AN IMPROVED HYBRID COMPUTATIONAL MECHANICS FRAMEWORK FOR COMPOSITE DAMAGE MODELING AND SIMULATION

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Key words: Composite Damage Modeling, X-FEM, CZM, Schapery Theory.

Abstract. In this study, an integrated modeling framework is proposed, combining continuum damage modeling (CDM), the extended finite element method (X-FEM), and the cohesive zone modeling (CZM) techniques, to model the progressive failure of fibre-reinforced composite laminates. This modeling framework has the capability to efficiently capture fibre failure, matrix cracking, and interlaminar delamination. The Schapery theory (to address polymer matrix viscoelastic behavior) is also incorporated to accurately simulate the pre-peak nonlinearity of the load-bearing response due to matrix microcracking. The proposed hybrid model is developed and implemented using Abaqus with user-defined subroutines. A multidirectional composite laminate with an open-hole notch configuration under tension (OHT) is examined as a case study. The simulation results are compared with the physical experiments in the open literature. The proposed framework represents a practical paradigm, which not only drastically reduces the pre-processing workload to build a physics-based high-fidelity damage model, but also largely decreases the computational cost.

1 INTRODUCTION

Fiber-reinforced polymer (FRP) composite materials have been replacing traditional metallic materials at an unprecedented rate for airframe structures, driven by the essential need for lightweight and improved structural performance to achieve high demands on aircraft sustainability objectives. Meanwhile, damage tolerance assessment of composite structures presents significant difficulties for airworthiness certification and aircraft sustainment due to their complex damage and failure mechanisms. Although considerable research has been devoted over the past decades to developing high-fidelity composite damage computational

models, having the capability to effectively and efficiently predict complex composite damage and failure behavior is still a daunting challenge. To the author's knowledge, existing mesoscale modeling strategies for composite damage suffer from either modeling cumbersomeness, lack of capability of accurately capturing certain intralaminar composite damage modes, or formidable computational cost. As a result, the current numerical models in the literature can barely be applied to real-world composite structures to solve practical problems. Therefore, a large gap still exists in developing an effective and efficient mesoscale damage modeling and simulation framework to practically assess composite damage tolerance and residual strength for actual composite structures.

This study aims to develop a hybrid computational mechanics framework to capture the major failure modes of each composite ply and predict their progressive damage evolutions in a composite laminate. An integrated modelling approach is proposed, combining continuum damage modelling (CDM), the extended finite element method (X-FEM), and the cohesive zone modeling (CZM) technique, to capture fibre fracture, matrix cracking, and interlaminar delamination. The Schapery theory (to address polymer matrix viscoelastic behavior) is incorporated criteria to accurately simulate the pre-peak nonlinearity of the load-bearing response due to matrix microcracking. The proposed hybrid model is developed and implemented using Abaqus with user-defined subroutines. A multidirectional composite laminate with an open-hole notch configuration under tension (OHT) is examined. The simulation results are compared with the physical experiments in the open literature and demonstrate the effectivity and practicability of the modelling methodology for composite progressive damage analysis.

2 DAMAGE AND FAILURE OF FIBRE-REINFORCED COMPOSITE LAMINATES

The complexity of failure mechanisms exhibited by FRP composite materials makes the characterization of their failure modes extremely difficult, particularly under aircraft in-service loading conditions. It is ultimately attributed to their intrinsic features: the heterogeneous microstructure of composites, the significant differences between the constituent properties, the presence of interfaces between fibres and polymer matrix, and the directionality of fibre reinforcement that induces anisotropy in overall mechanical properties[1, 2].

During a composite laminate service lifespan, micro-damage often proceeds to become macro-damage. The accumulation of damage throughout the material may cause the structure to reach a critical level, which makes it no longer able to perform its load-carrying function, such as an unacceptable drop in the modulus [1]. These critical states are defined as failures. Failures of a laminate can generally be categorized into two main groups: interlaminar failure and intralaminar failure.

Interlaminar failure, also called delamination, is a progressive separation between two adjacent plies of dissimilar orientation within the stacked laminate. Delamination can be a substantial problem in designing composite structures as it can diminish the role of strong fibres and make the weak matrix properties govern the structure's stiffness and strength [2]. Delamination can be caused by low-velocity impact, both in-plane and out-of-plane loadings, and intralaminar cracks. Delamination initiation is strongly related to the interlaminar strength, which is determined by the matrix and the interfacial strength [3]. The propagation of an interlaminar crack is governed by interlaminar fracture toughness. Consequently, interlaminar

stresses and shear stresses can cause the adjacent lamina to peel and slide between each other. As these stresses usually occur at the peak in the vicinity of the traction-free edge [4, 5], delamination most likely take place at holes, internal defects, and edges of structures [6, 7]. The free-edge stresses are the results of a mismatch in the thermo-elastic properties of adjacent plies, such as Poisson's ratio and shear coupling coefficient, with different stacking angles [7]. Delamination can also be caused by the growth of matrix cracks to ply interfaces. In most cases, delamination is dominated by fracture Mode I, Mode II, and the mixed mode (I&II).

Intralaminar failure take place within a ply and are idealized based on their dominant characteristic. Even though there is still a lack of consensus so far on intralaminar failure modes, most proposed failure modes in the literature are classified according to their dominant characteristic as either fibre or matrix related. Laminate tensile failure in the fibre direction is governed by the tensile strength of the fibres. Compressive failure in the fibre direction (either fibre splitting or fibre kinking) is governed by fibre misalignment and/or other local defects. Matrix fracture caused by transverse tensile stress is governed by the matrix tensile strength and the fibre-matrix interface strength, while matrix fracture caused by transverse compression and transverse shear is governed by matrix shear strength.

Damage initiation and evolution in a composite laminate depend on the characteristics and properties of the constituents, the fibre volume ratio, the ply thickness, the laminate layup configuration, and the loading condition. Each type of failure mode can act independently or interactively, thus tremendously increasing the difficulty of identifying, characterizing, and predicting the damage modes in an actual situation. Moreover, a lamina is stacked in different orientations in a real-world laminate configuration, which indicates the composite failure usually does not exhibit as an isolated failure mode. Instead, multiple failure mechanisms may coexist and interact with each other. One typical example is that transverse matrix cracks are often the origin of delamination [8].

3 HYBRID MODELING FRAMEWORK

To accurately capture the major composite material failure modes, four main components are structured in the hybrid modeling framework proposed in this study. They are presented in Figure 1. The Schapery Theory is used to predict the pre-peak nonlinear load response caused by matrix micro-cracking. The overall damage effect due to matrix micro-cracking is represented by a homogeneous damage field. The initiations of both fibre failure and major matrix cracking are predicted by the 3-D Hashin's failure criteria. While continuum damage modeling (CDM) is used to capture fibre failure, the extended finite element method (XFEM) is used to capture major matrix crack propagation. Irreversible modulus degradation is introduced to the elements based on the local strain. A linear stiffness degradation scheme is implemented to model fibre damage evolution with a scalar internal state damage variable. The cohesive zone modeling (CZM) technique has been shown to be effective for modeling interlaminar delamination of laminated composite structures in various studies. Therefore, it is also used in this study to model interlaminar failure. The implementations of each component are explained in the following subsections.



Figure 1: Hybrid modeling framework

3.1 The Schapery Theory

The Schapery Theory was initially developed to describe the nonlinear-elastic material behavior of solid viscoelastic polymers [9]. It was recently used to describe progressive micro-damage of matrix in carbon fibre reinforced composites [10]. Progressive micro-damage is the primary cause of gradual reduction in the matrix stiffness before the occurrence of macro damage, such as transverse matrix cracking, fibre kinking, and fibre breakage. In the Schapery Theory, the total applied potential energy is divided into two parts: the recoverable elastic strain energy and the dissipative potential energy due to micro matrix cracking when the structure is under loading conditions.

$$W_{Total} = W + W_s \tag{1}$$

Both *W* and W_s are functions of the internal state variable *S*. The total work potential (W_{Total}) is stationary with respect to internal state variable *S*. Since micro matrix-cracks only have effects on the transverse and shear moduli, E_{22} and G_{12} , we have the following expressions.

$$E_{22} = E_{220} e_S(S) \tag{2}$$

$$G_{12} = G_{120}g_S(S) \tag{3}$$

where $e_S(S)$ and $g_S(S)$ are polynomials.

Sicking [11] observed from the experiments that variable S is a function of ε_{ij}^3 , hence, he introduced a reduced internal state variable (S_{γ}^3) for better curve fitting purpose and it has the form of following.

$$S = S_{\gamma}^3 \tag{4}$$

$$e_{S} = e_{S0} + e_{S1}S_{\gamma} + e_{S2}S_{\gamma}^{2} + e_{S3}S_{\gamma}^{3}$$
(5)

$$g_{S} = g_{S0} + g_{S1}S_{\gamma} + g_{S2}S_{\gamma}^{2} + g_{S3}S_{\gamma}^{3}$$
(6)

The coefficients for each term are to be obtained from experiments. To simplify the problem, plane stress constitutive relationship is assumed

$$W_{Total} = \frac{1}{2} (E_{11}\varepsilon_{11}^2 + E_{22}\varepsilon_{22}^2 + G_{12}\gamma_{12}^2) + \nu_{12}E_{22}\varepsilon_{11}\varepsilon_{22}$$
(7)

Calculating the derivative of W with respect to S_{γ} yields:

$$\frac{\varepsilon_{22}^2}{2}\frac{\partial E_{22}}{\partial S_{\gamma}} + \frac{\gamma_{12}^2}{2}\frac{\partial G_{12}}{\partial S_{\gamma}} = -3S_{\gamma}^2 \tag{8}$$

Once S_{γ} is solved for each iteration, the degraded moduli can be obtained accordingly. Note that only the transverse and shear moduli are functions of *S* since matrix micro-damage only accrues in the matrix of the laminae.

3.2 Modeling of fibre failure and stiffness degradation

Fibre failures in tension and compression are modeled based on continuum damage mechanics. The 3-D Hashin's failure criteria are used to predict the damage onset. Fibre failure is categorized as tensile failure and compressive failure. The local failure mode is identified by local stress in the fibre direction, σ_{11} . The Cartesian coordinate system with the 1-axis aligned with the axis of the fibre direction is used to describe local stress and strain directions. A previous study conducted by Gu and Chen [12] has shown that the contributions of shear stresses σ_{12} and σ_{13} to fibre fracture are very small and can be neglected. Hence, in this study, the modified fibre tensile failure criterion is used:

Fibre tensile failure mode, $\sigma_{11} > 0$

$$\left(\frac{\sigma_{11}}{X_T}\right)^2 = 1\tag{9}$$

Fibre compressive failure mode, $\sigma_{11} < 0$

$$\left(\frac{\sigma_{11}}{X_c}\right)^2 = 1\tag{10}$$

where X_T and X_C are the fibre tensile and compressive strength, respectively.

Once the fibre failure criterion is satisfied, further loading will cause softening of the locally affected elements. The softening of material is modeled by reducing local element stiffness. The damage evolution law is based on fracture energy dissipation, and a linear stiffness degradation is assumed. The damage is represented by a scalar internal state variable named "damage factor". When the damage factor equals 0, it indicates there is no damage; when the damage factor equals 1, it indicates the element has been fully damaged. Various forms of stiffness degradation have been proposed for this purpose. In this study, a modified form referred to the work of Maimí et al. [13] is created to model fibre damage evolution.



Figure 2: Linear stiffness degradation

Since the material softening is based on the linear degradation (Figure 2), the damage factor, d, in the fibre direction is calculated using the following equations:

$$d = 1 - (1 - d_T)(1 - d_C)$$
⁽¹¹⁾

$$d_{I} = \frac{\varepsilon_{II}^{J}(\varepsilon_{1} - \varepsilon_{1I}^{0})}{\varepsilon_{1}(\varepsilon_{1I}^{f} - \varepsilon_{1I}^{0})}$$
(12)

$$I \in \{T, C\}$$

In the equations, subscript T and C represent tensile mode and compressive mode, respectively. ε_{1I}^0 is the equivalent element strain in the fibre direction when the damage initiation criterion is satisfied, and ε_{1I}^f is the equivalent strain at which the material is fully damaged ($d_I = 1$).

To alleviate mesh size dependency during material softening, the element characteristic length should be included in the formulation to express the constitutive law as a stress-strain relationship. The Bažant's crack-band theory [14] is incorporated into the model:

$$\varepsilon_{1I}^{f} = \frac{2G_{I}}{X_{I}L_{c}}$$

$$I \in \{T, C\}$$

$$(13)$$

where L_c is the characteristic length of the element and G_I/L_c represents the fracture energy dissipated by the element during crack propagation. The fracture energy G_T and G_c are material properties that can be obtained from experimental tests. In Abaqus, the element characteristic length is computed and can be directly passed to the user subroutines.

A 3-D form of linear stiffness degradation is developed in this study with the damage factor obtained above:

$$\begin{cases} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{12} \\ \sigma_{13} \\ \sigma_{23} \end{cases} = \begin{bmatrix} C_{11}' & C_{12}' & C_{13}' & 0 & 0 & 0 \\ C_{12}' & C_{22}' & C_{23}' & 0 & 0 & 0 \\ C_{13}' & C_{23}' & C_{33}' & 0 & 0 & 0 \\ 0 & 0 & 0 & G_{12}' & 0 & 0 \\ 0 & 0 & 0 & 0 & G_{13}' & 0 \\ 0 & 0 & 0 & 0 & 0 & G_{23}' \end{bmatrix} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{12} \\ 2\varepsilon_{13} \\ 2\varepsilon_{23} \end{bmatrix}$$
(14)
$$C_{11}' = \frac{1}{D} (1 - d)(1 - \nu_{23}\nu_{32})E_{11}$$
(15)

$$C_{12}' = \frac{1}{D} (1 - d)(\nu_{12} + \nu_{32}\nu_{13})E_{22}$$
(16)

$$C_{13}' = \frac{1}{D} (1 - d) (\nu_{13} + \nu_{12} \nu_{23}) E_{22}$$
⁽¹⁷⁾

$$C_{21}' = C_{12}' \tag{18}$$

$$C_{22}' = \frac{1}{D} (1 - \nu_{13} \nu_{31} (1 - d)) E_{22}$$
⁽¹⁹⁾

$$C_{23}' = \frac{1}{D} (\nu_{23} + \nu_{21}\nu_{13}(1-d))E_{33}$$
⁽²⁰⁾

$$C_{31}' = C_{13}' \tag{21}$$

$$C_{32}' = C_{23}' \tag{22}$$

$$C_{33}' = \frac{1}{D} (1 - \nu_{13} \nu_{31} (1 - d)) E_{33}$$
⁽²³⁾

$$G_{12}' = (1-d)G_{12} \tag{24}$$

$$G_{13}' = (1-d)G_{13} \tag{25}$$

$$G_{23}' = G_{23} \tag{26}$$

$$D = (1 - \nu_{12}\nu_{21}(1 - d) - \nu_{23}\nu_{32} - \nu_{31}\nu_{13}(1 - d) - 2\nu_{12}\nu_{23}\nu_{31}(1 - d))$$
(27)

3.3 Modeling of matrix major cracks

The Hashin's failure criteria are also used to predict matrix crack initiation. Matrix tensile and compressive failure modes are identified by the local stress status ($\sigma_{22} + \sigma_{33}$). The matrix major crack propagation direction is set along the fibre direction, the most common from experiment observations.

Matrix tensile failure mode, $(\sigma_{22} + \sigma_{33}) > 0$

$$\frac{1}{Y_T^2}(\sigma_{22} + \sigma_{33})^2 + \frac{1}{S_{23}^2}(\sigma_{23}^2 - \sigma_{22}\sigma_{33}) + \frac{1}{S_{12}^2}(\sigma_{12}^2 + \sigma_{13}^2) = 1$$
(28)

Matrix compressive failure mode, $(\sigma_{22} + \sigma_{33}) < 0$

$$\frac{1}{Y_C} \left[\left(\frac{Y_C}{2S_{23}} \right)^2 - 1 \right] (\sigma_{22} + \sigma_{33}) + \frac{1}{4S_{23}^2} (\sigma_{22} + \sigma_{33})^2 + \frac{1}{S_{23}^2} (\sigma_{23}^2 - \sigma_{22}\sigma_{33}) + \frac{1}{S_{12}^2} (\sigma_{12}^2 + \sigma_{13}^2) = 1 \quad (29)$$

where Y_T and Y_C are the tensile and compressive strength in the transverse direction, S_{12} and S_{23} are the longitudinal and transverse shear strength.

XFEM is coupled with CZM in this study to capture matrix major crack. Once the Hashin's failure criteria is satisfied, a matrix crack initiates and then its propagation is governed by a traction separation law. XFEM is employed for the mesh-independent discrete crack modeling, and the so-called "phantom node" approach is utilized in Abaqus to represent the discontinuity of the cracked elements [15]. Before the element is damaged, the phantom nodes are superposed on the original (real) nodes. When a crack propagates through an element, the damaged element will be divided into two elements. Each element is formed by some real nodes and some phantom nodes.

3.4 Modeling of delamination

Delamination is predicted using the cohesive zone modeling (CZM) technique with 3-D cohesive elements. Among the three fracture modes that cause delamination in a composite laminate, the opening mode (Mode I), the in-plane shear mode (Mode II), and the combination of both modes (Mixed-mode) are often found to be the dominant modes. The quadratic stress criterion (Quads) in Abaqus [15] is commonly used to predict damage initiation in cohesive elements [16, 17]. Damage is deemed to initiate when a quadratic interaction function involving the contact stress ratios reaches a value of one. This criterion is presented in the equation below:

$$\left(\frac{\langle t_n \rangle}{t_n^0}\right)^2 + \left(\frac{t_s}{t_s^0}\right)^2 + \left(\frac{t_t}{t_t^0}\right)^2 = 1$$
(30)

where t_n , t_s and t_t represent the nominal stress normal to the interface, and the shear stresses on the interface in the first and second shear directions, respectively. Macaulay brackets are used herein to signify that a pure compressive stress state does not initiate damage (delamination). After damage initiation, the element stiffness continuously softens with a bilinear traction separation law until the dissipated energy reaches the mixed-mode fracture toughness, as shown in Figure 3. In addition, the B-K law [18] is selected to model the coupled damage evolution behavior in the mixed-mode delamination.



Figure 2: Mixed-mode traction-separation behavior in cohesive elements [19].

3.5 Abaqus user subroutine

The computational mechanics framework of the hybrid modeling paradigm proposed above is developed and implemented in Fortran-coded "UMAT" and "UDMGINI" subroutines that are integrated with the Abaqus implicit solver. The user-subroutine runs during every time increment for each element, and the flowchart is shown in Figure 4. The reduced internal state variables for the Schapery's theory and damage factors used for failure evolution are stored as solution-dependent state variables (SDV). The saved SDVs are passed as input for the next time increment.



Figure 4: User-subroutine flowchart

4 FINITE ELEMENT MODELING AND RESULTS

The hybrid damage modeling and simulation methodology is applied to the progressive damage analysis of a multidirectional composite laminate with an open hole notch subjected to tensile loading. In accordance with the test conducted in the open literature [20], the length and the width of the specimen are 63.5 mm and 15.875 mm, respectively. The total thickness of the specimen is 1.162 mm, and the diameter of the hole is 3.175 mm. As shown in Figure 5, the panel with a quasi-isotropic lay-up [45/90/-45/0]s is modelled as eight layers of 3-D 8-node hexahedral elements (C3D8R), with each layer of solid elements representing one composite ply. One layer of 3-D cohesive elements (COH3D8) is embedded between each ply. Note that no cohesive elements are deployed between the two center 0° plies because delamination is not expected to take place between these two plies. The global mesh size is selected to be 0.23 mm based on an empirical study. The loads are applied to the specimen using a displacement control approach.



Figure 5: Open hole tension (OHT) FE model

The predicted matrix crack damage patterns are shown in Figure 6. The matrix damage factor is stored as a solution-dependent damage variable (SDV6). When it reaches a value of 1, it indicates that a crack has propagated through the element and the damaged element is divided into two elements. The delamination pattern is shown in Figure 7. Similarly, for the cohesive elements, when the Abaqus "scalar stiffness degradation" (SDEG) value reaches 1, it indicates two neighbouring composite plies are fully separated. Fibre failure is observed in the 0° plies and shown in Figure 8. According to the experiment conducted by Hallett et al. [20], it is observed that the initial damage occurs at the hole edge in the form of matrix cracking with associated delamination. As the crack propagates, it is followed by more extensive damage at the hole edge in the form of larger areas of delamination between plies. The stress relaxation is observed in 0° plies with matrix cracking. Finally, fibre failure is observed. The results from the FE model demonstrate similar damage sequences and damage patterns.



Figure 6: Matrix crack pattern of OHT panel configuration



Figure 7: Delamination pattern of OHT panel configuration



Figure 8: Fibre failure of OHT panel configuration.

5 CONCLUSIONS

An integrated FE modeling framework is proposed to predict the progressive failure of fibrereinforced composite laminates, combining continuum damage modeling (CDM), the extended finite element method (X-FEM), and the cohesive zone modeling (CZM) technique. Compared with the existing approaches in the literature, this framework is more accurate and efficient in capturing pre-peak nonlinearity due to matrix microcracking, fibre failure, matrix cracking, and interlaminar delamination. As a case study, a damage model is built for a multidirectional laminate with an open-hole tension (OHT) configuration. The simulation results correlate well with experimental observations in open literature. It demonstrates that the proposed framework represents a practical and efficient paradigm for high-fidelity modeling of progressive damage of composite laminates.

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