

COVER SHEET

Title: **Estimation of 3D Woven Design Sensitivities Using a Rapid Multiscale Analysis Technique**

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ABSTRACT

Highly-refined finite element models of three-dimension (3D) woven composite systems currently require excessive computational demands that limit their use in sensitivity analysis, uncertainty quantification, and optimization. An alternative analysis methodology was developed using the NASA Multiscale Analysis Tool (NASMAT) where multiscale models of a 3D woven composite (including inter-tow matrix voids and constituent failure) can be completed on a single central processing unit (CPU) on the order of ~ 30 s. To develop inputs and validation data for the NASMAT model, coupon and acid-digesting testing and x-ray computed tomography were performed. The NASMAT inputs were parameterized using a set of 25 input variables and distributions. These inputs were randomly sampled to generate a total of 100,000 NASMAT analyses that could be used to understand the influence of different material and geometric properties on the warp and weft-direction stiffness and strength. These analyses (including pre/post-processing) were performed in less than eight hours on a 120 CPU cluster. The computational efficiency of the NASMAT model enabled a sensitivity analysis to be performed, and dominant input variables were able to be identified. Key results were consistent with theoretical and experimental observations for the specific 3D woven system studied in this work.

INTRODUCTION

Three-dimensional (3D) woven composites have emerged as an alternative to traditional laminated composites by offering improved damage tolerance and customizability. NASA has developed multiple distinct 3D woven architectures for space missions as part of the Adaptive Deployable Entry Placement Technology (ADEPT) [1], 3D Multifunctional Ablative Thermal Protection System (3D-MAT) [2], Heatshield for Extreme Entry Environment Technology (HEEET) [3], and Composite Technologies for Exploration (CTE) [4, 5] projects. However, each of these weaves has predominately been evaluated experimentally due to the significant challenges associated with modeling 3D woven architectures. A few models have been developed to understand the effects of damage at the various length scales present in 3D woven composites [6–10]. When looking at the broader 3D woven literature, the trend is to use highly-refined finite element models of the woven architecture at a single scale, and

multiscale models are not employed [11–20]. As a result of the high computational demand for high-fidelity finite element models, it is currently challenging to perform sensitivity or optimization analyses for 3D woven composites based on this approach. Additionally, surrogate modeling likely is not a reasonable solution, particularly when damage and failure are considered, due to the significant runtimes since a large amount of training data are often required.

An alternative modeling methodology for 3D woven composites has been developed using the Multiscale Recursive Micromechanics (MsRM) approach within the NASA Multiscale Analysis Tool (NASMAT) [9] whereby accurate analyses can be obtained in ~30 s on a single central processing unit (CPU) compared to hours of analysis time on multiple CPUs for refined finite element models [18, 20]. This study will describe some of the initial efforts aimed at performing sensitivity analyses to better understand the influence of 3D woven design variables on the homogenized mechanical as well as the strength related properties of a 3D woven polymer matrix composite (PMC) developed under the NASA CTE project.

EXPERIMENTAL MATERIAL CHARACTERIZATION

During the NASA CTE effort, a wide variety of 3D woven composites were developed and characterized to various degrees including multiple fiber tow and matrix materials and weave designs [4, 5]. For this study, an IM7-6k/RTM6 3D orthogonal woven PMC was utilized. Woven preforms were made by Bally Ribbon Mills. and infused by North Coast Composites using a resin transfer molding process. A suite of coupon tests was performed on this material as well as acid digestion testing to characterize fiber and volume fractions. X-ray computed tomography (CT) data were also generated and used to determine defects and initial geometric parameters. The idealized weave geometry is shown in Figure 1. The designed unit cell size is approximately 8.23 mm x 4.80 mm x 3.18 mm in the warp, weft, and through-thickness directions, respectively. The unit cell is comprised of 24 warp tows (8 layers, 3 columns), 54 weft tows (9 layers, 6 columns), and three binder tows where each binder tow is located between each adjacent column of warp tows. Both warp and weft tows are predominantly aligned in their respective directions while the binder tows are aligned in the warp-direction, but periodically traverse through the thickness (TT) of the composite.

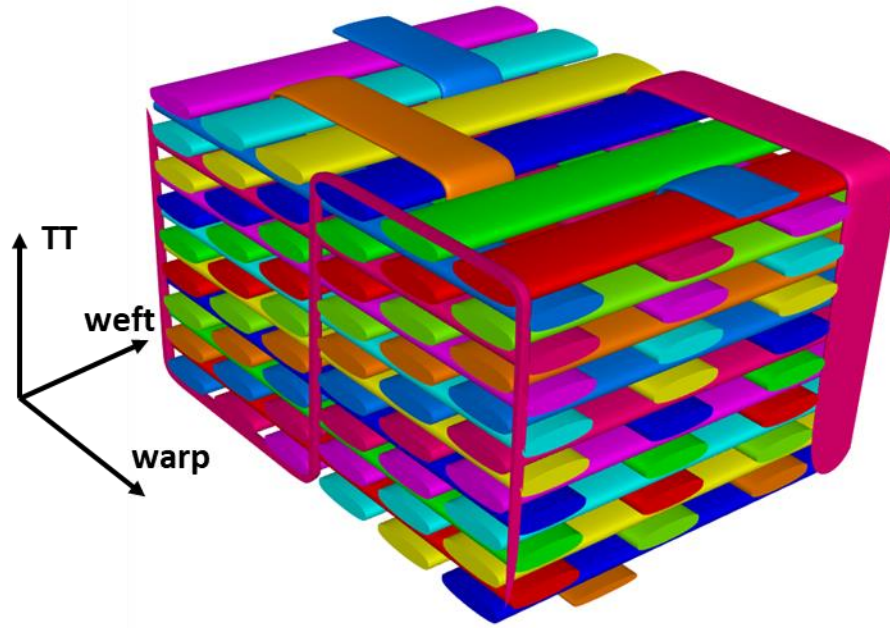


Figure 1. Designed IM7-6k/RTM6 3D woven geometry.

Coupon Testing

Standard composite tests were performed under room temperature ambient conditions by the National Institute for Aviation Research (NIAR). For this study, the relevant test data are comprised of five 254.0 mm x 25.4 mm ASTM D3039 tensile tests each performed in the warp and weft-directions. From these tests, the initial elastic modulus, Poisson's ratio, and strength were determined based on load cell and uniaxial strain gauge (SG) data (based on a 6.35 mm gauge length) and virtual extensometers (based on a ~66 mm initial gauge length) using a digital image correlation (DIC) system. Since significant disagreement was observed previously between predicted material properties and measured Poisson's ratio data, Poisson's ratio data were not utilized. Predicted Poisson's ratios from two independent finite element modeling approaches (Digimat and in-house methods) were in close agreement with the method of cells approach, and those approaches are described in more detail in Ref. [5]. An exact reason for the cause of this discrepancy is unknown, but it may be a result of the measurement averaging area not being a sufficient size compared to the unit cell dimensions and/or the highly localized strain fields observed from DIC data.

A summary of the panel modulus and strength data measured in the warp and weft-directions are shown in TABLE I and include calculated averages and standard deviations. For consistency with the NASMAT model coordinate system adopted in this study, the panel thickness is aligned with the x_1 -direction and the panel warp and weft directions are aligned with the x_3 and x_2 -directions, respectively. Processed DIC data for three specimens were unavailable. For the available DIC data, there were no significant disagreements between SG and DIC measurements. Since the weft-direction has more than double the number of fiber tows than the warp-direction, the

measured average modulus is higher in that direction. However, a significantly higher average strength in the weft-direction was not observed.

TABLE I. MEASURED TENSILE PROPERTIES ON AN IM7-6k/RTM6 3D WOVEN COMPOSITE

Specimen	Warp-Direction (x_3)			Weft-Direction (x_2)		
	Modulus (MPa) SG	Modulus (MPa) DIC	Strength (MPa)	Modulus (MPa) SG	Modulus (MPa) DIC	Strength (MPa)
1	58066	57549	915	67754	-	970
2	58497	56173	892	67088	68137	933
3	59778	56537	906	66680	-	905
4	58575	57864	871	69624	70919	894
5	58960	-	924	69198	70481	909
Average	58775	57031	902	68069	69846	922
St. Dev.	644	805	21	1293	1496	30

Acid-digestion Testing

Acid digestion testing based on ASTM D3171 Procedure B was used to characterize the bulk fiber volume fraction and void content. A total of nine specimens were tested. After testing, the fiber volume fraction was calculated to be 0.48 (0.01 standard deviation) and the void volume fraction was calculated to be 0.017 (0.003 standard deviation).

X-ray CT Characterization

For this particular IM7-6k/RTM6 3D woven system, x-ray CT images at a 13.4 μm resolution were generated on individual specimens both prior to and during various loading states of tensile testing [21]. Multiple types of cracks were present in pre-test images while some macroscale voids were observed [21]. These data are from panel “1Z” in Ref. [21], and readers are referred to that reference for more details regarding data generation and observed features. While the focus of this work is on pre-test x-ray CT data, the other sets of data are exceedingly valuable for evaluating damage progression and failure.

Based on features observed in the x-ray CT data, a number of key dimensions were identified and measured, and representative images are shown in Figure 2. These include the warp tow width (WaW) and height (WaH) and the weft tow width (WeW) and height (WeH). For sections of the binder tow aligned in the warp-direction, the elliptical binder tow shape is similar to those of the warp and weft fiber tows. As the binder transitions through the thickness, its width narrows and height elongates. To approximate this behavior, two sets of binder tow dimensions were measured: the width and height in the flat warp-aligned regions (BWf and BHf, respectively) and near the

mid-thickness (BWz and BHz, respectively). Statistical distributions of these eight dimensions were determined by repeatedly extracting dimensions from different locations near the appropriate tow centerline and from different cross-sectional planes if possible. For example, the warp tow width, WaW, can be found by measuring warp tows from images normal to the warp direction or normal to the thickness direction. These data are shown in Figure 3. Excluding the binder tow measurements at the through-thickness (TT) transition region, the measured tow widths and heights are similar. While this observation offers evidence to lump those dimensions together, separate measurements are maintained to better isolate the influence of key dimensions in the sensitivity analysis (SA). For simplicity, normal distributions are fit to these data and subsequently used in the SA. While the parameter BWz appears to be bimodal based on multiple x-ray CT images in Figure 2 and the histogram in Figure 3, these two measurements were not further isolated for this work and were lumped together instead. Additionally, while the distributions for parameters WaW, WeW, and BWf were similar, the binder tow was observed to overlap columns of warp tows.

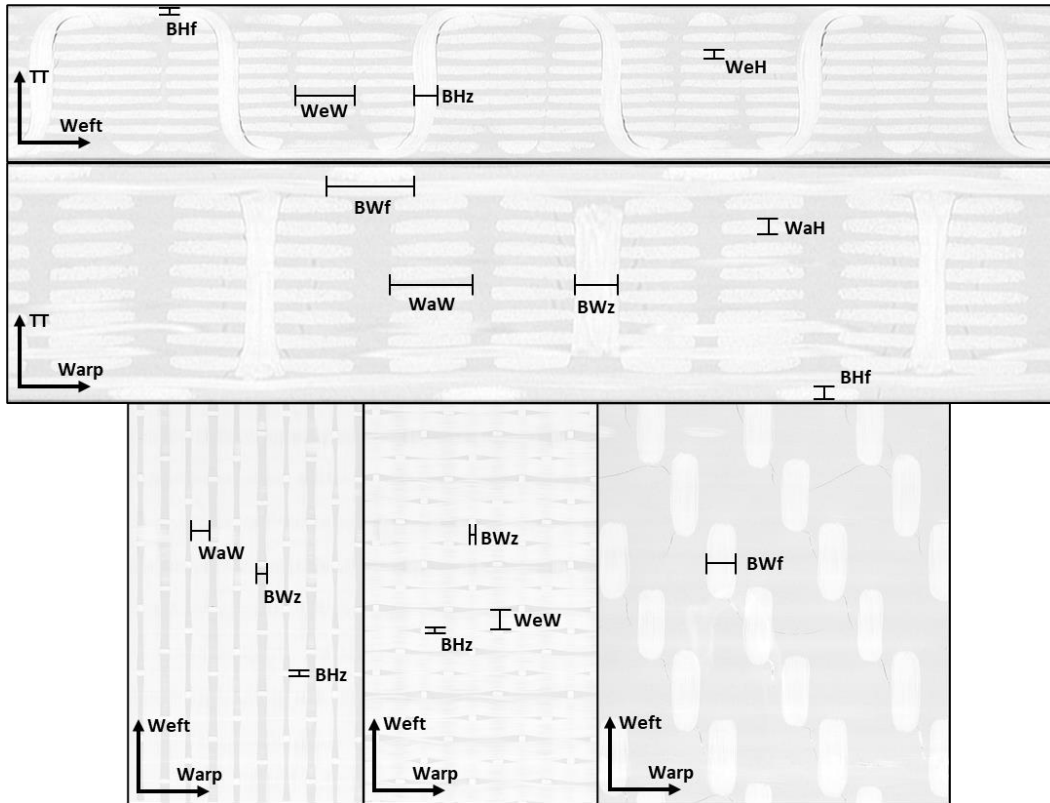


Figure 2. Representative x-ray CT images of an IM7-6k/RTM6 3D woven composite with possible measurement locations.

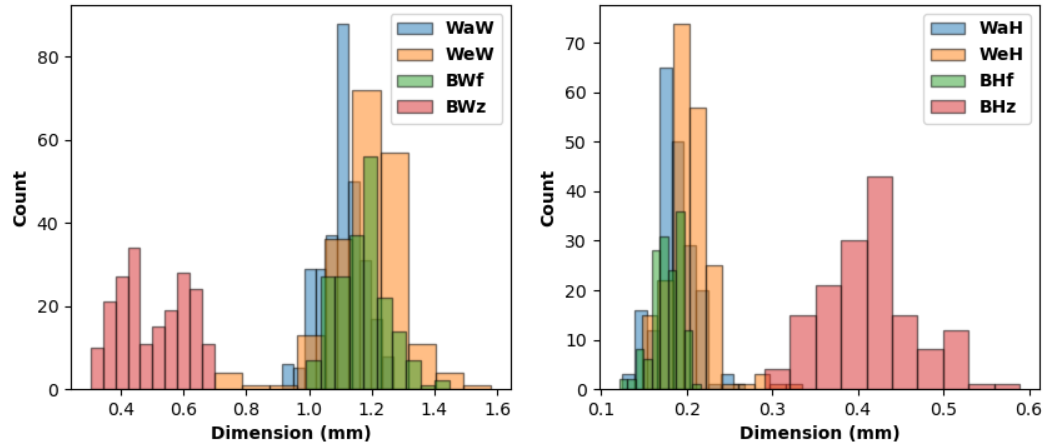


Figure 3. Histograms based on measurements extracted from x-ray CT images.

MULTISCALE MODELING PROCEDURE

The MsRM approach can be used to simulate materials with multiscale microstructures and is shown in Figure 4. Recursive procedures, subroutines, and data structures are extensively used in the NASMAT software. This permits an arbitrary number of scales to be defined, and data can be seamlessly transferred among the scales. Additionally, any micromechanics method can be utilized at any scale. Through a series of localization operations, successively lower levels are called until ultimately the individual constituents are reached. Once a subvolume at any level contains a constituent material, no further localizations can occur. After all localizations have occurred for a given level, properties are homogenized and passed up to the previous level. The highest level in the model, Level 0, represents the entry point for a NASMAT analysis and is where most data of interest are generated such as the effective composite moduli and effective stress/strain response. Currently, Level 0 calculations are performed using any of the available micromechanics theories, and periodicity is assumed. To relax the assumption of global periodicity, NASMAT can be called from a third-party tool (e.g., a finite element program) where the desired boundary conditions can be applied. More details on the MsRM formulation can be found in Ref. [9, 10].

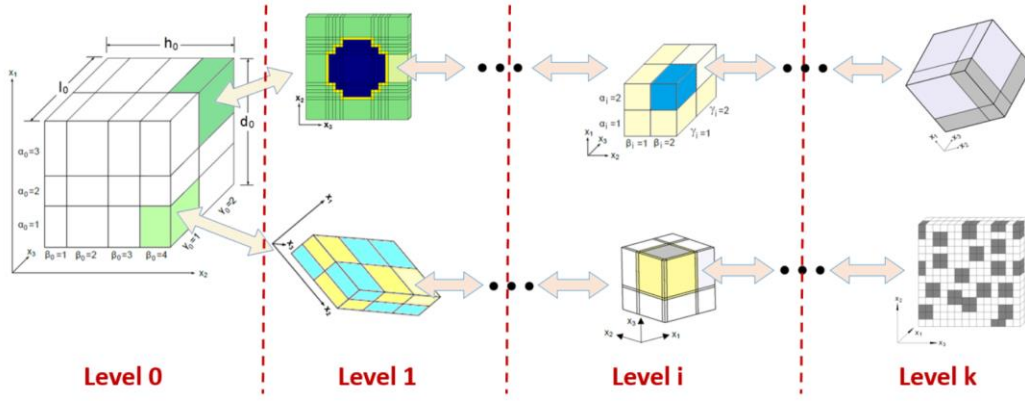


Figure 4. Schematic of the Multiscale Recursive Micromechanics (MsRM) approach wherein micromechanics models are embedded within each other to model microstructure at any number of length scales.

NASMAT MODEL DEVELOPMENT

Multiscale Modeling Approach

For a typical 3D woven composite, several unique length scales are present. The choice of a particular micromechanics theory at a given length scale can be chosen to balance overall model accuracy with computational cost. For the current study, the IM7-6k/RTM6 3D orthogonal textile architecture was analyzed using the 3D Generalized Method of Cells (GMC3D) micromechanics theory [22], the tows were modeled using the two-dimensional GMC (GMC2D) micromechanics theory [22] with a hexagonal arrangement of fibers, and the inter-tow matrix (matrix plus voids) is modeled using the Mori-Tanaka mean-field micromechanics theory [23]. Details on each of these micromechanics methods can be found in Ref. [22]. Level 1 and Level 2 represent a two-step homogenization procedure using the GMC3D micromechanics theory similar to the one adopted in Ref. [24]. The orientations of the fiber tows are included at Level 2. Additionally, homogenization at Level 1 is performed even though the material is not periodic in the thickness direction. A previous finite element study has shown that the relaxation of through-thickness periodicity does not significantly influence the in-plane results when using this multiscale modeling approach and give similar results to a legacy method of cells tool consistent with the one adopted in this study [5]. For this work, voids were assumed to only occur in the inter-tow matrix, and an expression was developed to calculate the amount of inter-tow void content required to yield a user-specified level of overall void content. Intra-tow void content could be additionally considered but was assumed to be negligible in this study.

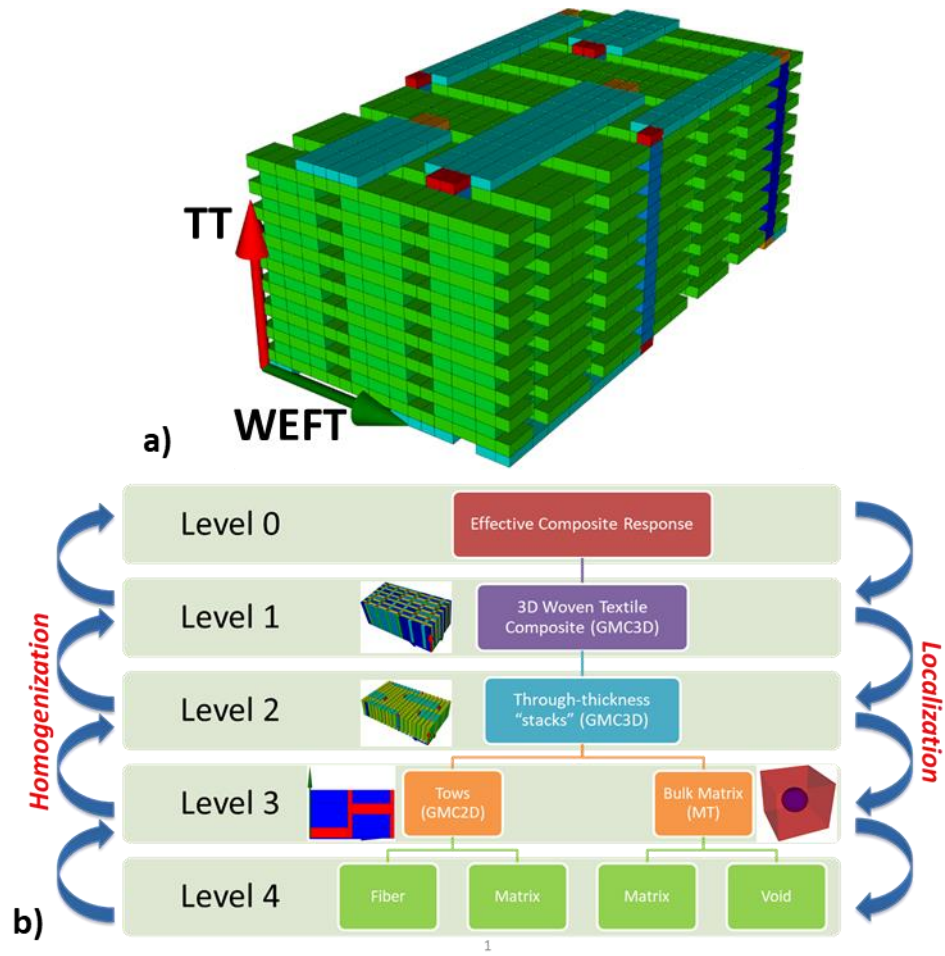


Figure 5. a) NASMAT model discretization (Levels 1/2) of an IM7-6k/RTM6 3D orthogonal woven composite with only tow materials shown and b) the multiscale modeling strategy.

Once an individual failure criterion is activated for a given constituent's subvolume, all components of the stiffness matrix for this subvolume are significantly reduced and is referred to as the subvolume elimination approach. Alternatively, progressive failure models (e.g., crack band [10, 25]) may be utilized to gradually modify the stiffness matrix of a subvolume. Both multiscale NASMAT approaches, which require on the order of seconds to minutes to complete on a single CPU, are significantly more efficient than single-scale high-fidelity finite element approaches which can take on the order of hours to complete on multiple CPUs. This speedup is key for running sensitivity analyses where on the order of tens of thousands of models may be required to obtain accurate and repeatable results.

Material and Geometric Input Properties/Parameters

A total of 25 inputs were varied as part of this study and include 15 material properties and 10 geometric inputs. These inputs are shown in TABLE II. The IM7 fiber was modeled as transversely isotropic resulting in five elastic constants, two normal tensile failure parameters, two normal compressive failure parameters, and two

shear failure parameters. The RTM6 matrix was modeled as isotropic resulting in two elastic constants, one normal tensile/compressive failure parameter (assumed to be equal), and one shear failure parameter. Void elastic properties were treated as isotropic with a negligible elastic modulus.

Truncated normal distributions were used to represent each of the inputs. IM7 fiber elastic properties and failure parameters were utilized from Ref. [26]. The RTM6 matrix elastic modulus, Poisson's ratio, and failure parameters were obtained from Ref. [27]. All elastic constants were assumed to have a 10% coefficient of variation while all failure properties were assumed to have a 20% coefficient of variation. Mean warp, weft, and binder tow dimensions and distributions were based on x-ray CT measurements. The overall void content mean and distribution were based on the previously described acid digestion tests. A tow fiber volume fraction of 0.7 was based on preliminary processed scanning electron microscopy (SEM) images for a similar weave of the same IM7-6k fiber tow and RTM6 matrix. A 10% coefficient of variation was assumed. All lower and upper bounds were set based on a plus/minus three standard deviation from each input's mean value (capturing 99.73% of the distribution). For most inputs, this avoids physically inadmissible inputs (e.g., negative volume fraction, Poisson's ratio greater than 0.5 for the isotropic matrix). However, since the binder width overlaps warp tow columns on the upper/lower surfaces of the composite, a constraint is introduced into the model that must be satisfied to have positive subvolume dimensions ($WaW - BWf + BWz > 0$). While this constraint can be satisfied by utilizing tighter bounds, it is primarily invalid near the parameters' extremes in the distributions. Rather than significantly restricting the design space for those parameters (to approximately plus/minus 1.7 standard deviations), samples were discarded that did not satisfy this constraint. Based on random sampling, an approximately ~0.1% sample rejection rate was observed.

TABLE II. INPUT MATERIAL PROPERTIES AND FAILURE PARAMETERS

Category	Variable	Description	Units	Mean	St. Dev.	Lower Bound	Upper Bound
Elastic properties	M-E	matrix modulus	MPa	2755.0	275.5	1928.5	3581.5
	M-v	matrix Poisson's ratio	-	0.380	0.038	0.266	0.494
	F-Ea	fiber axial modulus	MPa	262200.0	26220.0	183540.0	340860.0
	F-Et	fiber transverse modulus	MPa	11800.0	1180.0	8260.0	15340.0
	F-va	fiber axial Poisson's ratio	-	0.270	0.027	0.189	0.351
	F-vt	fiber transverse Poisson's ratio	-	0.210	0.021	0.147	0.273
	F-Ga	fiber axial shear modulus	MPa	18900.0	1890.0	13230.0	24570.0
Failure parameters	F-SIGF-FT	fiber tensile failure parameter (axial)	MPa	4335.0	867.0	1734.0	6936.0
	F-SIGF-TT	fiber tensile failure parameter (transverse)	MPa	113.0	22.6	45.2	180.8
	F-SIGF-X23	fiber shear failure parameter (in-plane)	MPa	128.0	25.6	51.2	204.8
	F-SIGF-X13	fiber shear failure parameter (out-of-plane)	MPa	138.0	27.6	55.2	220.8
	F-SIGF-FC	fiber compressive failure parameter (axial)	MPa	2608.0	521.6	1043.2	4172.8
	F-SIGF-TC	fiber compressive failure parameter (transverse)	MPa	354.0	70.8	141.6	566.4
	M-SIGFT	matrix normal failure parameter	MPa	87.0	17.4	34.8	139.2
	M-SIGFS	matrix shear failure parameter	MPa	76.1	15.2	30.4	121.8
Geometric inputs	WaW	warp tow width	mm	1.108	0.068	0.904	1.312
	WaH	warp tow height	mm	0.186	0.022	0.121	0.251
	WeW	weft tow width	mm	1.186	0.118	0.831	1.541
	WeH	weft tow height	mm	0.202	0.026	0.124	0.281
	BWf	binder tow width (flat region)	mm	1.171	0.081	0.928	1.413
	BHf	binder tow height (flat region)	mm	0.174	0.017	0.123	0.225
	BWz	binder tow width (TT region)	mm	0.501	0.105	0.186	0.817
	BHz	binder tow height (TT region)	mm	0.413	0.052	0.256	0.569
	Vv	overall void volume fraction	-	0.017	0.003	0.008	0.026
	Vf	tow fiber volume fraction	-	0.700	0.070	0.490	0.910

Model Evaluation at Mean Input Values

To evaluate the multiscale model's accuracy, mean values for each of the inputs in TABLE II were utilized to compare model results to experimental data. Strain-control loading in the warp or weft-direction was utilized, and the increment size was selected based on a convergence study. The same strain increment size (0.0004 mm/mm) was used for both the warp and weft-direction simulations. A key distinction of NASMAT analyses is that highly-detailed multiscale analyses can be completed in a short time. For this study, the warp-direction model ran in approximately 26 s and the weft-direction model ran in approximately 29 s.

The nominal fiber volume fraction from the model was 0.496 and agrees well with the measured value of 0.480 from acid digestion tests. The nominal warp and weft stiffnesses calculated from the model were 61780 MPa and 71692 MPa, respectively. This also compares favorably with the measured (DIC) warp and weft mean stiffnesses of 57031 MPa and 69846 MPa, respectively. Model and experimental stress/strain curves are shown in Figure 6, and in general, there is good agreement between the predicted and measured results. Final failure in the warp and weft-directions was driven by failure of the fibers within tows in the warp and weft-direction, respectively. The predicted warp strength (884 MPa) closely matches the average measured warp strength (902 MPa) while the predicted weft strength (1159 MPa) was higher than the average measured weft strength (922 MPa). The source of the discrepancy is being investigated but is likely due to the in-plane weft tow waviness not being captured (see the bottom middle image in Figure 2) in the NASMAT model.

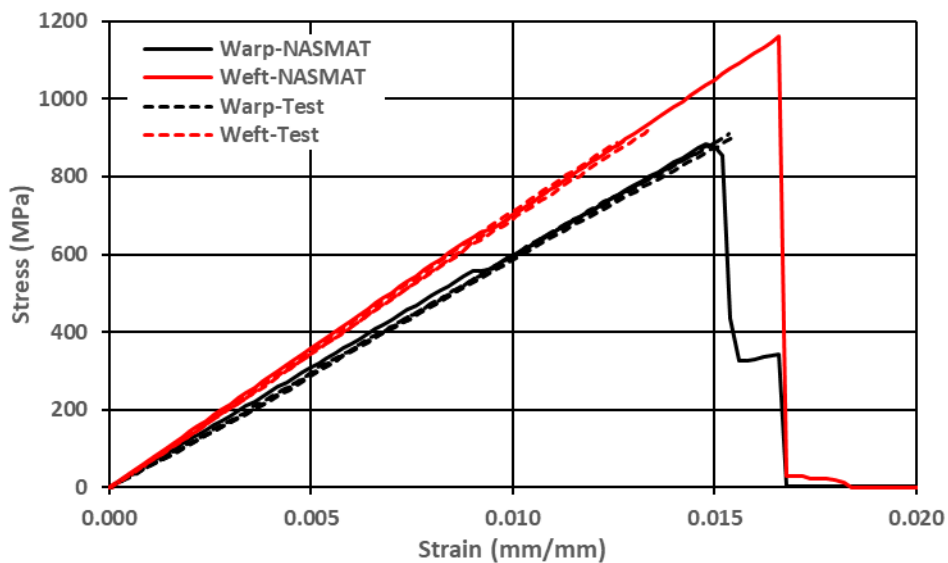


Figure 6. Predicted NASMAT and experimental stress/strain curves from tensile loading in the warp and weft-directions.

SENSITIVITY ANALYSIS

For this preliminary work, 50,000 unique combinations of input variables were randomly generated using a truncated normal distribution for each input variable and the values listed in TABLE II. Appropriate input files were created to run NASMAT. Since both warp and weft-direction loading were separately run, 100,000 NASMAT input decks were generated. This preprocessing step required ~31 min on a single CPU and can likely be significantly improved by writing inputs in parallel. Each NASMAT run was submitted to a cluster utilizing 120 Intel Xeon E5-2698 v4 (2.20 GHz) CPUs and the 100,000 NASMAT runs were completed in ~6.25 hours of wall-clock time. Similar to the input file generation, output results were processed on a single CPU in ~40 min – a time that also could be significantly improved by post-processing in parallel.

The utilized output from NASMAT consisted of the effective modulus in the warp and weft-directions as well as the stress/strain behavior in response to the applied loads. The damage initiation stress and the corresponding strain were determined by post-processing the NASMAT output text file to search for the first failure event. The output stress/strain response in the warp or weft-direction was processed to identify the ultimate failure stress and the corresponding strain.

To measure the sensitivity of the outputs to the inputs, the Pearson correlation coefficient (PCC), ρ , was calculated for each combination of input A and B using the built-in MATLAB function *corrcoef* [28]:

$$\rho(A, B) = \frac{1}{N} \sum_{i=1}^N \left(\frac{A_i - \mu_A}{\sigma_A} \right) \left(\frac{B_i - \mu_B}{\sigma_B} \right) \quad (1)$$

where μ_A and σ_A are the mean and standard deviation of A , respectively, and μ_B and σ_B are the mean and standard deviation of B , respectively. It is worth noting that the PCC can only capture a linear dependence between two inputs. Other measures of sensitivity such as Sobol indices [29–31] are currently being explored.

The dominant inputs (represented by a higher PCC) are shown in Figure 7 for the effective weft and warp-direction moduli, E22 and E33, respectively. As expected, for both loading directions, the tow fiber volume fraction (Vf) and fiber axial modulus (F-Ea) significantly impact the output moduli. Various other geometric parameters were found to be important to a lesser extent than Vf and F-Ea. The warp and weft tow heights were significant inputs in both loading directions. This observation may be due to the discretization choice of the NASMAT model. The TT discretization is solely based on individual tow heights and not combinations of input variables such as what is used to represent the warp and binder tow discretization across their widths. A thorough examination of the output sensitivities should therefore be carefully weighed against any modeling assumptions. Additionally, note that the void content was not found to significantly influence the warp/weft moduli. This is likely due to the mean void content being low (0.017) and offers evidence that future studies can neglect modeling the voids provided fiber dominated properties are being analyzed.

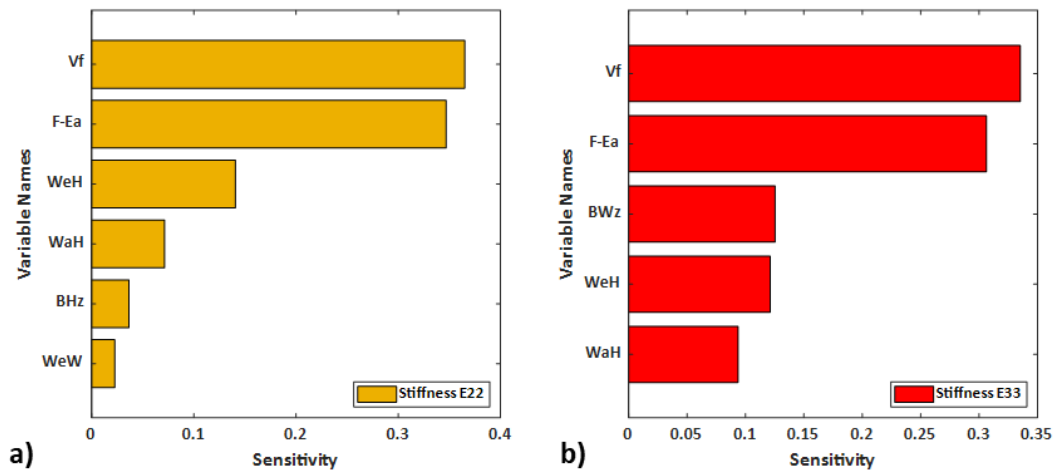


Figure 7. PCCs for a) weft and b) warp-direction moduli.

The PCCs for the weft and warp-direction damage initiation and ultimate strengths are shown in Figure 8. In terms of the damage initiation stress, the matrix tensile/compressive failure stress was the dominant input variable for both warp and weft-direction loading. From analyzing the text-based NASMAT output, this failure criterion was primarily activated due to tensile loading at the onset of damage in the model. The fiber axial and transverse moduli were also significant input variables for both loading directions. Since the damage initiation stress was primarily driven by matrix failure and the elastic material properties are completely decoupled from the failure criteria, the presence of dominant elastic properties (F-Ea and F-Et) suggests that the fiber tow properties may be playing a significant role in transferring stresses to the surrounding inter-tow matrix causing it to damage. Of course, a further study could be performed to isolate which individual tow properties (i.e., warp, weft, or binder) primarily contribute to the damage initiation stress. As expected, the ultimate strength of the composite in both the warp and weft-directions was primarily influenced by the fiber tensile failure strength and the tow fiber volume fraction. Although multiple failure criteria were specified for the fiber, these results align with the observation that the fiber compressive and shear failure criteria were not activated for these particular simulations. One interesting observation is that the same dominant geometric parameters for the warp and weft-direction moduli are reflected in their respective damage initiation stress and ultimate strength suggesting that out of the eight varied geometric dimensions, only half (WaH, WeH, BWz, BHz) significantly contribute to the output response.

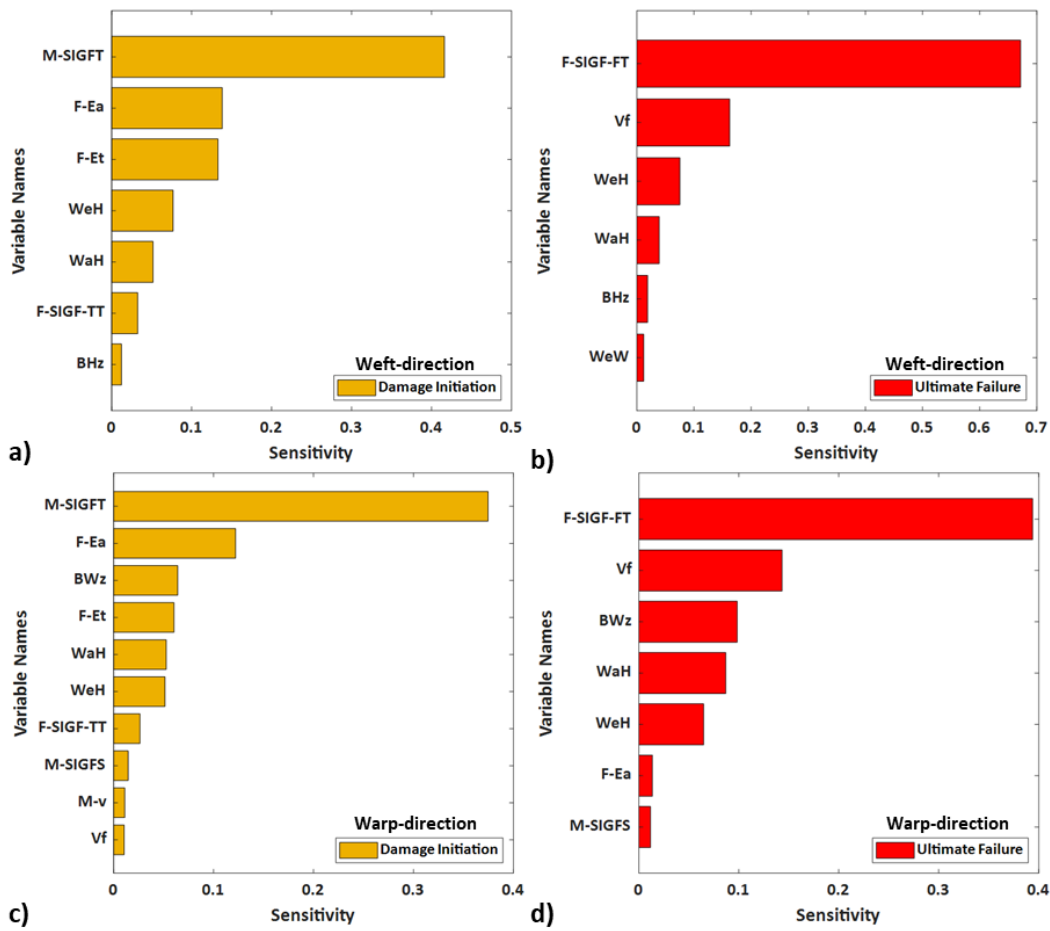


Figure 8. PCCs for weft-direction a) damage initiation stress and b) ultimate strength and warp-direction c) damage initiation stress and d) ultimate strength.

CONCLUSION

In this study, a methodology for performing rapid sensitivity analyses of three-dimensional (3D) woven composites is presented. Multiscale models including constituent failure were developed, and analyses were run using the NASA Multiscale Analysis Tool (NASMAT). Coupon and acid-digesting testing and x-ray computed tomography were performed to generate model inputs and provide validation data for the NASMAT model. In general, the stiffness and strength in both the warp and weft-directions agreed well with experimental data. It is expected that the weft-direction strength prediction can be improved by modeling the observed in-plane waviness of the weft tows. Individual analyses completed on the order of 30 s – significantly faster than highly refined finite element models. This significant efficiency enables thousands of simulations to be rapidly executed so that sensitivity analyses (SAs) can be performed for these composites. This SA methodology was demonstrated by running 100,000 NASMAT analyses based on 50,000 unique sets of 25 inputs (warp and weft-directions). Preliminary results demonstrated that the methodology was effective at

capturing relevant input sensitivities consistent with theoretical and experimental observations.

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