Modelling damage in fibre-reinforced thermoplastic composite laminates subjected to three-point bend loading

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ABSTRACT

It is important to account for nonlinearity in the deformation of a thermoplastic matrix, as well as fibre fracture and matrix cracking, when predicting progressive failure in unidirectional fibre-reinforced thermoplastic composites. In this research, a new high-fidelity damage model approach is developed incorporating elastic-plastic non-linearity. In order to validate the model, three-point bend experiments were performed on composite specimens, with a lay-up of [0₃/90₃]_{2s}, to provide experimental results for comparison. Digital Image Correlation (DIC) was employed to record the strain distribution in the composite specimens. The developed intralaminar damage model, which is implemented as a user defined material (VUMAT in Abaqus/Explicit) subroutine, is then combined with a cohesive surface model to simulate three-point bend failure processes. The simulation results, including the load-displacement curves and damage morphology, are compared with the corresponding experimental results to assess the predictive capability of the developed model. Good agreement is achieved between the experimental and numerical results.

KEY WORDS: Thermoplastic composites; Nonlinear behaviour; Damage mechanisms; Numerical simulation;

Nomenclature

Symbols	Definition
d_1, d_2, d_3 and d_s	Damage parameters defined in Hanshin's damage model
d_{inter}	Damage parameter defined in cohesive surface solution
f	The plastic potential
k_{33} , k_{31} and k_{32}	Cohesive stiffness
l_g	Gauge length of the composite specimens
l_t	Total length of the composite specimens
n	Non-linear parameter for defining the master curve
t	Thickness of the composite specimens
W	Width of the composite specimens
Α	Non-linear parameter for defining the master curve
E_{XX}	Apparent modulus of elasticity in the loading direction, x
$E_{ii}(i = 1, 2, 3)$	Elastic normal moduli in the material coordinate system
F_{iT} , F_{iC} and F_{iS} (<i>i</i> = 1,2,3)	Tension and compression failure indexes in NU theory
$G_{ij}(i,j=1,2,3,i\neq j)$	Elastic shear moduli in the material coordinate system
$G_{Ic} _{ft}$ and $G_{Ic} _{fc}$	Fibre-dominated tensile and compressive fracture toughness
$G_{Ic} _{mt}$ and $G_{Ic} _{mc}$	Matrix-dominated tensile and compressive fracture toughness
$G_{Ic} _{ms}$	Matrix-dominated shear fracture toughness
G_{Ic} and G_{IIc}	Interlaminar mode I and mode II fracture toughness
X^T and X^C	Longitudinal tensile and compressive strength
Y^T and Y^C	Transverse tensile and compressive strength
Z^T and Z^C	Through-thickness tensile and compressive strength
a_{ii} (<i>i</i> = 4,5,6)	The coefficients describing the extent of plastic anisotropy
a_{ij} (<i>i</i> , <i>j</i> = 1,2,3)	Coefficients in the quadratic stress-based yield function
$\gamma_{ij}(i,j=1,2,3,i\neq j)$	Shear strains in the material coordinate system
$\gamma_{12}^{p} (i,j=1,\!2,\!3, i\neq j)$	Plastic shear strains in the material coordinate system
$arepsilon_{eff}^p$	Effective plastic strain
$\varepsilon_{ii}(i = 1, 2, 3)$	Normal strains in the material coordinate system
$\varepsilon_{ii}^p (i = 1,2,3)$	Plastic normal strains in the material coordinate system
η	Benzeggagh–Kenane (B-K) coefficient
v_{ij} (<i>i</i> , <i>j</i> = 1,2,3)	Poisson's ratios in the material coordinate system
$\sigma_{ii} \ (i = 1, 2, 3)$	Normal stresses in the material coordinate system
σ_{eff}	Effective stress
$\tau_{ij}~(i,j=1,2,3,i\neq j)$	Shear stresses in the material coordinate system
FE	Finite element

* All given material properties are those for the composite material

1. Introduction

Continuous fibre-reinforced composites are becoming very attractive materials for application the commercial aviation industry. This is mainly due to their excellent mechanical, fatigue and corrosion resistant properties. In particular, two important performance criteria are high strength to weight ratio and high stiffness to weight ratio [1,2]. With regards to the matrix, fibre-reinforced composites can be categorised into two main types: thermoset matrix composites and thermoplastic matrix composites. Compared to thermoset matrix composites, thermoplastic matrix composites, which utilise polymers such as Poly(ether ketone ketone) (PEKK) and Poly(ether-ether ketone) (PEEK), show higher damage tolerance and better recycling capability [3,4]. The presence of a semi-crystalline polymer matrix results in the thermoplastic matrix composite exhibiting a more pronounced nonlinear stress-strain response in the matrix-dominated direction [5]. A high-fidelity model, for predicting this nonlinear behaviour and progressive failure, is proposed to better understand failure in thermoplastic composites and assist in the design of high-performance thermoplastic composite structures [6].

In developing efficient and reliable predictive tools for thermoplastic composite materials, a number of researchers have made considerable progress. Sun and Chen [7] developed a numerical, finiteelement analysis (FEA) model to predict the residual stresses in components manufactured using a carbon-fibre/PEEK composite where a multi-directional lay-up of the fibres was employed. The oneparameter flow rule for orthotropic plasticity [8] was successfully employed to describe the non-linear behaviour of the fibre-reinforced composite using a thermoplastic matrix.

Mokhtari et al. [9] investigated the compression failure of fibre-reinforced thermoplastic composites using a combined experimental and numerical method. In their experimental research, two laminate specimen lengths with different fibre orientations were considered, to analyse the response of thermoplastic composites subjected to compressive loading. Along with the experimental research, a numerical model was also developed to further understand the damage mechanisms and damage evolution in the thermoplastic composite laminates. The interlaminar damage (delamination) and the intralaminar damage (fibre fracture and matrix cracking) were modelled by the combination of the Cohesive Zone Model (CZM) and the Matzenmiller-Lubliner-Taylor (MLT) mechanical model. It was found that the loading conditions of composite laminates and the fibre orientation considerably affected the compression failure load of the thermoplastic composites.

With the aim of understanding and predicting the crush behaviour of thermoplastic composites, Tan and Falzon [10] conducted both experimental and numerical studies on AS4 carbon reinforced PEKK laminates. The damage mechanisms of thermoplastic composites, subjected to quasi-static crush loading, were investigated using digital microscopy and post analysed using Scanning Electron Microscopy (SEM). It was found that splaying and fragmentation were the primary failure modes. Based on further understanding from the experimental research, a mesoscale composite damage model was developed to capture the material response under crushing. In this way, Tan and Falzon demonstrated that the numerical approach developed could considerably reduce the extent of physical testing required for developing crashworthy composite structures.

In this research, an intralaminar damage model, which was implemented as a VUMAT subroutine within Abaqus/Explicit, was developed to capture the response of a thermoplastic composite ply. This intralaminar damage model was then combined with a cohesive surface model to form a FE model for predicting the mechanical response and progressive failure of thermoplastic composite laminates. Three-point bend experiments were performed on the thermoplastic composite specimens, manufactured using an Out-Of-Autoclave (OOA) route, to extract the experimental data for model validation. During the experiments, Digital Image Correlation (DIC) was employed to record the deformation and strain in the tested composite specimens. The experimental and numerical results, such as loading response and damage morphology, were compared to assess the capability of the developed FE model in predicting the mechanical response and progressive failure of a thermoplastic matrix composite.

2. The theoretical model

2.1. Introduction

The failure modes, presented by the unidirectional fibre reinforced composite laminates, are generally fibre fracture, matrix cracking and delamination [11], Fig. 1. In these three types of failure, the fibre

fracture/kinking and matrix cracking can be summarised as intralaminar damage, and the delamination can be defined as interlaminar damage.

Based on the observed failure modes in composite laminates, both interlaminar and intralaminar damage as well as nonlinear response were considered in the developed composite damage model, which was implemented as a VUMAT subroutine in Abaqus/explicit. The details of the developed composite damage model are given in the following sections.

2.2. Model for intralaminar damage

2.2.1. Intralaminar damage initiation

For the intralaminar failure, the North-western University (NU) damage criteria were employed to capture the damage initiation. The NU criteria were proposed by Daniel et al [12,13]. These 3D criteria are partially interactive failure criteria, in which more than one stress components have been used to evaluate the different failure modes. Failure indices for NU criteria involve eight failure modes. The failure modes included in the NU criteria are given by:

Longitudinal failure:

Tension-dominated :

$$F_{1T} = \left(\frac{\sigma_{11}}{X_T}\right)^2 + \frac{\sigma_{12}^2 + \sigma_{13}^2}{S_{12}^2} \le 1 \qquad , \tag{1}$$

$$F_{1C} = \left(\frac{\sigma_{11}}{X_C}\right)^2 \le 1 \qquad , \tag{2}$$

Transverse failure ($|\sigma_{22}| \ge |\sigma_{33}|$):

 $(|\sigma_{22}| \ge |\tau_{12}(\tau_{23})| \text{ and } \sigma_{22} \ge 0)$:

$$F_{2T} = \frac{\sigma_{22}}{Y_T} + \left(\frac{E_{22}}{2G_{12}}\right)^2 \left(\frac{\tau_{12}}{Y_T}\right)^2 + \left(\frac{E_{22}}{2G_{23}}\right)^2 \left(\frac{\tau_{23}}{Y_T}\right)^2 \le 1 \qquad , \tag{3}$$

Compression-dominated

Tension-dominated

Compression-dominated

$$(|\sigma_{22}| \ge |\tau_{12}(\tau_{23})| \text{ and } \sigma_{22} \le 0):$$

$$F_{2C} = \left(\frac{\sigma_{22}}{Y_C}\right)^2 + \left(\frac{E_{22}}{G_{12}}\right)^2 \left(\frac{\tau_{12}}{Y_C}\right)^2 + \left(\frac{E_{22}}{G_{23}}\right)^2 \left(\frac{\tau_{23}}{Y_C}\right)^2 \le 1 \quad , \quad (4)$$

Shear-dominated

 $(|\sigma_{22}| \le |\tau_{12}(\tau_{23})|)$:

$$F_{2S} = \left(\frac{\tau_{12}}{S_{12}}\right)^2 + \left(\frac{\tau_{23}}{S_{23}}\right)^2 + \frac{2G_{12}}{E_{22}}\frac{\sigma_{22}}{Y_C} \le 1 \qquad , \tag{5}$$

Through-thickness failure ($|\sigma_{33}| \ge |\sigma_{22}|$):

Tension-dominated

$$(|\sigma_{33}| \ge |\tau_{13}(\tau_{23})| \text{ and } \sigma_{33} \ge 0):$$

$$F_{3T} = \frac{\sigma_{22}}{Z_T} + \left(\frac{E_{33}}{2G_{13}}\right)^2 \left(\frac{\tau_{13}}{Z_T}\right)^2 + \left(\frac{E_{33}}{2G_{23}}\right)^2 \left(\frac{\tau_{23}}{Z_T}\right)^2 \le 1 \quad , \quad (6)$$
Compression-dominated

$$(|\sigma_{33}| \ge |\tau_{13}(\tau_{23})| \text{ and } \sigma_{33} \le 0):$$

$$F_{3C} = \left(\frac{\sigma_{33}}{Z_C}\right)^2 + \left(\frac{E_{33}}{G_{13}}\right)^2 \left(\frac{\tau_{13}}{Z_C}\right)^2 + \left(\frac{E_{33}}{G_{23}}\right)^2 \left(\frac{\tau_{23}}{Y_C}\right)^2 \le 1 \quad , \quad (7)$$
Shear-dominated

$$F_{3S} = \left(\frac{\tau_{13}}{S_{13}}\right)^2 + \left(\frac{\tau_{23}}{S_{23}}\right)^2 + \frac{2G_{13}}{E_{33}}\frac{\sigma_{33}}{Z_C} \le 1 \quad , \quad (8)$$

 $(|\sigma_{33}| \le |\tau_{13}(\tau_{23})|)$:

$$r_{3S} = \left(\frac{\tau_{13}}{S_{13}}\right)^2 + \left(\frac{\tau_{23}}{S_{23}}\right)^2 + \frac{2G_{13}}{E_{33}}\frac{\sigma_{33}}{Z_C} \le 1$$
, (8)

where σ_{ij} are the stress components. F_{iT} (i = 1,2,3), F_{iC} (i = 1,2,3) and F_{iS} (i = 1,2,3) are the tensiledominated, compression-dominated and shear-dominated failure indexes in three respective material directions, respectively. X_T , Y_T and Z_T denote the allowable tensile strength in the three respective material directions. Similarly, X_C, Y_C and Z_C are the allowable compressive strength in the three respective material directions. Further, S12, S13 and S23 represent allowable shear strengths in the corresponding principal material directions.

2.2.2. Intralaminar damage evolution

The damage evolution law, based on the energy dissipated during the damage process and linear material softening, was used to predict the evolution of the damage in the composite plies. Corresponding to the damage initiation mechanisms defined in NU damage criteria, eight damage parameters, d_{1t} , d_{1c} , d_{2t} , d_{2c} , d_{2s} , d_{3t} , d_{3c} and d_{3s} are defined in the damage evolution model. A general form of the damage variable for a particular damage initiation mechanism is given by:

$$d = \frac{\varepsilon^f(\varepsilon - \varepsilon^0)}{\varepsilon(\varepsilon^f - \varepsilon^0)}$$
(9)

where $d = d_{1t}$ represents the longitudinal tension-dominated failure, $d = d_{1c}$ represents the longitudinal compression-dominated failure. $d = d_{2t}$ represents the transverse tension-dominated failure, $d = d_{2c}$ represents the transverse compression-dominated failure and $d = d_{2s}$ refers to the transverse shear-dominated failure. Similarly, $d = d_{3t}$ represents the through-thickness tensiondominated failure, $d = d_{3c}$ and $d = d_{3s}$ refer to the through-thickness compression-dominated failure and the through-thickness shear-dominated failure, respectively. The strain, ε , is the equivalent strain in the composite ply. The strain values, ε^0 and ε^f , are the equivalent strains corresponding to initial failure and final failure, respectively. For longitudinal tension or compression failure, the strains ε , ε^0 and ε^f would be assigned to be $\varepsilon = \varepsilon_{11}$, $\varepsilon^0 = \varepsilon_{11}^0$ and $\varepsilon^f = \varepsilon_{11}^f$, respectively. For transverse tension or compression failure, strains ε , ε^0 and ε^f would be assigned to be $\varepsilon = \sqrt{\varepsilon_{22}^2 + \gamma_{12}^2 + \gamma_{23}^2}$, $\varepsilon^0 =$

 $\sqrt{\varepsilon_{22}^{0}^{2} + \gamma_{12}^{0}^{2} + \gamma_{23}^{0}^{2}}$ and $\varepsilon^{f} = \sqrt{\varepsilon_{22}^{f^{2}} + \gamma_{12}^{f^{2}} + \gamma_{23}^{f^{2}}}$, respectively. For through-thickness tension or

compression failure, strains ε , ε^0 and ε^f would be assigned to be $\varepsilon = \sqrt{\varepsilon_{33}^2 + \gamma_{23}^2 + \gamma_{13}^2}$, $\varepsilon^0 =$

 $\sqrt{\varepsilon_{22}^{0^2} + \gamma_{23}^{0^2} + \gamma_{13}^{0^2}}$ and $\varepsilon^f = \sqrt{\varepsilon_{22}^{f^2} + \gamma_{23}^{f^2} + \gamma_{13}^{f^2}}$, respectively. The final failure strain tensor, ε_{ij}^f (*i*, *j* = 1,2,3), can be determined through the following equation:

$$\varepsilon_{ij}^f = 2G_{ij}/(\varepsilon_{ij}^0 l_c) \quad , \tag{10}$$

Where G_{ij} is the fracture toughness corresponding to different principal materials directions, and ε_{ij}^{0} is the strain tensor corresponding to the damage initiation. l_c is the characteristic length, which can be determined based on the volume of the elements. For more details of the characteristic length calculation, please refer to [6,14–16].

During the intralaminar damage evolution, the elasticity matrix needs to be degraded to compute the values of the degraded stresses. The achieve this, four damage variables, d_1 , d_2 , d_3 and d_s , which reflect the state of longitudinal damage, transverse damage and through-thickness damage and shear damage, respectively, were derived from the damage parameters, d_{1t} , d_{1c} , d_{2t} , d_{2c} , d_{2s} , d_{3t} , d_{3c} and d_{3s} , corresponding to the failure types previously discussed, as follows:

Longitudinal damage:
$$d_1 = \begin{cases} d_{1t}, & \hat{\sigma}_{11} \ge 0\\ d_{1c}, & \hat{\sigma}_{11} \ge 0 \end{cases}$$
, (11)

Transverse damage: $d_2 = \begin{cases} d_{2t}, & |\sigma_{22}| \ge |\tau_{12}(\tau_{23})| \text{ a} \\ d_{2c}, & |\sigma_{22}| \ge |\tau_{12}(\tau_{23})| \text{ a} \\ d_{2c}, & |\sigma_{22}| \ge |\tau_{12}(\tau_{23})| \text{ a} \\ d_{2c}, & |\sigma_{21}| \le |\tau_{12}(\tau_{23})| \text{ a} \end{cases}$

$$\begin{aligned} d_{2t}, & |\sigma_{22}| \ge |\tau_{12}(\tau_{23})| \text{ and } \sigma_{22} \ge 0 \\ d_{2c}, & |\sigma_{22}| \ge |\tau_{12}(\tau_{23})| \text{ and } \sigma_{22} \le 0 \\ d_{2s}, & |\sigma_{22}| \le |\tau_{12}(\tau_{23})| \end{aligned}$$
(12)

Through-thickness damage:
$$d_{3} = \begin{cases} d_{3t}, & |\sigma_{33}| \ge |\tau_{13}(\tau_{23})| \text{ and } \sigma_{33} \ge 0\\ d_{3c}, & |\sigma_{33}| \ge |\tau_{13}(\tau_{23})| \text{ and } \sigma_{33} \le 0\\ d_{3s}, & |\sigma_{33}| \le |\tau_{13}(\tau_{23})| \end{cases}$$
(13)

Shear damage:
$$d_s = 1 - (1 - d_1)(1 - d_2)(1 - d_3)$$
 . (14)

The derived damage variables, d_1 , d_2 , d_3 and d_s , were employed to degrade the elasticity matrix to form the damaged elasticity matrix, C_d , which can be expressed as:

$$C_{d} = \frac{1}{D} \begin{bmatrix} (1-d_{1})E_{11} & (1-d_{1})(1-d_{2})v_{21}E_{11} & (1-d_{1})(1-d_{3})v_{31}E_{11} & 0 & 0 & 0\\ (1-d_{1})(1-d_{2})v_{12}E_{22} & (1-d_{2})E_{22} & (1-d_{2})(1-d_{3})v_{32}E_{22} & 0 & 0 & 0\\ (1-d_{1})(1-d_{3})v_{13}E_{33} & (1-d_{2})(1-d_{3})v_{23}E_{33} & (1-d_{3})E_{33} & 0 & 0 & 0\\ 0 & 0 & 0 & (1-d_{s})G_{12}D & 0 & 0\\ 0 & 0 & 0 & 0 & (1-d_{s})G_{13}D & 0\\ 0 & 0 & 0 & 0 & 0 & (1-d_{s})G_{23}D \end{bmatrix}$$
(15)

Where
$$D = 1 - (1 - d_1)(1 - d_2)v_{12}v_{21} - (1 - d_2)(1 - d_3)v_{23}v_{32} - (1 - d_3)(1 - d_1)v_{31}v_{13} - (1 - d_3)(1 - d_1)v_{31}v_{31} - (1 - d_3)(1 - d_3)v_{31}v_{32} - (1 - d_3)(1 - d_3)v_{31}v_{33} - (1 - d_3)(1 - d_3)v_{33}v_{33} - (1 - d_3)v_{33}v_{33} - (1 - d_3)(1 - d_3)v_{33}v_{33} - (1 - d_3)v_{33}v_{33}v_{33} - (1 - d_3)v_{33}v_{33} - (1 - d_3)v_{33}v_$$

 $2(1 - d_1)(1 - d_2)(1 - d_3)v_{12}v_{23}v_{31}$, E_{ii} (i = 1,2,3) is the elastic modulus in three respective material directions, and v_{ij} (i, j = 1,2,3 $i \neq j$) are the Poisson's ratios. Thus, the degraded stresses can be computed from $\boldsymbol{\sigma} = C_d \boldsymbol{\varepsilon}^e$, in which $\boldsymbol{\sigma}$ is the resulting stress tensor, $\boldsymbol{\varepsilon}^e$ is the current elastic strain tensor and the C_d is degradation matrix.

2.3. Model for interlaminar damage

2.3.1. Interlaminar damage initiation

For the interlaminar failure, a quadratic-traction criterion was employed to capture the damage initiation in the composite interface, given by:

$$\left(\frac{\langle t_{33} \rangle}{t_{33}^0}\right)^2 + \left(\frac{t_{31}}{t_{31}^0}\right)^2 + \left(\frac{t_{32}}{t_{32}^0}\right)^2 \le 1 \quad , \tag{16}$$

where t_i (i = 33, 31, 32) represent the current normal and shear tractions and t_i^0 (i = 33, 31, 32) represent the normal and shear cohesive strengths, when the separation is either purely normal (i.e. the 33) to the interface or purely in the first shear (i.e. 31) or the second shear (i.e. 32) directions, respectively. The interlaminar damage is assumed to initiate when the above quadratic interaction function reaches a value of one.

To determine a cohesive strength, which can ensure computation accuracy whilst avoiding a very fine mesh, Turon et al. [17] proposed a modelling methodology, in which an relatively lower interface strength may be used with a relatively coarse mesh size. Thus, a cohesive strength of $t_{33}^0 = 43$ MPa, for an interface between two unidirectional plies, was employed. The shear cohesive strength, $t_{31}^0 = t_{32}^0$, can be determined from [17],

$$t_{31}^{0}(t_{32}^{0}) = t_{33}^{0} \sqrt{\frac{G_{IIC}}{G_{IC}}} \quad , \tag{17}$$

where G_{Ic} and G_{IIc} are the interlaminar Mode I and Mode II critical energy release rates, respectively. Values of the cohesive stiffness and cohesive strength are shown in Table 2 for an interface between two unidirectional plies.

2.3.2. Interlaminar damage evolution

In the interlaminar damage model, the linear softening law was employed to model the damage evolution. During the interlaminar damage evolution, the cohesive stiffness needs to be degraded to compute the values of the degraded tractions. To achieve this, a damage parameter, d_{inter} , was defined to degrade the cohesive stiffness, given by:

$$d_{inter} = \frac{\delta^f (\delta - \delta^0)}{\delta (\delta^f - \delta^0)} \quad , \tag{18}$$

where $\delta = \sqrt{\delta_{33}^2 + \delta_{31}^2 + \delta_{32}^2}$ is the equivalent displacement in the composite interface. The strain values, $\delta^0 = \sqrt{\delta_{33}^0 + \delta_{31}^0 + \delta_{32}^0}$ and $\delta^f = \sqrt{\delta_{33}^f + \delta_{31}^f + \delta_{32}^f}$, are the equivalent displacements corresponding to initial failure and final failure, respectively. The calculated interlaminar damage parameter, d_{inter} , was employed to degrade the cohesive stiffness matrix to form the degraded cohesive stiffness matrix. Then, the degraded tractions can be computed from the following expression:

where $t_i(i = 33, 31, 32)$ represent the cohesive normal or shear tractions, and $\delta_i(i = 33, 31, 32)$ denote the cohesive normal or transverse displacements. $k_i(i = 33, 31, 32)$ are the cohesive stiffness defined in the cohesive surface model.

2.4. Model for nonlinear response

In the present research, an elastic-plastic constitutive model is employed to capture the nonlinear response of the composite ply. The global coordinate system is defined as X-Y-Z and the material coordinate system is defined as 1-2-3. To establish the relationship between a complex stress state and a simple experimental stress state an effective stress, σ_{eff} , and strain, ε_{eff}^{p} , for modelling the plastic constitutive relationships between the stress and strain need to be derived.

2.4.1. The effective stress, σ_{eff}

A quadratic stress-based yield function, arising from the results of a micromechanical FEA approach, has been proposed for a general 3-D fibre-reinforced composite [8,18]:

$$2f(\sigma_{ii}) = a_{11}\sigma_{11}^{2} + a_{22}\sigma_{22}^{2} + a_{33}\sigma_{33}^{2} + 2a_{12}\sigma_{11}\sigma_{22} + 2a_{13}\sigma_{11}\sigma_{33} + 2a_{23}\sigma_{22}\sigma_{33} + 2a_{44}\tau_{23}^{2} + 2a_{55}\tau_{13}^{2} + 2a_{66}\tau_{12}^{2}$$
(20)

where *f* is the plastic potential. The coefficients, a_{ij} (*i*, *j* = 1,2,3,4,5,6), which describe the extent of anisotropy in the plastic behaviour of the composite, are assumed to be constant and may be determined experimentally.

Now, Sun and Chen [5,8,19] have simplified Eq. (20) by incorporating the fact that for most unidirectional fibre composites the stress versus strain relation in the fibre direction is basically linearly elastic and they also considered the composite to be transversely isotopic material in the 2-3 plane. Further, to establish the relationship between a complex stress state and a simple experimental stress state, they defined an effective stress for modelling the plastic constitutive relationship between the stress and strain. Thus, the 3-D effective stress, σ_{eff} , for a transversely isotopic composite and linearly -elastic in the fibre direction is given by [20]:

$$\sigma_{eff} = \sqrt{\frac{3}{2}}(\sigma_{22}^2 + \sigma_{33}^2) - 3\sigma_{22}\sigma_{33} + 3a_{66}(\tau_{13}^2 + \tau_{12}^2 + \tau_{23}^2)$$
(21)

However, it may also be noted that, in off-axis tension tests of a unidirectional composite laminate, a state of plane-stress will be present. Hence, the expression in Eq. (21) for the effective stress can be reduced to a 2-D version which gives the one-parameter flow rule as [8,18]:

$$\sigma_{eff} = \sqrt{\frac{3}{2}\sigma_{22}^2 + 3a_{66}\tau_{12}^2}$$
(22)

where the stresses are given by:

$$\sigma_{11} = \cos^2\theta \sigma_{XX} \tag{23}$$

$$\sigma_{22} = \sin^2 \theta \sigma_{XX} \tag{24}$$

$$\tau_{12} = -\sin\theta\cos\theta\sigma_{XX} \tag{25}$$

and σ_{XX} is the uniaxial applied stress in the loading direction, x, and θ is the off-axis angle employed in the test. For tests with various off-axis angles, the in-plane stresses, σ_{22} and τ_{12} , and strains, ε_{22} and γ_{12} , can be calculated using the loading stress, σ_{XX} , and transition matrix, $[T(\theta)]$, more details are given in Appendix. Then, substitution of Eqs. (24) and (25) into (22) gives:

$$\sigma_{eff} = H(\theta)\sigma_{XX} \tag{26}$$

where [8,20]:

$$H(\theta) = \sqrt{\frac{3}{2}\sin^4\theta + 3a_{66}\sin^2\theta\cos^2\theta}$$
(27)

As will be shown later, the value of the single parameter, a_{66} , which is unknown in Eq. (27) can be readily determined experimentally from the off-axis tests conducted at different values of the off-axis angle, θ . Thus, this allows the value of σ_{eff} to be determined from Eq. (26). In the discussion below, it is again assumed that we have a transversely isotopic composite, which behaves in a linear elastic manner in the fibre direction and where a state of plane stress is present in our off-axis tension tests of a unidirectional composite laminate.

2.4.2. The effective plastic strain, ε_{eff}^p

The effective plastic strain, ε_{eff}^{p} , gives a measure of the amount of plastic, i.e. non-linear, strain in the composite. The total strain can be linearly decomposed into the elastic and plastic strains, assuming infinitesimal strain conditions, and for the normal strains may be expressed as:

$$\varepsilon_{ii} = \varepsilon_{ii}^e + \varepsilon_{ii}^p \tag{28}$$

and for the shear strains as:

$$\tau_{ij} = \tau^e_{ij} + \tau^p_{ij} \tag{29}$$

To define an effective plastic strain, ε_{eff}^{p} , a similar approach to that adopted above for the effective stress may be followed [8], which gives:

$$\varepsilon_{eff}^{p} = \frac{\varepsilon_{XX}^{p}}{H(\theta)}$$
(30)

where the term $H(\theta)$ is given by Eq. (27) and the term ε_{XX}^p is the plastic strain resulting from the uniaxially applied load in the X-direction, which is given by:

$$\varepsilon_{XX}^p = \varepsilon_{XX} - \frac{\sigma_{XX}}{E_{XX}} \tag{31}$$

In the above equation, E_{XX} , is the elastic modulus in the loading direction which can be calculated from the material properties and off-axis angle employed in the test as given in [8]:

$$E_{XX} = \frac{1}{\frac{1}{E_{11}}\cos^4\theta + \frac{1}{E_{22}}\sin^4\theta + (\frac{1}{G_{12}} - \frac{2\nu_{12}}{E_{11}})\sin^2\theta\cos^2\theta}$$
(32)

where E_{11} and E_{22} are the elastic moduli, v_{12} is the Poisson's ratio and G_{12} is the elastic shear modulus. To characterise the relationship between the effective plastic strain, ε_{eff}^p , and the effective stress, σ_{eff} , a power law function can be used to fit all the effective stress versus effective plastic strain ($\sigma_{eff} - \varepsilon_{eff}^p$) data points from the off-axis angle experiments. given by [8]:

$$\varepsilon_{eff}^{p} = A \sigma_{eff}^{n} \qquad (33)$$

where *A* and *n* are the nonlinear coefficients, which can give a best fit to the $\sigma_{eff} - \varepsilon_{eff}^p$ data points obtained from the different-angle off-axis tension experiments. The determination of the single parameter, a_{66} , and the nonlinear coefficients, *A* and *n*, facilitates the calculation of the elements in the incremental plastic strain tensor, $d\varepsilon_{ii}^p(i, j = 1, 2, 3)$, given by:

$$\begin{cases}
 d\varepsilon_{11}^{p} \\
 d\varepsilon_{22}^{p} \\
 d\varepsilon_{33}^{p} \\
 d\varepsilon_{12}^{p} \\
 d\varepsilon_{13}^{p} \\
 d\varepsilon_{23}^{p}
 \end{cases} = \frac{A n}{\sigma_{eff}^{n-1}} \begin{cases}
 0 \\
 3(\sigma_{22} - \sigma_{33})/2\sigma_{eff} \\
 3(\sigma_{33} - \sigma_{22})/2\sigma_{eff} \\
 3a_{66}\tau_{12}/2\sigma_{eff} \\
 3a_{66}\tau_{13}/2\sigma_{eff} \\
 3a_{66}\tau_{23}/2\sigma_{eff}
 \end{cases} d\sigma_{eff}$$
(34)

2.4.3. The elastic-plastic constitutive relation

The classic elastic constitutive equation for the stress versus strain relationship for orthotropic elasticity may be expressed as [21]:

$$\begin{cases} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \gamma_{12} \\ \gamma_{23} \\ \gamma_{23} \end{cases} = \begin{bmatrix} 1/E_{11} & -\nu_{21}/E_{11} & -\nu_{31}/E_{11} & 0 & 0 & 0 \\ -\nu_{12}/E_{22} & 1/E_{22} & -\nu_{32}/E_{22} & 0 & 0 & 0 \\ -\nu_{13}/E_{33} & -\nu_{23}/E_{33} & 1/E_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/G_{12} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/G_{13} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/G_{13} \end{bmatrix} \begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \tau_{12} \\ \tau_{13} \\ \tau_{23} \end{bmatrix}$$
(35)

where ε_{ii} are the normal elastic strains, σ_{ii} are the normal elastic stresses, γ_{ij} are the elastic shear strains, τ_{ij} are the elastic shear stresses, G_{ij} are the elastic shear moduli, v_{ij} are the Poisson's ratios and E_{ii} are the Young's moduli, either for tension or compression loading [22]. By combining the developed plastic model with the classic elastic model, the elastic-plastic constitutive relation for the response prior to damage initiation was obtained by:

$$\begin{pmatrix} d\varepsilon_{11} \\ d\varepsilon_{22} \\ d\varepsilon_{33} \\ d\varepsilon_{12} \\ d\varepsilon_{13} \\ d\varepsilon_{23} \end{pmatrix} = \begin{bmatrix} 1/E_{11} & -v_{21}/E_{11} & -v_{31}/E_{11} & 0 & 0 & 0 \\ -v_{12}/E_{22} & 1/E_{22} & -v_{32}/E_{22} & 0 & 0 & 0 \\ -v_{13}/E_{33} & -v_{23}/E_{33} & 1/E_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/G_{12} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/G_{13} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/G_{13} \\ 0 & 0 & 0 & 0 & 0 & 1/G_{23} \end{bmatrix} \begin{pmatrix} d\sigma_{11} \\ d\sigma_{22} \\ d\sigma_{33} \\ d\sigma_{12} \\ d\sigma_{13} \\ d\sigma_{23} \end{pmatrix} + \begin{pmatrix} d\varepsilon_{11}^{*} \\ d\varepsilon_{22}^{*} \\ d\varepsilon_{33}^{*} \\ d\varepsilon_{12}^{*} \\ d\varepsilon_{13}^{*} \\ d\varepsilon_{12}^{*} \\ d\varepsilon_{13}^{*} \\ d\varepsilon_{23}^{*} \end{pmatrix} , \quad (36)$$

where $d\varepsilon_{ij}$ (*i*, *j* = 1,2,3) are the incremental total strain tensors and $d\sigma_{ij}$ (*i*, *j* = 1,2,3) are the incremental stress tensors. E_{ii} (*i*, *j* = 1,2,3) are the Young's moduli, either for tension or compression

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loading. Parameters, $d\varepsilon_{ij}$ (i, j = 1, 2, 3), represent the incremental plastic strain tensors. Moduli, G_{ij} ($i, j = 1, 2, 3, i \neq j$), are the shear moduli and v_{ij} ($i, j = 1, 2, 3, i \neq j$) are the Poisson's ratios.

3. Experiments

3.1. Material characterisation

3.1.1. Fracture toughness characterisation

In this research, the results presented in [6,14,23,24] was employed to extract the fracture toughness required for the numerical modelling. Pre-cracks were introduced into the double-cantilever-beam (DCB), four-point end-notched-flexure (4ENF) and mixed-mode-beam (MMB) composite specimens by inserting the polytetrafluoroethylene (PTFE) into the laminated composites. The notches in the compact tension (CT) and compact compression (CC) specimens for intralaminar characterisation were machined using a milling cutter. The test configurations for material characterisation are shown in Fig. 2 and corresponding dimensions are presented in Table 1.

3.1.2. Nonlinearity characterisation

The off-axis tension experiments were employed to characterise the nonlinear behaviour of the composite ply. The geometry of the specimens for the off-axis tension experiments [25], are shown in Fig. 3, where X-Y refers to global coordinate system and 1-2 refers to material coordinate system. In this research, the lengthwise direction is parallel to the loading direction. All the composite specimens employed in the off-axis tension have the sample dimensions shown in Table 2.

3.2. Experimental validation

3.2.1. Material and specimen

Composite panels, for proceeding specimens used in the experimental validation, were manufactured using unidirectional AS4 carbon fibre reinforced PEEK prepregs, provided by CYTEC, United States. An Out-of-Autoclave (OOA) manufacturing route was employed to consolidate the CF/PEEK prepregs. A hydraulic press, manufactured by Mackey Bowley, United Kingdom, was employed to produce the CF/PEEK composite panels, Fig. 4a. A diagram of the APC-2 consolidation schedule for the CF/PEEK prepregs is shown in Fig. 4b.

As a widely-used material testing method, the three-point-bending tests are easy to perform and able to introduce various failure modes into specimens, such as tensile, compressive and shear failure, which are ideal to assess the predictive capability of the computational model. Based on this, in this research, the three-point-bending experiment was employed to conduct model validation. The composite specimens for three-point bend experiments were machined from the manufactured composite panels using a diamond saw, provided by MetPrep Ltd, United Kingdom. The sample geometry and testing apparatus described in ASTM D7265 [26] was employed , Fig. 5, where X-Y-Z refers to the global coordinate system. Details of the composite lay-up, the specimen dimensions and the testing configurations are summarised in Table 3. All of the thermoplastic composite specimens were initially painted using matt white paint before applying a speckle pattern using black dots to facilitate the application of DIC.

3.2.2. Experimental procedure

A screw-driven tensile testing Instron machine was employed to conduct the three-point bend experiments. The load cell has a range of 0 to 100 kN. During the experiments, a displacement control was applied, by setting the loading rate as 1 mm/s. A DIC system was used to measure the strain of the composite specimens under three-point bending. Four composite specimens were tested successfully, and good consistency was observed from those experimental results.

4. Numerical simulation

4.1. Finite element model

Fig. 6a shows the Computer-Aided Design (CAD) model created in Abaqus 2017, which was then converted to a FE model, Fig. 6b. The developed VUMAT subroutine was integrated with the cohesive surface model to simulate the three-point bend events performed on the composite specimens with a lay-up of [0₃/90₃]_{2s}. The virtual specimen was discretised using eight-node linear reduced integration (C3D8R) solid elements with a size of 1 mm × 1 mm. The total number of elements in the FE model for the three-point bend simulation was 16,224. The computational loading speed was set as 0.5 m/s to reduce the computing time and a smooth step was used to ensure the quality of the simulation was not affected by the inertial effects. A general contact algorithm was employed for the global contact and the cohesive surface solution was used for the interfacial contact

between the composite plies. Friction coefficients of 0.2 and 0.25 were defined for the global contact and cohesive contact, respectively [6,14]. Computational accuracy was set as double precision to reduce the accumulation error during simulation. Selective mass scaling was used to provide a compromise between computation time and accuracy. A stable time increment of less than 1e-08 s was achieved, yielding an approximate run time of 21 hours on a Linux Cluster consisting of 16 CPUs.

4.2. Properties for model input

The mechanical properties of the unidirectional CF/PEEK composite ply, such as strength and modulus, were obtained from the data sheet [27] provided by CYTEC, United States. The fracture toughness values were extracted from the results presented in [28] and [29]. The parameters for defining the nonlinearity of the composite ply were determined based on the results reported in [25]. The input parameters required for the developed FE model are presented in Table 4.

4.3. Model implementation

The flow chart of the developed FE model, which includes a cohesive surface model and an elasticplastic damage model, is schematically shown in Fig. 7a. The elastic-plastic damage model is also highlighted in Fig. 7b. In the flowchart, the time associated with the experiments enters the model with the 'Model state' being equivalent to a 'step time'. The numerical model is stopped when the defined total step time has expired. The above flow-chart shows one computation step for a single element. The computation process was performed for every appropriate single element in the FE model for mechanical response and progressive failure of thermoplastic composites.

5. Model validation

5.1. Load-displacement and major strain response

The load-displacement and major strain distribution, were obtained from both the experiments and simulation. Fig. 8a shows the comparison between the experimentally and numerically obtained load-displacement responses. It can be found that both the experimental and computational results followed a linearly elastic response at the initial stage, which was followed by a nonlinear state prior to the damage point. The experimentally measured average maximum load was compared with the corresponding computational results, which is shown in Fig. 8b. The average maximum load delivered

by the experimental results was 1.04 kN \pm 1.6%, and the computational maximum load was 1.02 kN, which is only 2% lower than the experimentally measured average value.

During the three-point bend experiments, the major strain of the thermoplastic composite specimens was recorded using a DIC system. A typical major strain history of the tested thermoplastic specimens is shown in Fig. 9, along with the numerically predicted major strain evolution of the thermoplastic composite specimen. During the experiments, it was observed that, prior to initial damage, the thermoplastic specimens evenly deformed over the span length, from displacement = 0 mm to displacement = 4 mm. Some localised strain was initially observed around the central area when the displacement reached 6 mm. This was observed in both the experimental and numerical results. This level of correlation between the experimentally recorded major strain and the numerically predicted major strain confirms that the developed composite damage model is capable of predicting the major strain for thermoplastic matrix composites.

5.2. Energy dissipation

Fig. 10 presents details of the energy dissipation obtained from the simulation. Prior to damage initiation, the energy was mainly stored as elastic energy, which was then released following the occurrence of damage. It was interesting to observe that the frictional energy, which was deemed to be mainly from the interaction between delaminated or fractured plies, also played a small role during the energy dissipation procedure. For comparison, the total energies measured from the experiments (shown as "Total energy-exp") in the figure were also presented in the figure, along with the computationally obtained total energy (shown as "Total energy-sim" in the figure). The comparison shows that the predicted total energy correlates well with the experimental total energy, which further confirms that the developed composite damage model is capable of predicting the energy dissipation of thermoplastic matrix composites.

5.3. Damage morphology

Fig. 11 shows a comparison of the interlaminar damage (delamination) obtained from the experiments and simulation. The side view of the tested specimen clearly showed that severe interlaminar damage (delamination) occurred within the composite laminates under three-point bend loading. The

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simulated interlaminar damage (delamination) delivered very good agreement with the experimentally observed interlaminar damage (delamination).

The developed damage model can also predict the intralaminar damage in the composite laminates. Fig.12 shows the matrix damage obtained from the experiments and simulation. From the photograph of the tested specimen, it can be observed that the matrix damage occurred in the central area of the tested specimens and this was also demonstrated by the numerical simulation results.

With regards to fibre damage on the top and bottom surfaces, Fig.13 shows the compressive fibre damage on the top surface and Fig. 14 shows the tensile fibre damage on the bottom surface, as obtained from the three-point bend experiments and simulation. It can be seen that fibre breakage occurred in the central area on both the top and bottom surfaces of the simulated specimens (compressive fibre damage on top and tensile fibre damage on bottom) which was consistent with the experimental coupons. The comparison shows that the predicted damage on the top surface has a width of about 7 mm, which is larger than the experimental y obtained damage, which has a width of about 4 mm. For damage on the bottom surface, the experimental and numerical results presented a damage area with a width of about 7 mm. The comparison of the experimental and simulation results indicates that the developed numerical model is able to capture well the failure modes, such as fibre breakage, matrix cracking and delamination, in the composite laminates and reproduce the overall damage morphology of the post-tested composite specimens.

6. Conclusions

An elastic-plastic damage model, which accounts for both the nonlinear behaviour and progressive failure of a thermoplastic composite ply, was implemented as a VUMAT subroutine in Abaqus/explicit, to predict the three-point bend behaviour of thermoplastic matrix composites. The developed elastic-plastic damage model was then combined with the Abaqus in-built cohesive surface model to form a complete Finite Element (FE) model to predict the mechanical response and progressive damage of thermoplastic composite laminates. The simulation results e.g. load response, deformation and damage morphology, were compared with the experimental results extracted from the three-point bend experiments performed on the composite specimens with a lay-up of [0₃/90₃]_{2s}. The comparison

showed that the computational results yielded good agreement to the experimental results. This confirmed the capability of the developed Finite Element (FE) model in predicting the nonlinear behaviour and progressive failure of thermoplastic composite laminates. It is considered this elastic-plastic damage model approach can be more widely applied to other loading configurations, including impact, and this will be developed in subsequent papers. This new high-fidelity damage model approach should be of much value in the design of high-performance thermoplastic matrix composite structures in the aviation industry.

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Fig. 1. The main failure types shown in the unidirectional fibre reinforced composite laminates: (a) experimental observed failure modes [12] and (b) schematically categorised failure modes.



Fig. 2. Testing configuration for (a) mode I (b) mode II (c) mixed-mode (d) modified compact tension and (e) compact compression.



Fig. 3. Dimensions of the samples employed in the off-axis tension experiments.



Fig. 4. Photograph and diagram: (a) photograph of the hot-press manufacturing system and (b) the diagram of APC-2 consolidation schedule for the CF/PEEK prepregs.



Fig. 5. Geometry of the composite specimens for three-point bend experiments.



Fig. 6. The developed CAD model and FE model: (a) the CAD model and (b) the FE model.



Fig. 7. The FE model implementation: (a) the flowchart of the main model and (b) the highlighted





Fig. 8. The overall response obtained from the experiments and simulation: (a) the loading response, (b) the maximum load.



Fig. 9. The comparison of major strain obtained from the experiments and simulation.



Fig. 10. Total energy obtained from experiments and simulation as well as the details of energy dissipation delivered by the computational model.



Fig. 11. The interlaminar damage (delamination) obtained from the physical and virtual post-tested

composite specimen.



Fig. 12. The comparison of matrix damage obtained from the physical and virtual post-tested

composite specimen.



Fig. 13. The comparison of fibre damage on the top surface, from physical and virtual post-tested composite specimen, showing compressive fibre damage.



Fig. 14. The comparison of fibre damage on the bottom surface, from physical and virtual post-

tested composite specimen, showing tensile fibre damage.

Table 1

Dimensions of specimens for material characterisation (mm)

Samples	L	h	a_0	W	R	d	l	r
DCB	140	1.6	45	N/A	N/A	N/A	N/A	N/A
4ENF	70	1.6	50	N/A	N/A	N/A	N/A	N/A
MMB	60	1.6	25	N/A	N/A	N/A	N/A	N/A
СТ	65	60	26	51	4	4	28	2
CC	65	60	20	51	4	10	12	2

Table 2

Nominal dimensions of specimens for off-axis tension and in-plane shear tests.

Items	Total length (l_t)	Gauge length (l_g)	Width (w)	Thickness (t)	Angle (θ)
Values	254 <i>mm</i>	190.5 <i>mm</i>	19 <i>mm</i>	1.27 <i>mm</i>	0°, 15° 30°, 45°, 90°

Table 3

The lay-up and dimensions of the composite specimens for three-point bend experiments.

Items	Lay-up	Length (L)	Width (W)	Thickness (T)	Radius (<i>R</i>)	Support span (D)
Values	[0 ₃ /90 ₃] _{2s}	120 <i>mm</i>	13 <i>mm</i>	3 <i>mm</i>	5 <i>mm</i>	96 <i>mm</i>

Table 4

Properties	Values			
Modulus (GPa)	$E_{11} = 127.6; E_{22} = E_{33} = 10.3; G_{12} = G_{13} = 6.0; G_{23} = 5.7;$			
Poisson`s ratios	$v_{12} = v_{13} = 0.32; v_{23} = 0.35;$			
Strength (MPa)	$X^{T} = 2023.4; X^{C} = 1234.1; Y^{T} = Z^{T} = 92.7; Y^{C} = Z^{C} = 176.0;$			
	$S_{12} = S_{13} = S_{23} = 186.0;$			
Intralaminar fracture	$G_{Ic} _{ft} = 201; \ G_{Ic} _{fc} = 128; \ G_{Ic} _{mt} = 5.6; \ G_{Ic} _{mc} = 9.3; \ G_{Ic} _{mc} = 128; \ G_{Ic} _{mt} = 5.6; \ G_{Ic} _{mc} = 9.3; \ G_{Ic} _{mc} = 128; $			
toughness (kJ/m^2)				
Interlaminar fracture	$G_{IC} = 5.6$; $G_{IIC} = 9.3$;			
toughness (kJ/m^2)				
B-K coefficient	$\eta = 1.89$			
Cohesive strength (MPa)	$\sigma_I = 43 MPa$; $\sigma_{II} = 55 MPa$;			
Cohesive stiffness (N/mm)	$k = 6.4 \times 10^5 N/mm$			
Nonlinear coefficients	$a_{66} = 1.5; A = 3.06e - 19; n = 7.5;$			

Input properties required for the modelling of AS4/PEEK composite ply.
