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A combined XFEM and cohesive zone model for composite laminate microcracking and permeability

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Abstract

A novel computational methodology for predicting three-dimensional microcracking and permeability in composite laminates is presented. The methodology simulates microcrack initiation and propagation using the extended finite element method (XFEM) and delamination using a mixed-mode cohesive zone model. Random microcrack initiation is modelled using a random (Weibull) distribution of fracture strengths. The Weibull distribution is adjusted to account for specimen volume, allowing mesh independent crack density predictions. An alternate method is also investigated, based on an elemental representation of defects using measured void geometry. The predicted microcracking and damage distributions are shown to correlate closely with 3D X-ray CT (computed tomography) scans of cryogenically cycled specimens. Crack opening displacements are consistent with laminate test measurements. Permeabilities, based on the dimensions of the leak paths, were found to be within the measured range for various CF (carbon fibre)/PEEK materials.

Keywords: Carbon Composites; Microcracking; Permeability; XFEM; Cohesive Zone model; Cryogenic Cycling

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1. Introduction

Due to their high specific strength and stiffness, composite materials are ideal for use in industries such as aerospace, automotive and renewable energy, amongst others. However, a major issue with using composite materials for such applications is their propensity to microcrack and delaminate under thermal and mechanical loads. Taken by themselves, these damage modes do not typically constitute full structural failure, with the early growth of microcracks and delaminations being difficult to detect [1-3]. However, this sub-critical damage build-up leads to a number of undesirable effects such as a multi-directional reduction in strength and stiffness, increased susceptibility to attack from solvents and the formation of gas leakage paths through the material [4-11]. Understanding the mechanisms of damage accumulation and how the various damage modes interact is particularly important for pressure vessel applications, including cryogenic fuel tanks for the next generation of re-useable space launch vehicles (RSLVs). The formation of through-thickness crack networks in such structures can allow cryogen leakage to occur, with catastrophic results [12].

Intra-laminar failure, in the form of transverse microcracking in off-axis plies, is usually the first noticeable damage mode encountered in composite laminates. Due to the multi-axial nature of thermal loading, cracks may form in multiple ply groups simultaneously and below the failure strength of the material [13-15]. Overlapping microcrack families in adjacent plies allow the formation of leakage paths through a damaged laminate, with factors such as stacking sequence and laminate thickness being known to influence crack density and permeability [16-19]. With more severe loading, inter-laminar damage in the form of delamination may develop, which can link microcracks in adjacent plies, leading to the formation of leakage paths that might not have developed through microcracking alone. The interaction between delaminations and microcracks has been found to affect transverse crack opening at ply interfaces [20, 21]. Delamination growth in laminates with existing transverse cracks under thermal fatigue loading has previously been modelled by the authors, showing a direct correlation between delaminated crack opening displacement and laminate permeability [22, 23].

The complexity of multiple failure modes acting simultaneously within a composite, in addition to random crack initiation due to variations in material properties, lay-up, loading and the presence of manufacturing defects, calls for a sophisticated and flexible modelling methodology. Attempts at developing finite element models capable of predicting both intra-laminar and inter-laminar failure in composites have used a partition of unity approach for microcracks and a cohesive approach for delaminations [24, 25]. However previous studies have not been able to model or predict the formation of random 3D crack networks in laminates. The ability to predict this sub-critical damage build-up in a single model is of prime importance to understanding composite structure failure. Existing permeability models have been based on repeating 2D and 3D geometries, with pre-existing cracks defined [20, 21, 26-28]. This study, through meso-level modelling of laminates, presents a novel methodology to predict random (Weibull and defect based) crack initiation and growth in composites laminates. The 3D models developed allow mesh independent prediction of crack density, the direct measurement of crack opening displacement and crack overlap areas, and
hence, laminate permeability. The methodology is developed on a globally applicable platform allowing the potential of up-scaling the approach to deal with large structures, including cryo-tanks. A parallel programme of experimental work on cryogenic cycling of CF/PEEK laminates has been conducted and some of these results are presented here for comparison and calibration purposes. 3D X-ray CT (computed tomography) scans of pristine and damaged laminates have been used to provide input in terms of defect distributions and as a means of comparing resulting damage accumulation. The permeability of modelled laminates is also compared to previously measured leak rates from test specimens.

2. Methodology

The methodology developed in this work is based on a combined XFEM (extended finite element method) and SCZM (surface cohesive zone model) approach to damage modelling in composite laminates. XFEM is used for microcrack initiation and propagation (intra-laminar failure), with a Weibull strength distribution being used to account for the random nature of the distribution of matrix microcracking. This approach is predicated on the random distribution of laminate strength within the finite element model of the laminate. An alternate method, based on using an experimental defect distribution to represent material discontinuities, is also presented. Here, a distribution of a priori micro-voids (ellipsoidal) is defined within the finite element mesh, based on measured distributions of these micro-voids. Delamination growth between plies (inter-laminar failure) is based on a mixed-mode SCZM. A globally applicable XFEM platform is essential due to the 3D requirements for future modelling of large-scale fuel storage tanks and material defect distributions which will require crack propagation analysis to be undertaken via a user interface. Fig. 1 gives a general overview of the method.

2.1 Experimental work

In order to develop accurate models of crack growth behaviour, an extensive programme material and damage characterisation regime was undertaken, as described in [29]. Optical microscopy and 3D X-ray CT were used to determine the void contents of a range of CF/PEEK materials of varying thickness (8-ply, 16-ply and 32-ply) and lay-up. Subsequently these laminates were cryogenically cycled in liquid nitrogen (+40°C to -196°C), with damage progression monitored, also using optical microscopy and 3D X-ray CT. The thicker laminates were found to crack extensively after one cycle, with no subsequent crack growth observed after 50 cycles. The resulting crack patterns and dimensions measured from this experimental work, as well as the defect distributions obtained, are employed directly in this present work to define the inputs to the micro-void models and to compare the predicted microcrack distributions against, i.e. for both calibration and independent validation of the models.

2.2 Intra-ply microcracking XFEM model

The extended finite element method is an extension of the classical finite element method, based on the concept of partition of unity [30], which allows modelling of discontinuities through the use of special enrichment functions which are incorporated into the finite element
approximation. XFEM is effective and efficient for modelling material discontinuities in general, such as voids, grain boundaries, dislocations and crack growth problems [31, 32]. Conventional methods of analysing such discontinuities require that the finite element mesh conforms to the discontinuity. This becomes an issue when modelling crack growth, where the dimensions of the discontinuity may change considerably over the course of the analysis, so that constant re-meshing is required in order to represent crack growth. With XFEM, the discontinuity is defined separately from the mesh, allowing a crack of arbitrary shape and location to be modelled effectively without the need for re-meshing and without the usual extensive mesh refinement required [33]. Knowledge of the crack location or propagation path is not required a-priori, allowing the user to forego costly mesh refinement and continual updating of the mesh in the area of interest. This feature is critical to the ability of the methodology to predict microcrack growth due to random inherent material defects in composite laminates, which forms the basis of this work.

The proposed methodology is implemented here within the general purpose, non-linear finite element code, Abaqus [34]. This has significant benefits due to the widespread use of Abaqus in both academic and industrial applications. Phantom nodes are defined within enriched elements to represent the jump in crack surfaces, where real and corresponding phantom nodes separate when the prescribed fracture criterion has been satisfied. The degree of separation of the nodes is defined via a traction-separation cohesive behaviour, whereby the cohesive strength of an enriched cracked element decays to zero. The traction–separation model used here comprises a linear elastic behaviour phase and a subsequent damage progression phase. The constitutive matrix for the elastic phase, relating the stresses and separations in an enriched element are given by Eq. (1) [34],

$$
\begin{bmatrix}
\delta_n \\
\delta_s \\
\delta_t
\end{bmatrix} =
\begin{bmatrix}
K_{nn} & 0 & 0 \\
0 & K_{ss} & 0 \\
0 & 0 & K_{tt}
\end{bmatrix}
\begin{bmatrix}
\delta_n \\
\delta_s \\
\delta_t
\end{bmatrix}
$$

where $t_n$ is the normal component of the stress traction vector and $t_s$ and $t_t$ are the two shear tractions along the local 1- and 2-directions, respectively. $K_{nn}, K_{ss}$ and $K_{tt}$ are the stiffness components that relate the element stresses to separations and $\delta_n, \delta_s$ and $\delta_t$ are the element separations related to the aforementioned normal and shear stresses.

XFEM can be used to model inter-laminar failure. However, in order to accurately capture the transition between inter-ply and intra-ply failure modes using XFEM, it is necessary to use an increased mesh density at the ply interfaces, due to the constraint of one crack surface per element in XFEM. A computationally inexpensive alternative proposed here is to combine an XFEM-based microcracking prediction methodology with a SCZM methodology for inter-laminar failure. This method allows a relatively straightforward interaction between adjacent plies and cracks using pre-defined delamination surfaces. This combined approach is necessary to facilitate large-scale structural damage modelling, e.g. for cryogenic fuel tank structure models, and for subsequent associated permeability predictions. Fig. 2 illustrates the
significant difference in mesh densities required for combined microcrack and delamination prediction using (a) a pure XFEM approach and (b) the proposed XFEM-SCZM approach.

2.3 Delamination SCZM model

The SCZM simulates the decohesion of initially-bonded delamination surfaces which correspond to the outer layers of adjacent ply groups in a laminate. The interfaces between such adjacent ply groups are assumed to be of negligible thickness. A generalized traction-separation behaviour is implemented for the surface decohesion is defined, similar to the XFEM cohesive behaviour. This method allows the modelling of delamination at interfaces, with failure of the cohesive bond characterized by progressive degradation of the cohesive stiffness. The traction-separation model used here assumes initially linear elastic behaviour followed by the initiation and evolution of damage based on mixed-mode fracture. The elastic behaviour is based on a constitutive matrix similar to that of Eq. (1). Due to the complex multi-axial loading during cryogenic cycling, damage evolution is described by the Benzeggagh and Kenane criteria [35] for mixed-mode fracture, which defines an equivalent critical energy release rate, $G_{\text{equivC}}$, combining energy release rates from all three fracture modes ($G_{I}$, $G_{II}$ and $G_{III}$) as follows:

$$G_{\text{equivC}} = G_{IC} + (G_{IIIC} - G_{IC}) \left( \frac{G_{II} + G_{III}}{G_{I} + G_{II} + G_{III}} \right)^\eta$$  (2)

where $\eta$ is a curve fitting parameter.

2.4 Microcrack initiation

Being an intra-ply failure mode, microcracking is modelled using XFEM. A crack is assumed to initiate when the relevant fracture criterion, $f$, is exceeded. In this work, the maximum nominal stress criterion is used, whereby a crack initiates when the value of $f$ exceeds a pre-defined tolerance as follows:

$$f = \max \left\{ \left( \frac{t_n}{t_n^0} \right), \left( \frac{t_s}{t_s^0} \right), \left( \frac{\tau_\theta}{\tau_\theta^0} \right) \right\}$$  (3)

where $t_n^0$, $t_s^0$ and $\tau_\theta^0$ define the peak values of the nominal stress in the normal direction and local 1- and 2- (shear) directions. The surface of newly formed cracks is orthogonal to the normal component of the stress traction vector, which depends on the local material orientation assigned to the enriched element. The X-ray CT scans of the cryogenically cycled CF/PEEK laminates show that transverse microcracks align with the fibre direction in each ply of a damaged laminate, as shown in Fig. 3.

This dependence of crack-growth direction on the local fibre orientation allows for a simplified modelling methodology, whereby a single set of material properties and fracture parameters is defined for the 0° ply. Material property definitions can then be applied to off-axis plies by transformation via local co-ordinate systems relative to the base 0° definition (Fig. 4).
In order to develop a realistic random damage model, manufacturing defects and discontinuities need to be integrated into the simulation. Optical microscopy has shown that voids, inclusions, resin-rich areas and other defects within the plies are possible crack nucleation points, whereby initiation may occur locally at stress levels below the fracture strength of the bulk material. The presence of these discontinuities was found to have a direct correlation to crack formation in the cryogenically cycled laminates [29]. The principle method of representing these defects and discontinuities within the material space is based on a Weibull strength distribution. An alternative method, based on an elemental representation of defects, is also presented. These methods are discussed below.

The first approach is based on the inherent random distribution of the material fracture strength, to simulate microcrack initiation [15, 25, 36]. A continuous probability Weibull distribution is used to represent this distribution of fracture strength [37, 38]. For a given load, \( \sigma \), the strength distribution is given by:

\[
F(\sigma) = 1 - \exp \left[ -\left( \frac{\sigma}{\sigma_0} \right)^m \right]
\]

where \( \sigma_{th} \) is the threshold stress below which failure does not occur, \( \sigma_0 \) is the normalised material strength and \( m \) is the Weibull modulus. The distribution associated with the material is assigned randomly to enriched elements in the finite element mesh. Under loading, cracks are predicted using XFEM to initiate and propagate from and through areas of lower strength, specifically below the fracture strength of the bulk material. Fig. 5 shows a Weibull distribution of random fracture strengths assigned to a 1,000 element mesh, generated using Python code for a carbon-fibre composite material with a mean transverse tensile strength of 85 MPa and a Weibull modulus of 12 [25].

Python is a multi-paradigm, open source programming language [39] which is used here to generate random distributions such as the Weibull distribution, through built-in functions. It was chosen here as a scripting language due to its compatibility for use with Abaqus FE analyses.

The second approach for capturing material defects and discontinuities is based on an elemental representation of defects. A customised Python code was written to randomly vary the elastic properties in a finite element mesh of the composite lay-up according to the measured Gaussian distribution of voids, inclusions and resin-rich areas [29].

Voids can be represented by ellipsoids within an element volume. Knowing the size range of voids within a given laminate, it is possible to randomly distribute voids within this size range throughout the laminate. The effect of voids is to degrade various material properties [40-43], including stiffness, of the surrounding material in an element in proportion to the maximum cross-sectional area of the void as viewed from orthogonal reference planes. To this end, it is assumed that the major and minor axes of the ellipsoids align with the primary directions (x, y, z), corresponding to the fibre and transverse directions, as shown in Fig. 6.
Based on the measured size ranges of voids from X-ray CT scans of the CF/PEEK laminates [29], Gaussian distributions are used to assign appropriate random x (length), y (width) and z (height) values for each ellipsoid. These distributions can be expressed in terms of the following probability density function for a variate:

\[ P(x) = \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \]  

where \( \mu \) is the mean and \( \sigma \) is the standard deviation. Expressing the reduction in stiffness of a material element as a proportion of the element occupied by a void, the corresponding reduced element stiffnesses \( E_i^* \) are thus calculated as follows:

\[ E_1^* = (1 - \pi y z) E_1 \]  
\[ E_2^* = (1 - \pi x z) E_2 \]  
\[ E_3^* = (1 - \pi x y) E_3 \]

where \( E_1 \) is the fibre direction modulus and \( E_2, E_3 \) are the transverse moduli. Fig. 7 shows the trend in void morphology in terms of the relationship between sphericity, \( S \), and void radius, \( r_{void} \), from the measured data, where sphericity is defined as the ratio between the surface area of a sphere with the same volume as a defect and the surface area of the defect. This relationship can be expressed as:

\[ S = -a \ln r_{void} + b \]

where \( a \) and \( b \) are constants. In general, the greater the void volume, the more elongated the void.

The effect of inclusions and resin-rich regions within the material is dealt with in the same way as voids. However, instead of reducing the stiffness of an element based on the presence of a void, the properties of the element are altered to represent those of the discontinuity. In the case of large resin-rich areas in composites, as shown by the dark regions in Fig. 8, the properties of entire elements are replaced by those of the polymer.

2.5 Size effect and mesh dependence

The effect of specimen size on strength is a well-known physical phenomenon [37, 44, 45], arising from the higher probability of occurrence of a critical flaw in larger specimens than in smaller specimens of the same material. Consider the FE analysis of composite laminates with the specimen discretised into a number of individual elements, based on the assigned mesh density. If size effects are not taken into account, the same strength distribution would be applied to the elements in meshes of different densities, resulting in mesh-dependent crack density predictions. Fig. 9 further explains this effect.

On average, a larger volume should contain more defects than a smaller volume. The two meshes in Fig. 9 have equal volumes but different mesh densities. Given that the total meshed volume is
the same, the probability of failure for both meshes should be equal. However, during material property assignment, if the same strength distribution is assigned to the single large element as to each of the 8 smaller elements, the probability of there being a defect in the denser mesh increases relative to the coarse mesh. This is due to the statistical effect whereby there is likely to be a larger variance in 8 distributions than in a single distribution. This means the likelihood of failure of one or more elements in the equivalent 8 element mesh is greater, leading to a direct correlation between crack density and mesh density. In order to correct for this effect, a single large element should therefore have a higher probability of failure than a single small element from the equivalent 8-element mesh. To account for size effect and mesh dependency in crack density predictions here, the Weibull distribution is normalised with respect to the reference element volume. The volume adjusted mean strength, $\bar{\sigma}_s$, for the distribution is therefore given as:

$$\bar{\sigma}_s = \bar{\sigma}_0 \left(\frac{\nu}{V_0}\right)^{-1/m}$$  \hspace{1cm} (10)

where $\nu$ is the element volume and $V_0$ is the reference element volume. Fig. 10 shows this theoretical variation of Weibull mean strength parameter, $\bar{\sigma}_s$, against element volume for a carbon composite material with a mean fracture strength, $\bar{\sigma}_0$, of 75 MPa and a Weibull modulus, $m$, of 12, based on Eq. (10) for a reference element volume of 1 mm$^3$.

In order to demonstrate the mesh independence of this approach, a sensitivity study was carried out to determine the number of elements, in a given finite element mesh, with fracture strengths below the mean fracture strength of the material. A number of Weibull distributions were generated for meshes of different densities, giving different element volumes, as shown in Table 1.

The mean fracture strength was defined to vary with element volume $\nu$, as defined by Eq. (10). The results of the sensitivity study are shown in Fig. 11.

The effect of mesh density on the number of elements below the mean fracture strength is shown to be invariant, within the bounds of normal statistical scatter, for element volumes below 0.01 mm$^3$. Predicted microcrack density is directly controlled by the total number of elements below the mean fracture strength, i.e. a larger number of weaker elements leads to a higher crack density at a given load. Fig. 11 shows that the number of low-strength elements remains constant for high mesh densities (element volume < 0.01 mm$^3$), i.e. that the methodology is capable of capturing the effect of element volume on mean element fracture strength. Above a certain threshold (element volume < 0.01 mm$^3$, number of elements < 10,000), mesh independency is achieved. Hence, mesh independent prediction of crack density is only possible for a specific range of mesh densities. It is necessary, therefore, to establish mesh convergence for reliable results.

### 2.6 Permeability prediction

The extreme thermal stresses arising from cryogenic cycling are sufficient to cause extensive through-thickness microcracking and delamination in composite laminates. Overlapping
crack networks in adjacent plies can lead to permeation of the cryogen though the laminate thickness. Fig. 12 shows an X-ray CT scan of these crack networks present in a cryogenically cycled CF/PEEK laminate [29].

Due to the prevalence of these crack networks in damaged laminates, permeability predictions are typically focused on determining the magnitude of crack openings and the overlap area between adjacent damaged plies [20, 21, 26, 27]. Following [21], an expression for material permeability for an $N$-ply composite laminate, $\beta_0$, is given as:

$$\beta_0 = C \left[ \sum_{K=1}^{N} \left( \frac{\sin \theta}{C_{DK}C_{DK+1}D_{COD_K}D_{COD_{K+1}}} \right) \right]^{-1} \quad (11)$$

where $C$ is the material conductance, $\theta$ is the ply angle, $C_{DK}$ and $C_{DK+1}$ are the crack densities of adjacent plies and $D_{COD_K}$ and $D_{COD_{K+1}}$ are the delaminated crack opening displacements (DCOD) of adjacent plies. Fig. 13 illustrates the overlap area formed by two adjacent microcracks.

Modelling the following three key damage characteristics, as well as the interaction between them, is crucial to developing a methodology capable of predicting laminate permeability:

- Crack density - $C_{DK}$, $C_{DK+1}$
- Delaminated crack opening displacement - $D_{COD_K}$, $D_{COD_{K+1}}$
- Overlapping crack families - $\theta$

2.7 Finite element implementation

In order to implement the above methodology combining XFEM and SCZM, the Abaqus FE code is employed along with customised Python code. A flowchart of the modelling process is shown in Fig. 14:

- Step 1: Weibull parameters or defect distributions are obtained from the literature/experimental work
- Step 2: An Abaqus macro is developed in Python script containing relevant commands and the model geometry
- Step 3: The geometry and mesh are generated within the FE programme, with the model being partitioned into individual plies or ply groups
- Step 4: Separate Python scripts are then used to define a volume-adjusted Weibull fracture strength distribution or a defect/discontinuity distribution
- Step 5: The relevant material/fracture properties of the composite are then updated on an element-by-element basis, based on whichever distribution will be used in the analysis and are then randomly assigned to each element in the previously generated FE mesh
- Step 6: A number of XFEM assignment sets are used to automatically enrich all elements in the mesh (Fig. 15)
- Step 7: The SCZM interactions are defined between each ply group (Fig. 15)
• Step 8: Loading and boundary conditions are defined within the FE software and the model is then run
• Step 9: A Python macro can also be included to run multiple iterations of the model using different random distributions for use in Monte Carlo simulations

In step 10, permeability calculations are carried out based on Eq. (11), using the calculated DCOD and overlap areas from the FE model using an integrated Python code:

- Read nodal connectivity from mesh
- Read x, y, z nodal displacements from output database
- Cross reference connectivity with cracked XFEM elements
- DCOD calculation based on relative x, y, z displacements of adjacent nodes in crack elements
- Calculation of crack-overlap area for individual crack networks
- Sum over the entire laminate and calculate permeability

The Python code calculates laminate permeability based on co-incident crack networks. For more complex crack networks, the process is augmented by direct identification and measurement of leakage path dimensions.

3. Test cases

3.1 Transverse tension test

The transverse tension test for composites was used to verify the mesh independent microcrack initiation aspect of the methodology. In this test, a CF/PEEK coupon 2.5 mm thick, 25 mm wide and with a 150 mm gauge length, is loaded in tension. The uni-directional composite lay-up is such that the fibres are aligned perpendicular to the direction of extension. A volume-adjusted Weibull strength distribution was assigned to the elements in a number of similar specimens with mesh densities varying from 4,000 to 36,000 elements. A limit was placed on the distributions such that no element could be assigned a fracture strength greater than 110 MPa, which was assumed to be the upper limit of the transverse strength of the material, based on the strength of pure PEEK. 3D solid reduced integration elements were used in the analysis, with displacement-control. A uniform mesh density was used throughout each specimen. The base case CF/PEEK properties used in this and subsequent analyses are given in Table 2. The analysis results for six different mesh densities are shown in Fig. 14.
In Fig. 16, fully open transverse cracks can be seen extending partially or fully across the specimens, as signified by the presence of red elements. Numerous partially cracked cyan-coloured elements are also visible in each specimen, representing the extent of local damage formation, prior to failure. Fig. 17(a) shows the result of the size-effect adjustment made to the fracture Weibull distributions for each mesh density. All distributions yield approximately 500 elements with a fracture strength below the pre-assigned threshold of 110 MPa. Fig. 17(b) shows that apart from the specimen with the lowest mesh density of 4,000 elements, all other meshes produced results consistent with a bulk transverse stress at failure of approximately 98 MPa. This result indicates that above a certain density limit (4,000 elements), mesh independence is achieved, with specimen failure occurring at a similar, but statistically-varying, load point for all models.

3.2 Cryogenic permeability prediction

3.2.1 Overview

The specimens investigated for this case are similar to the rectangular (34 mm× 27 mm) CF/PEEK laminates tested in [29]. Of the 8-ply, 16-ply and 32-ply laminates which were tested, the thickest 32-ply specimens were found to crack after a single cryogenic cycle (ΔT = -236 °C) in liquid nitrogen, leading to the formation of extensive through-thickness crack networks and associated crack overlap areas. This result was observed through the use of 3D X-ray CT. At sufficient scan resolution (15 μm), it was possible to examine overlapping crack groups in damaged specimens, and to directly measure individual crack opening displacements and crack overlap areas, as shown in Fig. 18.

The proposed modelling methodology allows the prediction of laminate permeability based on the physical opening of 3D XFEM cracks in adjacent plies, similar to the method by which the overlap area is calculated in Fig. 18. The technique is illustrated in Fig. 19, where a single crack network has been modelled using the combined XFEM-SCZM approach, with the DCOD values being directly measured at the overlap area.

3.2.2 Weibull distribution method

The first test case uses a Weibull distribution of fracture strengths to simulate random microcrack initiation. The distribution is size dependent and is based on the transverse tensile strength of Suprem IM7, given in Table 2, for a specimen volume of approximately 9375 mm³. Two 32-ply lay-up configurations were modelled: [0/90/0/90]S and [0/45/135/0/90]S, each with a volume of 4112 mm³. The part geometries were uniformly meshed with 120,000 3D elements, with a surface interaction defined between each of the ply groups. A thermal load, ΔT = -339°C, based on the difference between the glass transition temperature of the material and the temperature of liquid nitrogen, was applied directly to the mesh. In addition, symmetry conditions were applied to the specimen edges to mitigate against computationally expensive edge effects.

The simulations were performed on 24 2.4GHz Intel Ivy Bridge cores on an SGI ICE X system at the Irish Centre for High Performance Computing (ICHEC), with each simulation
typically requiring 1,150 CPU hours. Extremely small time increments, on the order of $10^{16}$ units, were required in order to ensure solution convergence, due to the rapid growth of multiple cracks simultaneously. Specialised general solution controls were also required, including increased number of allowable increment cutbacks in line with the discontinuous nature of the analyses. Figs. 20 and 21 shows the results of the simulations in terms of the resulting surface cohesive forces and the XFEM crack surfaces.

As expected, crack nucleation occurred in low-strength elements first. The degradation in stiffness of cracked elements was found to cause an altered stress field in the vicinity of the initial crack, leading to an increased likelihood of crack initiation and propagation in adjacent elements and ply groups. In the case of the cross-ply laminate (Fig. 20), the initial nucleation sites subsequently developed into the hubs of through-thickness crack networks. As observed in cryogenic experiments, transverse microcracks were able to propagate across the entire specimen. The majority of cracks grew simultaneously within an extremely small time increment ($<10^{10}$), with the exception of some cracks in the inner $0^\circ$ plies, which took slightly longer to grow across the entire specimen width. This action suggests near-instantaneous crack formation on an experimental time-frame. Interfacial damage was non-existent, except for relatively minor delaminations along crack paths and overlap areas.

The quasi-isotropic laminate (Fig. 21) was found to exhibit more complex crack network formation. Like the cross-ply laminate, initial nucleation sites influenced crack formation in adjacent plies; however, not all of these sites resulted in co-incident through-thickness cracking. Several inter-connected leakage paths were predicted, comprised of spatially disparate cracks throughout the laminate. Other cracks, particularly in the $90^\circ$ plies, were predicted to form in isolation, not connected to any crack network. Again, the majority of the crack growth was predicted to occur simultaneously and near-instantaneously, with the exception of the slightly slower growth of cracks in the outer $0^\circ$ plies. Minor delamination was also predicted at crack overlap areas.

Fig. 22 compares COD values from experimental work with the above simulations. The crack openings calculated from the models were found to follow the same general trend measured in the test specimens, where the microcracks in the outer ply groups of laminates were consistently found to be wider than those in inner ply groups. This trend also shows, with regards to co-incident crack networks, that permeability of the laminate would be restricted by the relatively narrow crack openings found in the inner and off-axis plies. Permeability output for the laminates using the Weibull strength distribution method is given in Section 3.2.2.

### 3.2.2 Defect distribution method

The input data for the defect distribution method is based on the void content analyses from [29] for 32-ply CF/PEEK laminates, which provide the range and variation in void dimensions in terms of x-y-z coordinates. As described in the previous section, full cross-ply and quasi-isotropic laminates were modelled using the same thermal load. However, a reduced mesh of approximately 46,000 elements was used for these simulations. In order to
reduce computational expense, the void range was subject to a lower bound, below which the smaller voids (< 0.025mm³ in volume) were assumed to have a negligible effect on the surrounding material properties. Due to the lower mesh density, input processing was generally completed in less than 0.5 hours, with the simulations being run over the same system described in Section 3.2.1. Difficulty in achieving solution convergence within the 48 hour processing window for this method required using a reduced toughness Suprem IM7 material model, with the fracture toughness values being reduced by an order of magnitude. Figs. 23 and 24 shows the results of the simulations in terms of the resulting surface cohesive forces and the XFEM crack surfaces.

Crack nucleation for this method was found to occur in the region surrounding high void content elements. This is the result of the low stiffness of high void content elements, which leads to the formation of local stress concentrations. Elements in the direct vicinity of these voids are therefore subjected to stress levels above those present in the bulk material. As mentioned previously, achieving full crack propagation using this method proved computationally more expensive than for the Weibull method. In order to ensure prompt crack growth in this case, with a focus on qualitative trends in terms of distributions and orientations of microcracking, the material toughness was artificially reduced by a factor of 10. Fig. 23 shows the extensive microcrack formation for the 32-ply cross-ply laminate. As with the Weibull method, crack growth is predicted across the laminate within an extremely small time increment. However, a small number of cracks were predicted to not propagate fully across the specimen width prior to the simulation terminating. This trend was more noticeable for the quasi-isotropic laminate shown in Fig. 24, where only cracks in the centre plies were predicted to undergo significant growth within the simulation run-time. Crack nucleation was predicted in off-axis and outer ply groups, but these cracks were not predicted to grow through more than a few elements.

3.2.3 Permeability calculations

Permeability calculation was implemented though the customised Python code discussed in Section 2.5 and by direct computation of crack opening displacements from the simulation deformed geometry, depending on the complexity of the resulting leak paths. Predictions for the Weibull and defect distribution simulation methods were compared with leak rates for a number of CF/PEEK 8-ply laminates exposed to a single cryogenic cycle (Table 3).

The predicted leak rates for the simulations were found to lie between the bounds of the most and least permeable test specimens. For the Weibull simulations, the cross-ply laminate was predicted to have a slightly higher permeability, based on a predicted general trend of wider adjacent overlapping cracks. Although the cross-ply defect simulations had a significantly greater crack density compared to the cross-ply Weibull simulations, the leak rates for the laminates were quite similar. This is due to a ‘bottleneck’ effect, whereby the centre ply group of the defect laminate has a relatively low crack density, thus limiting the potential for leakage as a function of these crack dimensions, in spite of higher crack densities in the outer ply groups. Given the limiting effect of low crack density plies on leak rates for laminates, identification of these low-damage ply groups is of prime importance for the design of
composite cryogenic storage vessels. While the quasi-isotropic defect simulation laminate predicted fully propagated microcracks, no through-thickness crack networks were predicted, resulting in zero leak rate.

4. Conclusions

A combined XFEM and cohesive zone methodology for predicting composite laminate microcracking distributions and permeability is presented. The method uses XFEM for random microcrack initiation and propagation (intra-laminar failure) and SCZM for the delamination between plies (inter-laminar failure). The methodology allows for complex 3D crack networks to be modelled and enables direct computation of DCOD values and crack overlap areas for permeability prediction.

Given the inherently random nature of the potential microcracking features in composite materials, two distinct methods of predicting random microcrack initiation were investigated. In the first method, a Weibull distribution, for stochastic characterisation of the fracture strength of a material was used to represent the presence of defects within the material. Based on the strength distribution, a random fracture strength, adjusted to account for size effects, was assigned to each element in the FE mesh. Mesh independence was established via a series of transverse tensile test simulations using a range of mesh densities. The second approach was based on an elemental representation of defects. This involved the reduction in a given element stiffness based on the dimensions of defects, specifically voids, within its bounds. The size range of voids was taken from measurements via 3D X-ray CT characterisation of CF/PEEK laminates.

Full 3D simulations of 32-ply cross-ply and quasi-isotropic laminates, subjected to a cryogenic load history, using both methods of defect representation, predicted extensive through-thickness crack networks consistent with X-ray CT scans of similar tested specimens. Average COD values taken from the models were found to follow the same trends as those measured experimentally, with inner ply groups having consistently narrower crack openings than outer ply groups. Permeability calculations for the damaged laminates fell within the range of measured leak rates from tested CF/PEEK specimens, indicating the applicability of the methodology to complex damage accumulation prediction for composite materials.

Future work will include modelling of realistic cryogenic pressure vessel structures to determine the optimum composite lay-up for minimal gas leakage. The models will incorporate transient heat transfer to examine the effects of tank wall thickness on damage formation.

Acknowledgements

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Transportation. Access to computational resources was provided by the Irish Centre for High-End Computing (ICHEC).

References


[39] Available at www.python.org


Figure captions

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Figure 7 Relationship between sphericity and void radius from test data [29] for a CF/PEEK laminate for $a = b = 0.167$

Figure 8 Filtered X-ray CT scan of a CF/PEEK laminate with resin-rich regions shown as dark cuboids within the bulk material

Figure 9 The effect of mesh density on the strength of an element. The probability of failure in the 8-element model is greater than for the 1-element model, for equal fracture strength distributions applied to each constituent element. This is shown by the difference in fracture strength ranges between the 1-element and the 8-element distributions

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Figure 16 Results of the transverse tension tests on uni-directional laminae for the 4,000 element and 21,000 element specimen models. The specimens are shown at failure, with the horizontal red rows of elements signifying fully open cracks

Figure 17(a) Number of elements below the threshold fracture strength limit, set at 110 MPa, for each mesh. (b) Bulk transverse stress at failure for each mesh density

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<th>Number of elements</th>
<th>Element volume $v$ (mm³)</th>
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Table 2

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<th>Property</th>
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<tr>
<td>$0^\circ$ Tensile Modulus (GPa)</td>
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<td>Poisson’s ratio</td>
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<td>GIIC (J/m$^2$)</td>
<td>1355</td>
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<td>Weibull modulus ($m$)</td>
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<table>
<thead>
<tr>
<th>Material</th>
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<th>Leak rate (scc/s/m²)</th>
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<td>Cytec AS4 (8-ply QI)</td>
<td>Experiment</td>
<td>$8.5 \times 10^{-3}$</td>
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<tr>
<td>Tencate AS4 (8-ply QI)</td>
<td>Experiment</td>
<td>$1.0 \times 10^{-4}$</td>
</tr>
<tr>
<td>Suprem IM7 (8-ply QI)</td>
<td>Experiment</td>
<td>$2.5 \times 10^{-1}$</td>
</tr>
<tr>
<td>Suprem IM7 (32-ply CP)</td>
<td>Weibull simulation</td>
<td>$8.42 \times 10^{-3}$</td>
</tr>
<tr>
<td>Suprem IM7 (32-ply QI)</td>
<td>Weibull simulation</td>
<td>$3.6 \times 10^{-3}$</td>
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<tr>
<td>Suprem IM7* (32-ply CP)</td>
<td>Defect simulation</td>
<td>$1.18 \times 10^{-2}$</td>
</tr>
<tr>
<td>Suprem IM7* (32-ply QI)</td>
<td>Defect simulation</td>
<td>-</td>
</tr>
</tbody>
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