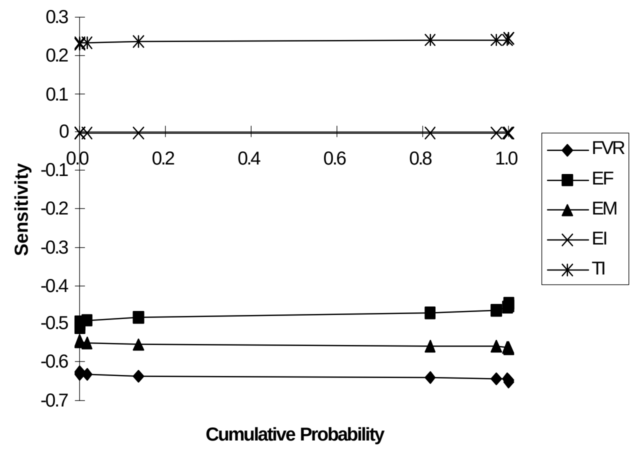

Figure 4. Sensitivity factors for E_{c11} for $[0]_8$ SiC/RBSN composite

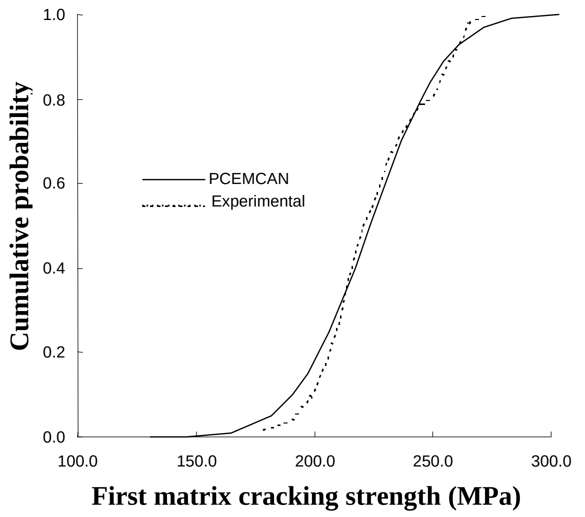

Figure 5. Comparison of first matrix cracking strength CDF simulation with the Experimental data for a $[0]_8$ SiC/RBSN composite laminate.

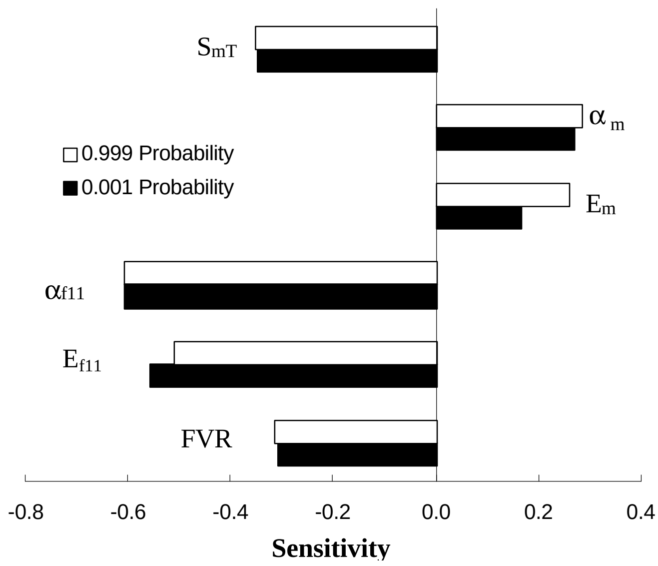

Figure 6. Sensitivity of the first matrix cracking strength to the primitive random variables of a $[0]_8$ SiC/RBSN composite laminate

The computationally obtained mean first matrix cracking strength is 225 MPa that matches with 221 MPa from the test data. The coefficient of variation (COV) for the FMCS is about 11.34%. The predicted probabilistic scatter in the FMCS range from 124 to 303 MPa as compared to 172 to 276 MPa obtained experimentally. The experimentally observed scatter based on 60 samples fall within the predicted scatter. From Figure 6 it is seen that the FMCS is sensitive (in the descending order) to the thermal expansion coefficient (CTE) of the fiber (α_{f11},), longitudinal fiber modulus (E_{f11}), matrix strength in tension (S_{mT}), fiber volume ratio

(FVR), matrix thermal expansion coefficient (α_m), and matrix modulus (E_m). In a composite in which the modulus and CTE of the fiber are greater than those of the matrix, compressive residual stresses are generated in the matrix after cooling the composite from the fabrication temperature. In this case the compressive residual stress in the matrix increases the FMCS. In contrast, in a composite in which the modulus and CTE of the fiber are lower than those of the matrix, tensile residual stresses are generated. This will decrease the FMCS. Therefore, the thermal residual stresses significantly affect FMCS in composites. Thus, the processing temperature plays an important role in affecting the design strength. Also, to obtain a reduced scatter in the design strength, the uncertainty in these variables should be controlled. Furthermore, processing techniques to reduce the residual stresses should be developed. Note that the stress free temperature is considered deterministic in the current analysis. Similar results for cross-ply and angle-ply laminates were also generated and can be found in Reference 9.

Probabilistic behavior simulation of 5-harness 0/90 Sylramic Fiber/CVI-SiC/MI-SiC woven CMC material system:

The enabling propulsion material (EPM) project team of NASA/LeRC was involved in evaluating a woven composite CMC system as a possible candidate material for combustor lines. A 5-Harness 0/90 Sylramic Fiber with CVI (chemical vapor inflation) SiC matrix and MI (melt infiltration) matrix was chosen as the candidate material. This composite system consists of two mutually orthogonal sets of fiber tows inter-laced with each other, to form a layer. The layer is then coated with Boron Nitride (BN coat) through a CVI process. Subsequently SiC is deposited through CVI process to fill the fiber tows till it forms a thin coating around the fiber tow. Melt-infiltration process is then used to deposit the SiC matrix between fiber tows (MI-SiC).

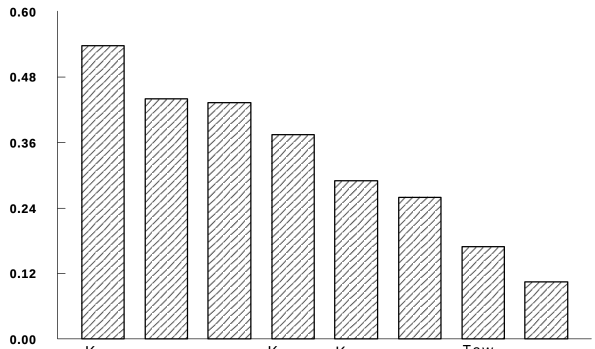

Figure 7. Importance ranking of variables contributing to the scatter in through-the-thickness thermal conductivity for a 0/90 Sylramic Fiber/CVI-SiC/MI-SiC 5 HS woven CMC at 2200 ^{0}F

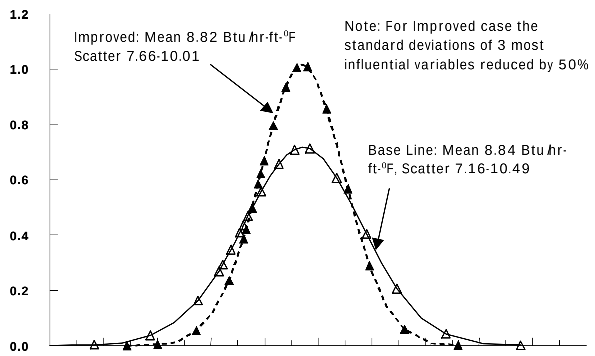

Figure 8. Probabilistic density function of through-the thickness thermal conductivity for a 0/90 Sylramic Fiber/CVI-SiC/MI-SiC 5 HS woven CMC at 2200 ^{0}F

In order to analyze this CMC system, CEMCAN was modified with micromechanics for woven composites, which is then utilized to study the probabilistic behavior of the EPM material. The details of the analytical modeling, property predictions and comparison with experimental data were reported in Reference [8]. The details of probabilistic material modeling and results can be found in Reference [9]. The sensitivity information and probabilistic density functions are presented for through-the-thickness thermal conductivity (K_{C33}) at 2200 ^{0}F of the woven CMC system considered at are shown in Figures 7 and 8. The sensitivity analysis results for through-the-thickness thermal conductivity are shown in Figure 7. The influence of various properties with uncertainties are ranked according to their sensitivity magnitude. The sensitivity information can be utilized to improve the material. For example, one can study the effects of reducing the scatter on the property by computational simulation. In this work, this was performed by reducing the scatter in the three most influential properties. The results are shown in Figure 8. The probability density function for the base line case and for the improved case are shown with solid and dashed curves. The dashed line indicates, the result obtained for the case where the scatter in the top three most influential variables is reduced by 50 percent. This resulted in a reduction of 29% in scatter for the through the thickness thermal conductivity. Such information could be very valuable for material development effort, since, it defines where to expend efforts and resources to optimize key material response variables.

CONCLUSIONS

An overview of the various in-house activities pertaining to computational simulation of probabilistic ceramic matrix composite behavior is presented through several examples. Sample results are presented with comparison to experimental data where available for two different CMC composite systems. Collectively the results show the versatility and usefulness of the simulation approach. In addition, the results show that the present technique can provide qualitative as well as quantitative information that can be used as a guide in the fabrication and testing of the material. A means to possibly reduce observed scatter and thereby improve the quality of the material is illustrated through an example. The scatter observed in the through the thickness thermal conductivity is reduced by about 30 percent using this procedure.

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