Composite Laminate Failure Parameter Optimization Through Four-Point Flexure Experimentation and Analysis

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Abstract

Fiber-reinforced composite materials offer light-weight solutions to many structural challenges. In the development of high-performance composite structures, a thorough understanding is required of the composite materials themselves as well as methods for the analysis and failure prediction of the relevant composite structures. However, the mechanical properties required for the complete constitutive definition of a composite material can be difficult to determine through experimentation. Therefore, efficient methods are necessary that can be used to determine which properties are relevant to the analysis of a specific structure and to establish a structure's response to a material parameter that can only be defined through estimation. The objectives of this study deal with demonstrating the potential value of sensitivity and uncertainty quantification techniques during the failure analysis of loaded composite structures; and the proposed methods are applied to the simulation of the four-point flexural characterization of a carbon fiber composite material. Utilizing a recently implemented, phenomenological orthotropic material model that is capable of predicting progressive composite damage and failure, a sensitivity analysis is completed to establish which material parameters are truly relevant to a simulation's outcome. Then, a parameter study is completed to determine the effect of the relevant material properties' expected variations on the simulated four-point flexural behavior as well as to determine the value of an unknown material property. This process demonstrates the ability to formulate accurate predictions in the absence of a rigorous material characterization effort. The presented results indicate that a sensitivity analysis and parameter study can be used to streamline the material definition process as the described flexural characterization was used for model validation.

Keywords

A. Carbon fibre; C. Computational modeling; C. Finite element analysis (FEA); C. Statistical properties/methods

1. Introduction

Computer simulations can be used to model the behavior of a loaded composite structure assuming the structure's materials are well defined. Specifically, sophisticated material models are being developed that will accurately simulate the complex progressive damage and failure behaviors commonly observed in fiber-reinforced composite materials. However, while these material models offer the capability for realistic simulations, their use requires the definition of numerous material parameters (i.e., elastic moduli and failure strengths in the different material directions). Ideally, these input parameters would be determined via a thorough experimental characterization program for the composite materials of interest. Unfortunately, given realistic time and cost constraints, the experimental determination of such a large number of material model parameters is not generally feasible. However, through the application of methods investigating the individual input parameter sensitivities and uncertainties, such thorough characterization techniques may not be necessary. A sensitivity analysis can be used to quantify the individual effect that each input parameter has on a simulation's output, effectively identifying those material parameters critical to the modeled response. Also, uncertainty quantification methods can be used to enumerate the influence of unknown input parameters on a simulated output response, allowing for reliable predictions in the absence of an exact material characterization.

Many examples exist in literature demonstrating the value of parametric sensitivity studies in the process of modeling various physical phenomena. The applications for this type of analysis have proven to be fairly far reaching with sampled references demonstrating relationships to many different scientific fields. For example, within the field of material science, Gunawan, et. al., utilized a sensitivity analysis to measure the activation energies most critical to computer simulations of boron diffusion in silicon [1]. In separate studies completed by Binici, et. al., Zheng, et. al., and Bryson, et. al., parametric sensitivity analyses were shown as applicable to civil engineering applications. Specifically, Binici, et. al., utilized sensitivity studies to determine which uncertain material parameters have the most profound effect on the behavior of reinforced concrete columns, Zheng, et. al., studied the influence of model parameters in simulations of the long-term deflection of continuous, rigid frame bridges, and Bryson, et. al, applied a sensitivity study to computer models of soils and clays loaded in compression [2-4]. Similar studies have also been utilized for vehicular and automotive applications. Hua, et. al., measured the effect of geometrical parameter variations of a dynamically loaded vehicle frame and Huang, et. al., examined the effect of material input parameters in models simulating the presence of "squeal" in automotive brakes [5-6].

Additional relevant studies have also been found in composites research. Namely, Radebe, et. al., and Daneshpayeh, et. al., demonstrated the use of sensitivity analyses in their studies of the effect of material property uncertainty on the performance of nanostructures and nano-composites [7-8], Vu-Bac, et. al., utilized a sensitivity analysis to assess the effect of uncertain material parameters on mechanical properties determined through multi-scale modeling [9], and Islam, et. al., utilized a sensitivity study in the process of optimizing manufacturing parameters for particleboards [10]. In another example from literature, Kenis, et. al., demonstrated the usefulness of a sensitivity study to geological applications as simulations modeling the development of specific rock formations were completed within a parameter study [11]. Finally, Zhang et. al., demonstrated the negative effect that material porosity and increasing void content can have on a composite's structural performance due to the variability that such material inconsistencies can create in the composite's mechanical properties [12]. This variability can be difficult to account for in finite element simulations when continuum methods are applied. Therefore, the application of uncertainty quantification techniques and parameter studies can be utilized to account for the inconsistencies voids can create in a composite material.

Examples from literature have demonstrated the usefulness of parameter studies within diverse scientific fields. Therefore, the objectives of this study deal with the application of sensitivity and uncertainty quantification techniques within the structural analysis of composite parts. Specifically, a sensitivity analysis will be completed for simulations of a carbon fiber composite material loaded in four-point flexure. The corresponding simulations will utilize a phenomenological composite material model that was recently developed and implemented into the production version of the Sandia National Laboratories' solid mechanics finite element analysis code. This model is capable of capturing such important composite material behaviors as progressive damage and post-failure softening, but requires the input of 77 separate material parameters. Therefore, the sensitivity analysis will be used to determine which of the material inputs are most critical to predictions of failure and only those critical parameters will be rigorously defined using experimental methods. Then, uncertainty quantification will be used to propagate any input parameter unknowns through to the predicted output response effectively predicting the material's flexural behavior in the absence of a complete experimental characterization of the model's 77 separate input parameters. Furthermore, the modeling methods verified with the uncertainty quantification simulations will be used to develop a surrogate, or approximation, model that can be used in conjunction with the experimental data to determine unknown material properties of interest.

2. Flexure Experiments

To demonstrate the proposed techniques and to provide validation data for the simulations, experiments were completed to characterize a carbon fiber/epoxy composite material in four point flexure. The flexural loading scheme was deemed desirable as the applied bending conditions provide for a complex and interesting response, which offer a good measure of the proposed technique's value through the planned computer simulations. Furthermore, experiments of this type are easily prepared for and conducted.

2.1 Composite Materials and Specimen Preparation

The flexural test specimens were composed of a carbon fiber reinforced polymer (CFRP) material consisting of an 8-harness textile, pre-impregnated carbon fabric with an epoxy based resin. Laminates for testing were manufactured with a hand lay-up process with precut ply kits, which were prepared with a CNC cutter in order to control the geometry and fiber orientation. The flat laminates were cured with a standard autoclave process under vacuum with an applied temperature and pressure of 350°F and 45 psig, respectively, as suggested by the manufacturer. Several specimens were cut from the consolidated laminates with a wet saw outfitted with a diamond blade. A total of four specimens were considered as part of this study and their average dimensions and stacking sequence are given in table 1.

2.2 Experimental Procedure

The described specimens were tested to failure in four-point flexure with an applied load span of 50 mm and support span of 100 mm (quarter-point loading). The tests were completed under displacement control with a crosshead descent rate of 5 mm/min and, throughout each test, displacement and load data were recorded directly from the testing machine crosshead and load cell with an acquisition rate of 10 Hz.

Upon testing completion, the measured specimen dimensions and recorded load-displacement data were used to determine the flexural stress and flexural strain as well as the flexural modulus. For this quarter point loading configuration, the maximum displacement and the crosshead displacement differences are accounted for, allowing the flexural strain, ε , and flexural modulus, E_f , to be expressed as:

$$\varepsilon = \frac{6t}{L^2} V_c \quad (1)$$

$$E_f = \frac{L^3}{8wt^3} \left(\frac{P}{V_c} \right) \quad (2)$$

Where the thickness, t , width, w , and length, L , are all specified from the specimen geometry, and the crosshead displacement, V_c , and applied load, P , are directly measured during the experiment. The flexural stress, σ_f , can be computed from equation 1 and equation 2, and is independent of the crosshead displacement. Also, the stiffness of the experimental load frame and fixturing was taken into account with respect to the flexural rigidity of the specimen, allowing the crosshead displacement to be used in all calculations rather than a direct measure of the central span deflection, simplifying the analysis procedure.

2.3 Experimental Results

With the methods described in the preceding section, flexural stress versus flexural strain and flexural modulus versus flexural strain curves were generated for each of the tested specimens in order to identify important characteristic features, as shown in figure 1. As evident in this figure, the elastic response is relatively linear and results in a peak flexural modulus of approximately 66 GPa at a strain of 0.8%. These curves further demonstrate a point of initial softening, or the point at which the rate of flexural stress increase begins to decrease. This occurrence was experimentally determined to correspond to the initiation of buckling on the top-most surface of the test specimen as the compressive strength of the outer, free-surface ply was exceeded (refer to sub-figure C in figure 1). Therefore, as the ability to formulate accurate predictions of a composite material's compressive behavior is both challenging and valuable, the simulation of this observed softening response was the focus of this study. Specifically, referring to figure 1, the sequence from A through C was the focus of this investigation. The additional sequences of events, from D through F, are included in figure 1 only for completeness.

3. Computational Methods

The four-point flexure characterization data presented in the preceding section was used to verify the potential usefulness of sensitivity analysis and uncertainty quantification during the definition of a simulated material's constitutive model. Specifically, a sensitivity analysis was completed to determine the critical input parameters, effectively identifying which parameters required the most thorough characterization, and uncertainty quantification was applied to measure the effect of input parameter unknowns on predictions of the composite's flexural response.

3.1 Description of Finite Element Model

3.1.1 Analysis Software

All simulations were completed using Sandia National Laboratories' Sierra Solid Mechanics code Adagio. Adagio is a Lagrangian, three-dimensional code for the finite element analysis of solid structures and is suitable for implicit, quasi-static analyses. Sierra Adagio makes use of a multi-level solver, the solution core of which is a nonlinear, conjugate gradient algorithm that can iteratively find a solution that is within some user-defined tolerance of equilibrium. Use of the multi-level solver within Adagio aids in the solution of problems containing such challenging aspects as contact, materials with non-linear responses or extreme differences in stiffness, and material failure with element death [13].

3.1.2 Element Formulation

All of the modeled components were simulated with eight-noded, hexahedral elements. For ease of application and decreased computational time, the element formulation default to Sierra Adagio was used. This formulation conducts the volume integration with single-point Gaussian quadrature. While the 1-point integration approach does represent a significant savings in computer time, it has a noteworthy disadvantage in the form of zero energy modes or hourglass modes. However, a simple method of controlling this spurious activity is to apply a small elastic stiffness that is capable of stopping the formation of any anomalous modes without affecting any global modes. Sierra Adagio is automatically equipped with a default "hourglass stiffness" of 0.05 and this value was used in all of the completed analyses [13].

3.1.3 Material Models

The three-dimensional components of the flexural experiment simulations were modeled with just two materials: the load rollers were made of steel and the flexural specimens were made of a carbon fiber/epoxy composite. The steel material was modeled with Sierra Adagio's elastic model as no yielding or failure was expected for the load rollers. This model describes a simple linear elastic behavior and the only material properties required for its use are: density, Young's modulus and Poisson's ratio [13].

Alternatively, the carbon fiber/epoxy material was modeled with a phenomenological composite constitutive model capable of capturing such relevant behaviors as non-linear damage, post-failure softening, and strain rate dependency [14]. With this model, the non-linear damage response is activated according to a set of partially interactive, quadratic failure criteria and, once initiated; damage evolves according to user defined damage moduli and hardening exponents. When the simulated damage is complete, the modeled material softens linearly according to user defined values describing the composite's strain energy densities. Specifically, a quadratic strain

criterion is used for both damage initiation and failure. Damage activation functions are evaluated in both tension and compression, in both the matrix and fiber modes, and on each of the material planes. As an example, the 11-plane matrix mode damage activations functions, ϕ , are given by equations 3 and 4 [15-18].

$$\text{Tension:} \quad \phi_{11+}^m = \sqrt{\left(\frac{E_{11}\langle\varepsilon_{11}\rangle}{X_{11+}^m}\right)^2 + \left(\frac{G_{12}\gamma_{12}}{S_{12}^m}\right)^2 + \left(\frac{G_{13}\gamma_{13}}{S_{13}^m}\right)^2} \quad (3)$$

$$\text{Compression:} \quad \phi_{11-}^m = \sqrt{\left(\frac{E_{11}\langle-\varepsilon_{11}\rangle}{X_{11-}^m}\right)^2 + \left(\frac{G_{12}\gamma_{12}}{S_{12}^m}\right)^2 + \left(\frac{G_{13}\gamma_{13}}{S_{13}^m}\right)^2} \quad (4)$$

Where, E_{ij} , G_{ij} , ε_{ij} , γ_{ij} , X_{ij} , and S_{ij} represent the material's moduli, strains, and strengths, respectively.

Once damage is initiated, the composite's stiffness is progressively degraded through damage variables, which are introduced to each of the material's stress components. The corresponding compliance tensor has the following form:

$$\mathbf{S} = \begin{bmatrix} \frac{1}{E_{11}(1-d_{11})} & \frac{-\nu_{21}}{E_{22}} & \frac{-\nu_{31}}{E_{33}} & 0 & 0 & 0 \\ \frac{-\nu_{12}}{E_{11}} & \frac{1}{E_{22}(1-d_{22})} & \frac{-\nu_{32}}{E_{33}} & 0 & 0 & 0 \\ \frac{-\nu_{13}}{E_{11}} & \frac{-\nu_{23}}{E_{22}} & \frac{1}{E_{33}(1-d_{33})} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2G_{12}(1-d_{12})} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2G_{13}(1-d_{13})} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2G_{23}(1-d_{23})} \end{bmatrix}$$

Where, d_{ij} represent the damage variables and E_{ij} and G_{ij} represent the elastic and shear moduli, respectively. Correspondingly, the stresses and strains can them be determined with $\boldsymbol{\sigma}=\mathbf{S}^{-1}\boldsymbol{\varepsilon}$. Note that the compliance tensor, $\mathbf{S}$, becomes singular when $d=1$, therefore the model is written such than the limit of stiffness as $d \rightarrow 1$ exists. The evolution of the damage variables, d_{ij} , is controlled by user-defined damage moduli and damage exponents. As an example, the evolution of matrix mode failure in each of the tensile, compressive, and shear directions is governed by the damage variable, d , given by equation 5.

$$d = 1 - \frac{K_m}{E} + \left(\frac{K_m}{E} - 1\right) \frac{1}{r_m^n} \quad (5)$$

Where, K_m and n represent the user-defined matrix mode damage moduli and exponents, respectively. Also, r_m represents the damage evolution variable, which is related to the monotonically increasing load function. In its simplest form, this load function would represent the ratio of the current model strain to the strain at failure.

Lastly, once the fiber mode strength is exceeded, the material is linearly softened according to user-defined quantities related to the material's strain and fracture energies. Refer to [14] for a more complete discussion of the material model.

As described by the equations above, this failure model requires the definition of numerous parameters related to a composite's behavior elastically as well as in failure. Specifically, 77 separate input parameters are required and are summarized in table 2. Note, regarding the material subscripts given in table 2, the 11-direction corresponds with the span direction of the flexural specimens, the 22-direction corresponds with the specimen widths, and the 33-direction refers to the specimen depths.

3.1.4 Model Geometry

Simulations of the four-point flexure experiments were completed with three-dimensional geometries and meshes created using Cubit, which is a robust software toolkit capable of creating both two- and three-dimensional geometries and meshes, and were based upon the dimensions shown in table 1. Also, as both the test specimen and loading conditions were symmetric across the specimens' widths and lengths, quarter model symmetry conditions were applied for simplicity and efficiency in calculation. The simulation geometry representative of the first flexural specimen tested is shown in figure 2 without mesh lines.

3.1.5 Boundary Conditions

Boundary conditions were applied to the flexural experiment simulations to model both the physical loading of the specimen through the steel rollers as well as to apply the symmetry boundary conditions. To emulate the physical loading conditions, constraints were applied to the flexural simulation models mimicking the actual test conditions. Specifically, the bottom-most, flat surface of the support roller was rigidly fixed in all degrees of freedom while the top-most, flat surface of the load roller was vertically displaced by 10 mm. This 10 mm displacement was chosen according to the load-displacement data recorded during the actual experiments. Specifically, an applied vertical displacement greater than 8 mm would guarantee the initiation of failure (points B through C in figure 1) in the simulated flexural specimens.

3.1.6 Contact Definitions

In addition to the boundary conditions, contact definitions were also specified for the flexural experiment simulations. Within Sierra Adagio, different contact algorithms exist that attempt to prevent any unrealistic interpenetration of adjacent model parts. The default contact algorithm in Adagio, which was used for all of the completed analyses, is the augmented Lagrange approach. This technique is similar to the commonly used penalty based approach, which applies a penalty force at points of contact experiencing spurious penetrations to eliminate the unwanted behavior.

In addition to specifying the contact algorithm for the simulations, specific contact interactions were also defined for all pairs of surfaces that were initially or that could potentially come into contact. These would be such surface pairs as the top surface of the specimen and the upper load roller and the bottom surface of the specimen and the lower load roller.

3.2 Mesh Convergence Study

In order to verify the finite element analysis methods described in the preceding sections and to allow for quantitative predictions of the flexural response, a grid convergence study was completed to confirm that the simulated solutions were converging to the same continuum value. Furthermore, this mesh study was also used to determine the appropriate mesh size for all ensuing models. To begin this investigation, the geometry corresponding to the first flexural specimen, represented by figure 2, was discretized with three different mesh sizes. The element sizes in these models were made progressively smaller through uniform refinement as the in-plane element length was reduced from approximately 1.11 mm to 0.556 mm to 0.137 mm. Figure 3 shows a portion of each of the three meshed models.

Next, the models represented in figure 3 were processed according to the boundary conditions and contact definitions described in the previous sections. The material parameters used to define the orthotropic-elastic-failure model were specified with plausible values found in literature. For the purposes of this verification study, the accuracies of the simulations' predictions were not as important as demonstrating that the three discretization levels converged to the same continuum solution. Therefore, the exactness of the properties defining the composite material model was not significant. Upon successful completion of these three simulations, an estimation of the exact value, or solution corresponding to an element size of zero, of the predicted softening load was determined with Richardson's Extrapolation. This method allows for the approximation of a higher order estimate of a

continuum value given a series of lower order, discrete values [19-20]. As shown in equation 6, with this technique, a discrete solution, f_k , can be thought of as the exact solution plus some error terms:

$$f_k = f_{exact} + g_1 h_k + g_2 h_k^2 + g_3 h_k^3 + \dots \quad (6)$$

Where g_i represents the i -th term error coefficient and h_k represents a measure of the grid spacing, or element size.

Then, if a second order method is assumed ($g_1 = 0$) for the above equation and if the discrete solutions exist for at least two different mesh sizes, the above equation can be solved for the exact, or continuum, solution with equation 7:

$$f_{exact} \approx f_1 + \frac{f_1 - f_2}{r^2 - 1} \quad (7)$$

Where r is the ratio of grid sizes, h_2/h_1 , and f_k represents the two discrete solutions. Then, the Richardson extrapolation given by the above equation can be generalized for any p -th order method (equation 8):

$$f_{exact} \approx f_1 + \frac{f_1 - f_2}{r^p - 1} \quad (8)$$

In equation 8, p is the order of convergence, or the order of accuracy, and it is related to the behavior of the solution's error. Given at least three solutions corresponding to three different mesh sizes, the value of p can be estimated through the solution of equation 9, in which r is again the ratio of discrete solution mesh sizes and ε_{ij} represents the differences in the discrete solutions, or $f_i - f_j$.

$$\frac{\varepsilon_{23}}{r_{23}^p - 1} = r_{12}^p \left(\frac{\varepsilon_{12}}{r_{12}^p - 1} \right) \quad (9)$$

For the described flexural experiment simulations, the Richardson's extrapolated exact solution was estimated to be 2363.6 N. Figure 4 shows a plot of the percent error calculated for each grid solution as a function of mesh size and figure 5 shows a comparison of the three simulated responses.

As shown in the above plots, the percent error decreases with each level of mesh refinement, indicating that these three initial simulations are converging to the calculated exact value and this lends confidence to the modeling procedure. Also, as there is a much smaller decrease in the percent error with the second level of mesh refinement, it has been assumed that a mesh size of 0.556 mm or smaller is adequate for this study's ensuing models.

3.3 Sensitivity Analysis

3.3.1 Overview and Methodology

As discussed in the preceding sections, the orthotropic-elastic-failure model requires the definition of up to 77 separate material input parameters. This number of parameters cannot easily or inexpensively be determined through experimental characterization. Rather, a sensitivity analysis can be applied to determine which of these parameters are truly influential to the simulated response, and then only those critical parameters must be rigorously defined.

As a first step, prior to initializing the sensitivity study, engineering judgment can be used to eliminate any of the parameters intuitively insignificant to a specific load case of interest. Then, with the remaining k parameters, a set of computer experiments can be designed in which the k -dimensional parameter space is sampled numerous times and each sampled parameter set is processed within a structural simulation utilizing a deterministic code, such as Sierra Adagio. Furthermore, if the high-dimensional parameter space is sampled in a representative and organized fashion, a minimum number of sample sets and simulations can be used to develop and recognize trends and relationships between the individual k input parameters and the simulated output.

There are many different approaches that can be taken to efficiently sample the k -dimensional parameter space. One such approach is the Box Behnken Design method (BBD). This approach, which was chosen for all ensuing sensitivity studies, offers a highly stable sampling method. Specifically, the BBD methodology avoids overly extreme parameter combinations and, unlike similar methods (e.g. central composite design method), it does not sample outside of the process space. Additionally, when compared to other similar approaches, this method seems to require fewer overall samples to develop trends between the input parameters and the output, as the number of computer experiments designed with the BBD approach, N , for k input parameters is given by

$N = 2k(k - 1) + 1$ [21]. Upon completion of the N simulations, the individual parameter sensitivities can be assessed. This assessment can be readily conducted with a multi-way analysis of variance (ANOVA). Specifically, the ANOVA represents a model independent, probabilistic sensitivity analysis method that can be used to determine the existence of statistical associations between an output response and one or more input parameters [22].

3.3.2 Sensitivity Analysis Results

The methods described in the preceding section were used to conduct a sensitivity analysis of the orthotropic-elastic-failure model. The study specifically examined the influence of this material model's parameters on the predicted softening load due to the four-point flexural loading scenario (figure 1). The sensitivity analysis made use of the geometry and boundary conditions corresponding to the first flexural experiment conducted (figure

2) and, due to similarities observed during the characterization process, the material model parameters specified as critical for this single experiment were assumed as critical for the remaining experiments as well.

As mentioned, the first step in the sensitivity analysis process was to eliminate any unnecessary material parameters with engineering judgment. Of the 77 material parameters listed in table 2, 30 were deemed insignificant for this quasi-static, flexure load case. These neglected parameters as well as justifications for their eliminations are shown in table 3.

With the remaining material input parameters, the BBD method was used to develop a 47-dimensional parameter space and design 4,325 computer experiments. These experiments, or simulations, were processed within Sierra Adagio utilizing the verified geometry and medium refinement mesh shown in figure 3. The 4,325 resulting softening load predictions are shown in figure 6.

As shown in the figure, horizontal trends are evident. As this indicates the presence of critical material parameters, a multi-way ANOVA was applied to the presented data to identify which of the 47 parameters were in fact influencing. The completed analysis of variance indicated that only 11 of the 47 examined material model inputs were critical. A summary of the ANOVA results for these 11 critical parameters is given in table 5. Since the ANOVA tests the null hypothesis that the variance associated with a specific input parameter is equal to that of the overall population, low probability values, or p-values less than 0.05, indicate sufficient evidence to reject this hypothesis. Therefore, the input parameters described in table 5 are demonstrably critical to the simulated response. Furthermore, these parameters are primarily related to in-plane compression and out-of-plane crush, and this seems to agree with intuition in terms of which composite material properties are relevant to a flexural loading scenario.

4.1 Uncertainty Quantification

4.1.1 Overview and Methodology

Upon completion of a sensitivity analysis, some of the original k input parameters will be specified as influential to the simulated response. Then, significant effort can be expended in the process of characterizing these critical input parameters exactly. However, it is possible that certain critical material parameters cannot be determined experimentally, possibly due to cost constraints or lack in experimental expertise. For example, lacking suitable test fixtures, the out-of-plane compressive and shear properties for a fiber-reinforced, polymer composite material are difficult to determine experimentally. Nonetheless, it is likely that through additional numerical analyses or thorough literature surveys, accurate ranges for which the critical parameters may fall within can be

determined. Then, given uniform or normal distributions that describe the influential input parameters, uncertainty quantification can be used to propagate input parameter uncertainties through a simulation to determine the corresponding uncertainty in the predicted output response. This is readily achieved by sampling each input parameter range n times, creating n sets of sampled parameters. Then, n simulations can be processed in which the material model is defined with the n parameter sets. The resulting distribution of n simulation responses will represent the output range corresponding to the input parameter uncertainties [23].

The statistical method used to create the n parameter sets sampled from the input ranges is important as full coverage of the parameter space needs to be guaranteed. A sampling method that is commonly used to construct computer experiments is the Latin Hypercube Sampling (LHS) approach. Given a predefined number of sample points, the LHS method can be used to ensure that a random ensemble of sampled variables is truly representative of reality [24]. Therefore, this approach was chosen for the ensuing uncertainty quantification studies associated with this presented work.

4.1.2 Uncertainty Quantification Results

It was not possible to experimentally determine all 11 parameters found to be critical for the flexural load case. Specifically, just three of the influential parameters were characterized through physical testing. These properties, E_{11} , ν_{12} , and G_{12} , were readily determined with standardized, in-plane tension testing and their values are shown in table 5.

The remaining eight critical parameters were specified within plausible ranges through either a micromechanical model representing a unit cell of the composite material [25] or with a thorough literature review. Table 6 summarizes these defined ranges.

As several of the influencing material model parameters were defined within plausible ranges, uncertainty quantification was used to determine the corresponding ranges in the softening loads predicted for the tested flexural specimens. With the methods described in the previous section, the LHS method was used to sample the ranges of values given in tables 5 and 6 100 times, creating 100 sets of sampled parameters. These 100 parameter sets were then applied to the material models in 100 simulations and these simulations were processed with Sierra Adagio.

This process of creating and processing 100 simulations was completed for the tested specimens described in table 1. For each specimen, upon completion of the computer experiments, the distribution created by the 100 simulated responses was tested for normality with the adjusted Anderson-Darling statistic [32]. The distributions of

softening loads predicted for each of the four test specimens were verified as normal. Therefore, a histogram and normal distribution was fit to each set of 100 simulations and the mean value of the distribution was compared to the experimentally observed load at initial softening. Figure 7 shows a histogram and normal distribution representative of the uncertainty quantification process and table 7 summarizes the simulation and experimentally observed data.

Several observations can be made regarding the softening load predictions presented in table 7. First, it is important to note that the percent differences between the predicted responses and the experimentally observed behaviors are small, as no specimen presented a percent difference greater than 10%. This perhaps indicates that the uncertainty quantification, coupled with the sensitivity study, can be used to make accurate predictions in the absence of exact material property values. There is also only a small difference in the mean values predicted for the softening loads for the four modeled flexural specimens, with the largest deviation occurring with specimens #1. According to the specimen dimensions given in table 1, this could indicate that, while the small dimensional deviations observed between tested specimens do not largely affect the simulated response, the measured difference between the individual specimens' depths have the most noticeable effect on the simulated responses. Specifically, perhaps this observation could be related to the decreased span-to-depth ratio specimen #1 exhibits. As a final observation, the predicted softening loads are consistently lower than the experimentally observed values. Through the application of the two-sample t-statistic, there is only a 2.6% chance of a softening load prediction exceeding an experimentally observed value [33]. Although this behavior can likely be attributed to parameter variations not accounted for during the study, such as variations in the experimental set-up (i.e., support span variations), it could lend confidence to the presented methodology for a conservative prediction of the onset of failure in a flexurally loaded composite.

4.1.3 Surrogate Modeling for Material Parameter Estimation

The uncertainty quantification results presented in the previous section indicate that the developed modeling approach provides a reasonably accurate simulation of reality. Therefore, an additional Latin Hypercube Sampling (LHS) study was completed to allow for the estimation of an unknown material property through the application of a response surface method. Specifically, a response surface, or surrogate, model of the simulations discussed in the preceding section was used to provide an estimate of the COMPRESSIVE_FIBER_STRENGTH_11, which corresponds with the observed buckling behavior.

As previously discussed, the orthotropic-elastic-failure model is difficult to experimentally characterize. However, as discussed by [34], a conventional method of estimating an unknown mechanical property is to approximate a physical response through finite element analysis. Specifically, an experiment, such as the four-point flexure characterization discussed in section 2 of this paper, is conducted. Then, a validated finite element model of the experiment, such as the model discussed in section 3, is solved several times in an attempt to reproduce the measured physical response. In each execution of the finite element model, a trial value is used to define the unknown mechanical property and the model response is compared to the experimentally observed behavior. While this approach for parameter estimation is valuable, the repeated solution of a high-fidelity finite element model can be prohibitively computationally expensive. Therefore, a response surface model, or a surrogate model, which represents a regression analysis of a higher fidelity model, can instead be developed and implemented.

To generate the surrogate model, three different regression types (constant, linear, and quadratic) were applied to the LHS study. Then, the Leave-One-Out-Cross-Validation (LOOCV) method was implemented to provide an evaluation of the relationships developed by each of the three regression types. LOOCV simply removes one observation from the simulation set and defines it as the “testing set.” Then, the regression is applied to the remaining simulated observations to generate a surrogate model. The surrogate model is then applied to the “testing set” to measure whether or not it is capable of producing a prediction close to the value associated the high-fidelity model [35]. The LOOCV completed for the LHS study of the flexural experiments generated mean absolute errors for each of the three regression types. These errors were 1.90%, 1.86% and 2.61% for the constant, linear, and quadratic regression types, respectively.

Utilizing the linear regression model, as it presented the lowest LOOCV error; a new LHS study was completed to determine the buckling strength of the topmost composite layer, or the COMPRESSIVE_FIBER_STRENGTH_11 material property. Specifically, given the known experimental data and the data ranges presented in tables 5 and 6, the surrogate model was solved to determine the composite’s buckling strength. The final result was a distribution of values corresponding to the desired compressive strength. A histogram of these values and its corresponding normal distribution is shown in figure 8 and the mean and standard deviation are 840.7 MPa and 47.8 MPa, respectively.

As a means of validated this prediction, the standard deviations associated with the experimental characterization of the fiber direction dominated properties, partially represented by the data in table 5, were

compared with the standard deviation predicted for the compressive fiber strength (47.8 MPa). Specifically, physical experiments to determine the TENSILE_FIBER_STRENGTH_11 parameter resulted in a measured standard deviation of 37.3 MPa. This value compares well with the predicted deviation and helps provide confidence in the surrogate model method of parameter estimation, as similar deviations indicate that the strength prediction accurately represents the physical material.

5. Summary and Conclusions

A sensitivity analysis and a parameter study were completed with finite element simulations of four-point flexural experiments to demonstrate the ability to make accurate predictions of a loaded structures response and unknown material properties without a comprehensive experimental material characterization program. Specifically, a sensitivity analysis was used to indicate which of a recently implemented composite material model's input parameters were most critical to accurately predicting the flexural response of a composite. Through the application of the Box Behnken Design method and a multi-way ANOVA, the necessity to define the material model's 77 input parameters was decreased to only 11. The uncertainties in these inputs were then propagated through the model in order to provide a statistical distribution of the output response. These results provided sufficient statistical evidence in the model's ability to formulate reliable predictions in the absence of an exact material characterization, as only three of the 11 critical input parameters could be defined exactly. The results of the verified uncertainty quantification were then used to develop a surrogate model that was used to estimate an unknown material parameter, which was experimentally validated.

This sensitivity analysis procedure can be used to help optimize and streamline the material definition process for future simulations involving any material model requiring a large number of unknown input parameters. The timely completion of this analysis can be used to prioritize material characterization efforts as well as to eliminate the need to expend unnecessary effort in the determination of material properties insignificant to a simulated load case of interest.

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Figure Captions

Figure 1: Summary of experimental results with characteristic features identified

Figure 2: Representative geometry of four-point flexure simulations

Figure 3: Three models with mesh refinement for mesh convergence study

Figure 4: Error between softening loads predicted for three mesh sizes and the exact solution

Figure 5: Simulated responses for three mesh sizes with representative displacement contour

Figure 6: Predicted initial softening loads for 4,325 simulations

Figure 7: Representative distribution of uncertainty analysis simulation output

Figure 8: Histogram of estimated compressive strengths

Table 1: Typical dimensions for flexural specimens

Width (mm)	Length (mm)	Thickness (mm)	Stacking Sequence
24.57	135	2.93	$[(0/90)_4]_5$

Table 2: Orthotropic-elastic-failure material model input parameters

<u>Elastic Properties</u> E11, E22, E33 NU12, NU13, NU23 G12, G13, G23	<u>Post-Failure, Damage Evolution Properties (Cont'd)</u> COMPRESSION_COUPLING_FACTOR_11, _22, _33 TENSILE_DAMAGE_MODULUS_11, _22, _33 COMPRESSIVE_DAMAGE_MODULUS_11, _22, _33 SHEAR_DAMAGE_MODULUS_12, _23, _13 HARDENING_EXPONENT_11, _22, _33 HARDENING_EXPONENT_12, _23, _13
<u>Initial Failure Properties</u> TENSILE_MATRIX_STRENGTH_11, _22, _33 COMPRESSIVE_MATRIX_STRENGTH_11, _22, _33 TENSILE_FIBER_STRENGTH_11, _22, _33 COMPRESSIVE_FIBER_STRENGTH_11, _22, _33 SHEAR_MATRIX_STRENGTH_12, _23, _13 SHEAR_FIBER_STRENGTH_12, _23, _13	<u>Strain Rate Dependency Properties</u> REFERENCE_STRAIN_RATE ELASTIC_RATE_COEFFICIENT_11, _22, _33 ELASTIC_RATE_COEFFICIENT_12, _23, _13 FIBER_STRENGTH_RATE_COEFFICIENT_11, _22, _33 FIBER_STRENGTH_RATE_COEFFICIENT_12, _23, _13 MATRIX_STRENGTH_RATE_COEFFICIENT_11, _22, _33 MATRIX_STRENGTH_RATE_COEFFICIENT_12, _23, _13 FIBER_STRENGTH_RATE_COEFFICIENT_12, _23, _13 MATRIX_STRENGTH_RATE_COEFFICIENT_11, _22, _33
<u>Post-Failure, Damage Evolution Properties</u> TENSILE_FRACTURE_ENERGY_11, _22, _33 COMPRESSIVE_FRACTURE_ENERGY_11, _22, _33 SHEAR_FRACTURE_ENERGY_12, _23, _13 CHARACTERISTIC_LENGTH MAXIMUM_COMPRESSIVE_DAMAGE_11, _22, _33	

Table 3: Parameters eliminated from sensitivity analysis with engineering judgment

<i>Property</i>	<i>Justification</i>
TENSILE_MATRIX_STRENGTH_11, _22 COMPRESSIVE_MATRIX_STRENGTH_11, _22 TENSILE_DAMAGE_MODULUS_11, _22 COMPRESSIVE_DAMAGE_MODULUS_11, _22 HARDENING_EXPONENT_11, _22, _33	<p>These 10 parameters define the “knee” point behavior observed in composites materials. However, since most carbon fiber/epoxy composites are linear to failure in in-plane tension and compression, these parameters can be ignored.</p>
CHARACTERISTIC_LENGTH	<p>This is a mesh dependent variable and is not a measurable material property.</p>
REFERENCE_STRAIN_RATE ELASTIC_RATE_COEFFICIENT_11, _22, _33 ELASTIC_RATE_COEFFICIENT_12, _23, _13 FIBER_STRENGTH_RATE_COEFFICIENT_11, _22, _33 FIBER_STRENGTH_RATE_COEFFICIENT_12, _23, _13 MATRIX_STRENGTH_RATE_COEFFICIENT_11, _22, _33 MATRIX_STRENGTH_RATE_COEFFICIENT_12, _23, _13	<p>These 19 parameters define strain rate dependencies. Since the flexural tests were completed at quasi-static loading rates, these parameters can be ignored.</p>

Table 4: Summary of critical material model input parameters

Input Parameter	ANOVA p-value
E11	0.0000
E33	0.0000
NU12	0.0000
NU13	0.0011
G12	0.0000
G13	0.0000
COMPRESSIVE_FIBER_STRENGTH_11	0.0002
COMPRESSIVE_MATRIX_STRENGTH_33	0.0000
SHEAR_MATRIX_STRENGTH_13	0.0004
SHEAR_FIBER_STRENGTH_13	0.0000
SHEAR_DAMAGE_MODULUS_13	0.0000

Table 5: Critical material parameters determine through testing

Parameter	Mean	Standard Deviation
E_{11}	63.9 GPa	2.40 GPa
ν_{12}	0.050	0.019
G_{12}	3.93 GPa	0.110 GPa

Table 6: Plausible ranges defined for unknown critical parameters

Parameter	Minimum	Maximum	Reference
E33	8.19 GPa	8.98 GPa	[25]
NU13	0.399	0.416	[25]
G13	3.00 GPa	3.53 GPa	[25]
COMPRESSIVE_FIBER_STRENGTH_11	517 MPa	917 MPa	[26]
COMPRESSIVE_MATRIX_STRENGTH_33	150 MPa	325 MPa	[27-29]
SHEAR_MATRIX_STRENGTH_13	25 MPa	70 MPa	[30-31]
SHEAR_FIBER_STRENGTH_13	60 MPa	83 MPa	[26]
SHEAR_DAMAGE_MODULUS_13	166 MPa	345 MPa	[30-31]

Table 7: Summary of experimental and simulation results

Specimen #	Actual Softening Load	Predicted Softening Load	% Difference
1	2185.8 N	2098.2 N	4.1%
2	2181.9 N	2087.1 N	4.4%
3	2237.6 N	2087.4 N	6.9%
4	2243.4 N	2087.6 N	7.2%

Figure 1

A Experiment Begins

B Elastic Bending

C Buckling
Compressive Tows

D Load
Redistribution

E Buckling
at Load Point

F Load
Redistribution

Figure 2

Figure 3

Figure 4

Figure 5

Figure 6

Figure 7

Figure 8