DEVELOPMENT AND IMPLEMENTATION OF A PARAMETER ESTIMATION AND POST-PROCESSING TOOL FOR THE FAILURE ANALYSIS OF COMPOSITE MATERIALS

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KEYWORDS

Composite Materials, Failure Analysis, Parameter Estimation.

ABSTRACT

In engineering practice, the barrier for the application of a superior, mode based, failure model like for example the Puck Criterion [1] is still quite large compared to simpler phenomenological models like the Tsai-Wu criterion [2]. The reasons being that the latter is often applicable as a user sub-routine in finite element codes and since the related experimental data naturally shows a large scatter, a robust routine for the parameter estimation is needed to exploit the advantages of a more sophisticated failure mode based model.

In this paper a free to use numerical tool is presented that helps to overcome the aforementioned barriers and facilitates the application of Puck's Failure criterion for structural integrity analysis. The tool offers two modules: the first helping with the parameter estimation and determination of the related confidence intervals, the second module performing a structural integrity analysis using FE stress data. The latter giving both, the critical failure location and the leading failure mode which are important information for a design optimization.

1. INTRODUCTION

For the failure analysis of composite structures and components different failure criteria have been presented and analyzed in the literature. The simplest of them are the maximum strain or the maximum stress criteria and quadratic criteria like the Tsai-Wu criterion [2]. However, even though these criteria might give a good estimate of the critical loading state for multi-axial stress-states, they are formulated purely phenomenologically without any knowledge of the critical failure modes. In contrast to this, the Puck Failure Criterion [1] is advantageous since it combines different individual failure criteria for different failure modes. The Puck failure criteria for example differentiates between tensile and compressive fiber-failure and inter fiber-failure. The latter is further divided into tensile failure, shear failure and compressive failure.

For the practical application such a failure mode-based criteria has two main advantages: first of all, the fit to experimental data is generally much better and thus the modeling error will be smaller. As an example, this has been shown by the present authors for tests under cryogenic conditions in [3]. Second, the application of a failure-mode based criterion gives the designer important information not only on where the component might fail, but also on how this component (failure-mode) might fail. This in turn gives important information on how the component can be optimized with respect to its overall strength.

Despite these advantages, in engineer practice the simpler maximum stress or strain criterion and the quadratic Tsai-Wu criterion are often preferred. In the authors opinion there are two reasons for this: first of all, the simpler criteria are often available as a material model in finite element codes and are therefore applicable directly without the need to program additional post-processing routines or user sub-routines. Secondly, experimental results used to determine material parameters of a failure criterion naturally shows a large scatter, therefore a robust routine to determine these material parameters is needed to exploit the advantage of the Puck failure criterion.

In this paper a numerical tool is presented that helps to overcome the aforementioned barrier and facilitates the application of Puck's Failure criterion for structural integrity analysis. The tool consists of two modules that can be applied together or individually. The first module is a numerical fitting routine offering different optimization strategies to determine the requested material parameters together with related confidence intervals. The second module can be used for the structural integrity analysis itself using numerical results from a FE Stress analysis using the finite element solver

MSC Nastran [4]. The tool can be downloaded from ESA [5] and is free to use.

2. PUCK FAILURE CRITERION FOR PLANE STRESS

In most cases in the integrity analysis of composite laminates, the consideration of plane stress states with $\sigma_{33} = \sigma_{23} = \sigma_{13} = 0$ is sufficient since for plane structures, no pronounced stresses acting transversely to the laminate plane develop. In this case, an analytical solution to the optimization problem for the determination of the failure plane angle Θ_f can be derived (Puck and Schürmann [2,6]). In this case, the inter fiber failure criteria are obtained for the three inter fiber failure modes A, B and C. In this context, mode A describes a tensile failure mode with a complete separation of the specimen. Mode B describes a shear failure mode without or with limited friction of the failure surfaces due to a possible compressive normal load. Mode C describes a failure of the laminate ply under compression, occurring locally by means of a wedge-like shearing mode. The failure surface together with the individual failure modes is illustrated Figure 1. Together with the fiber failure modes $f_{\mathrm{ff}}(\boldsymbol{\sigma})$, the individual failure criteria for inter fiber failure $f_{\mathrm{iff}}(\boldsymbol{\sigma})$ are assembled to a continuous, but not necessarily smooth, joint failure surface as follows:

$$f(\boldsymbol{\sigma}) = \frac{f_{\mathrm{iff}}(\boldsymbol{\sigma})}{f_{\mathrm{w}}(\boldsymbol{\sigma})} \quad \text{with} \quad f_w(\boldsymbol{\sigma}) = 1 - \left(0.9 f_{\mathrm{ff}}(\boldsymbol{\sigma})\right)^n, \; n > 0. \tag{1}$$

Where $n > 0$ describes the narrowing of the failure envelope along the fiber axis $\mathbf{e}_1$ (Figure 2). As illustrated in Figure 1 and Figure 2 the failure envelope is described by the following material parameters: S_{22}^t, S_{22}^c and S_{12}^s, the inter fiber tensile compressive and shear strength respectively, S_{11}^c, S_{11}^t, the fiber compressive and tensile failure stress, p_{21}^+, p_{21}^-, describing the slope of the inter fiber failure envelope towards the positive and negative side of the σ_{12}-axis and p_{22}^- implicitly describes the position of the intersection between modes B and C. This parameter is not an independent parameter and related to the other parameters by

$$p_{22}^- = \frac{1}{2}\left(\sqrt{1 + 2p_{21}^- \frac{S_{22}^c}{S_{21}^s}} - 1\right) \tag{2}$$

Further details on the implemented equations for plane stress are not repeated here and can be found in the tool documentation that can be accessed from [5].

3. PARAMETER ESTIMATION METHODS

To get an estimation for the material parameters two numerical methods are available in the PuckFailure Tool. The first method is a very simple and robust approach using the method of least square optimization. The second approach is a more sophisticated approach using the maximum likelihood method.

Applying the maximum likelihood method [7] an estimation for the parameter vector $\theta = (S_{11}^c, S_{11}^t, S_{22}^c, S_{22}^t, S_{12}^s, p_{12}^+, p_{12}^-)$ is obtained by maximizing the logarithm of the likelihood function $L(\boldsymbol{\Theta}; \boldsymbol{\sigma})$

$$\begin{aligned} \boldsymbol{\theta} &= \arg\max_{\boldsymbol{\theta}\in\mathcal{G}}(\ln\left(L(\boldsymbol{\theta}; \boldsymbol{\sigma})\right) \\ &= \arg\min_{\boldsymbol{\theta}\in\mathcal{G}}(-\ln\left(L(\boldsymbol{\theta}; \boldsymbol{\sigma})\right). \end{aligned} \tag{3}$$

The Likelihood function itself is defined by assuming a probability density function $\rho(\boldsymbol{\sigma}_i, \boldsymbol{\theta})$ for the scatter of the experimental data $\boldsymbol{\sigma}_i, i = 1, \ldots, n$. By further assuming statistical independence of the individual measurements the joint probability of all measurements can be written as

$$L(\boldsymbol{\theta}; \boldsymbol{\sigma}) = \prod_{i=1}^{n} \rho_i(\boldsymbol{\theta}; \boldsymbol{\sigma}_i). \tag{4}$$

In general, the user of this tool will have access to insufficient data to perform a statistic hypothesis test. But since the experimental data $\sigma_i, i = 1, \ldots, n$ represent the measurements from uniaxial tensile tests and these are found to follow a normal distribution in [8], the assumption that the test data follows a normal distribution is adopted here.

Compared to the least square approach, this method offers further options for the parameter estimation described next.

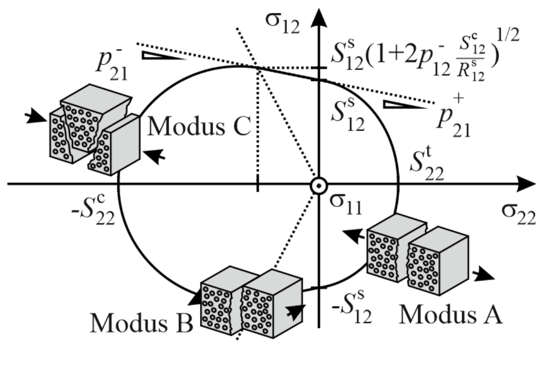

Figure 1: inter fiber failure envelope

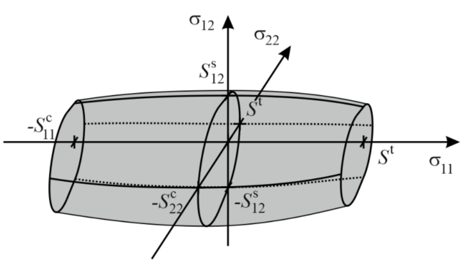

Figure 2: Complete failure envelope for plane stress states

3.1. Confidence Interval Estimation

A confidence interval for the estimated parameters can be calculated applying the so-called Profile-Likelihood method [9].

For this an α-confidence interval $CI_i = [\theta_L^i, \theta_U^i]$ is calculated for every parameter θ^i such that this parameter lays within this interval with a probability of α:

$$P(\theta_L^i \leq \theta^i \leq \theta_U^i) = \alpha. \quad (5)$$

In the context of the Profile-Likelihood method the upper and lower bounds θ_U^i and θ_L^i for every parameter θ^i are calculated individually such that

$$CI_i = [\theta_L^i, \theta_U^i] = \{\theta^i : L_{PL}(\Theta_i) - L(\widehat{\boldsymbol{\Theta}}) \leq q_k(\alpha)\}. \quad (6)$$

In here, $\widehat{\boldsymbol{\Theta}}$ is the solution from (3), $q_k(\alpha)$ is the (α)th quantile of the χ^2 distribution for k degrees of freedoms and $L_{PL}(\Theta_i)$ is the profile likelihood function for the parameter of interest θ_i:

$$L_{PL}(\Theta_i) = \max_{\boldsymbol{\Theta} \in \Psi(\Theta_i)} L(\boldsymbol{\Theta}), \quad (7)$$

which is nothing else then the maximum likelihood problem where the parameter Θ_i is held constant. In the implementation Θ_i according to (6) is found by incrementally increasing (decreasing) by $\Theta_i = \Theta_i \pm h$ for the lower (upper) bound until a Θ_i is found that fulfills

$$L_{PL}(\Theta_i) - L(\widehat{\boldsymbol{\Theta}}) \leq q_k(\alpha) \quad (8)$$

As a default value the tool tries to determine the 95% confidence interval ($\alpha = 0.95$), however if the scatter of the experimental data is large, this can result in unphysical (negative) Puck material parameters, that are violating (9)) or Puck material parameters that are resulting in failure envelopes limits that are crossing each other. In such a case α is automatically reduced (until α = 0.3) until upper and lower limits are found that result in physically admissible upper and lower limits.

3.2. Conservative Estimation

Furthermore, the parameter estimation based on the maximum likelihood approach, with or without the confidence interval calculations, requires the solution of the optimization problem (3). By applying an optimization algorithm suitable for the solution of a constrained optimization problems further boundary conditions can be considered for the parameter estimation. This is used to constrain the slope of both, the Mode A, and the Mode B failure condition to be negative at $\sigma_{22} = 0$, which is equivalent to

$$p_{21}^- > 0 \text{ and } p_{21}^+ > 0. \quad (9)$$

The mechanical interpretation of this condition is that the shear strength is increased (decreased) by a superimposed compressive (tensile) stress σ_{22} (see also Figure 1). Beside this mechanical motivated constraint, the constrained optimization algorithm is used to realize a conservative estimation method where all n experimental data points $\boldsymbol{\sigma}_i$ should lay outside of the estimated failure envelope. Mathematically this is written as

$$f(\boldsymbol{\sigma_i}) \geq 1 \quad \forall \mathrm{i} = 1, \ldots, \mathrm{n}. \quad (10)$$

To solve the optimization problem (3) as well as the optimization problems resulting from the Profile-Likelihood method a sequential least squares programming method complemented with a basin-hopping approach is used. This implementation is provided from the “basinhopping” method together with the SLSQP method from the Python Scipy library. Details of the implementation can be found in the Scipy documentation. This optimization algorithm is chosen since it allows to find the global minima of nonlinear constrained optimization problems considering the boundary conditions given in Equations (9) and (10).

4. IMPLEMENTATION

Both modules of the PuckFailure structural integrity analysis tool, *i.e.*, the parameter estimator and the post processing module, are implemented using Python. A stand-alone executable of the Implementation can be obtained from [5]. The tool is started from a command line and the individual modules, together with further control keywords, are controlled in an ini-type job file. Using the estimator module, both, experimental input and estimated material parameters, are given and received in the yaml file format. The latter can directly be used as an input for the second module to perform the structural integrity analysis. For this, stress field data from a Finite Element analysis using MSC Nastran [4] must be provided in the hdf5 file format. The results of the failure analysis are given as the commonly used margin of safety λ. With $f_{\max} = \max\{f_{\mathrm{ff}}, f_{\mathrm{iff}}\}$, the margin of safety λ can be written as

$$\lambda = \frac{1 - f_{\max}(\boldsymbol{\sigma})}{f_{\max}(\boldsymbol{\sigma})} \quad (11)$$

The margin of safety as well as additional information on the leading failure mode is written to an extended copy of the hdf5 input as well as a csv data file. The hdf5 output file can directly be used for further post-processing analysis or to simply generate contour plots using the post-processor Patran. Importantly the parameter estimation module can be used as a stand-alone tool and is therefore of great general interest also for users not using Nastran and or Patran for their structural integrity analysis.

Since the material strength generally shows a large temperature dependency, the PuckFailure tool can also handle temperature dependent data to perform a temperature dependent structural integrity analysis. For this, multiply experimental datasets for different temperatures can be used as an experimental input. For every given temperature dataset, a corresponding set of material parameters is obtained and can thereafter be used for the structural analysis. Material parameters for missing temperatures, if needed, are inter- or extrapolated from the existing dataset.

5. EXAMPLES

To demonstrate the implemented methods some examples are investigated in the following. For this a test campaign on a unidirectional carbon fiber reinforced epoxy, fabricated by Nieke Composites, is used for a parameter estimation showing some of the implemented functionalities. The test campaign includes unidirectional tensile and compression tests with unidirectional reinforced samples having an angle between reinforcement and loading axis of 0,15,30,60 75 and 90 degrees. Additionally shear experiments using double-notched samples have been conducted. The Test campaign was repeated at 295- and 4.2-degree Kelvin. Further details of the test campaign can be found in [10].

The failure envelope from the Maximum Likelihood estimation for both temperatures are compared to the experimental data in Figure 3 and Figure 4, whereas for reasons of clarity the failure envelope is only plotted for zero fiber stress ($\sigma_{11} = 0$). Since fiber stress interaction is not considered in this example, the represented failure envelope does not vary with $\sigma_{11} \neq 0$ and therefore also the experimental data points with $\sigma_{11} \neq 0$ are added to Figure 3 - Figure 6.

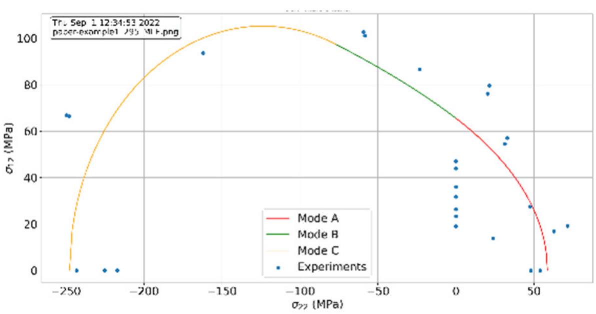

Figure 3: Maximum Likelihood estimation of the Puck failure envelope for inter-fiber failure at ambient temperature T = 295K.

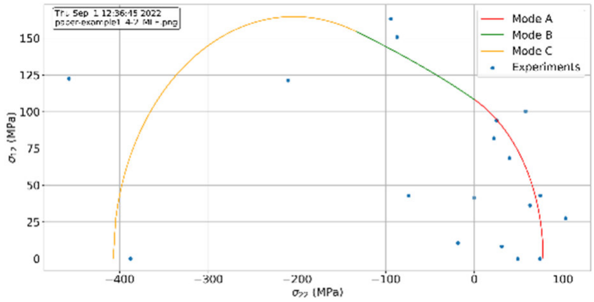

Figure 4: Maximum Likelihood estimation of the Puck failure envelope for inter-fiber failure at cryogenic temperature T = 4.2K.

Figure 5 and Figure 6 show some additional variants of the maximum likelihood estimation. In Figure 5 the conservative estimation of the Puck failure envelope is calculated incooperating the conservative constraint (10). An example of the confidence interval estimation using the profile Likelihood method is shown in Figure 6. In this example the probability α (see Equation (5)) was automatically reduced to 35% to result in physically admissible boundary failure envelopes. Partly this can be a attributed to the large scatter of the data itself which is also seen in the large variance of the estimated material parameters (see Table 1), but can also be attributed to the approach itself (discussed next).

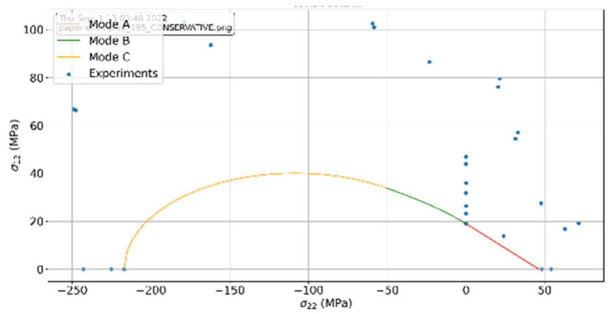

Figure 5: Conservative Maximum Likelihood estimation of the Puck failure envelope for inter-fiber failure at ambient temperature T = 295K.

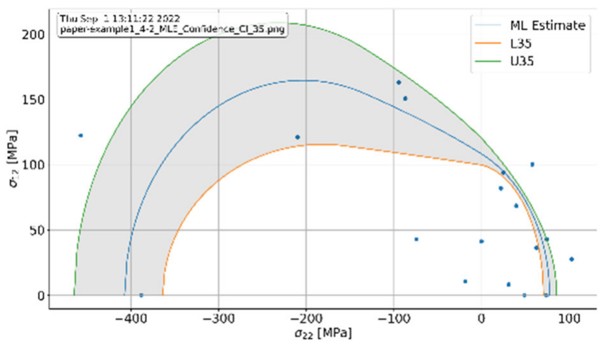

Figure 6: Maximum Likelihood estimation of the 35% confidence interval for the Puck failure

envelope for inter-fiber failure at cryogenic temperature T = 4.2K.

Table 1: Summary of the estimated Puck material parameters applying different methods

	p_{12}^{-}	p_{12}^{+}	S_{12}^{s}	S_{22}^{c}	S_{22}^{t}
295K MLE	0.5	0.5	65.5	247.5	58.6
295K MLE, conservative	0.41	0.41	19.0	217	46.3
4.2K MLE	0.42	0.42	108.3	407.1	77.7
4.2K MLE, upper bound	0.66	0.74	120.3	464.5	85.7
4.2 MLE, lower bound	0.1	0.16	99.8	363.5	70.6

6. DISCUSSION

This work presented a structural integrity analysis tool called PuckFailure that is available for free. The tool not only helps with the structural failure analysis, applying the Puck failure criterion, itself, but also provides various possibilities to easily perform the related parameter fitting based on experimental data from uniaxial tensile and shear tests. In practice, the parameter fitting to scatted data is often done intuitively by hand not following any repeatable procedure. In this work several examples applying some of the implemented methods showed a large variance of the estimated parameters. This underlines the importance of a parameter estimation methods that repeatable determine material parameters for a given experimental dataset. Only by such a method it is possible to systematically compare the multiaxial strength of different materials and also their influence on the failure load (and failure mode) of components.

To quantify (and compare) the confidence of the estimated material parameters the Profile-Likelihood method has been implemented. Beside measuring the confidence of the parameters, themselves, this can also be used to quantify the confidence of a structural integrity analysis simply by repeating the post-processing step for both, the upper and lower limit, using the provided material parameters. However, it has turned out that the estimation of a confidence interval with a large probability α often leads to physically non feasible bounds of the failure envelope. The reason for this is, that the profile likelihood method calculates bounds for each material parameters individually and the envelopes of the confidence interval limits are restricted to also follow the form of the puck failure envelope. This in turn is a strong assumption which might need to be relaxed.

For the future it is planned to continuously improve the tool. On the one side, further even more sophisticated parameter estimation methods can be implemented. For example, parameter estimation based on Bayesian statistics is a promising alternative which directly provides confidence interval estimations, however, is often computational expensive [11]. On the other side, the tool can also be generalized for other failure criteria, or more generally even for the parameter fitting for other material models. The latter is a task that is always difficult to handle in the engineering practice and often excludes the use of elaborated material model, simply because the material parameter estimation is such a difficult task.

7. REFERENCES

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