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# Discrete ply modelling of aeronautical intermediate-scale notched carbon fibre reinforced thermoplastic specimens subjected to multiaxial loading

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## Abstract

Several finite element models developed at the mesoscale level are available for predicting the strength and failure progression of composite materials. However, this kind of damage models are commonly validated by comparing with typical coupon-scale testing specimens under uniaxial loading, which are not fully representative of aeronautical structures subjected to complex multiaxial loads. In this work, the Discrete Ply Model (DPM) is employed to reproduce intermediate-scale experimental tests carried out on carbon fibre reinforced thermoplastic samples, with a sharp central notch of 100 mm, tested in the VERTEX rig under tension, shear, and combined tension and shear loading. The tests show early buckling (particularly for the shear and combined cases) and development of post-buckling for almost the entire loading. The numerical results obtained demonstrate that the strengths, the fluxes as a function of the applied strains, deformed shapes, buckling modes, crack propagations and failure patterns are predicted with reasonable accuracy.

*Keywords:* Thermoplastic, Finite element analysis (FEA), Multiaxial loading, Structural scale specimens

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## 1. Introduction

Carbon Fibre Reinforced Polymer (CFRP) composites are nowadays widely used for lightweight applications, such as in aerospace, wind turbines, automotive, etc., thanks to their excellent stiffness and strength to weight ratio [1–3]. Nonetheless, one major drawback of CFRP is their inherent brittle and complex failure behaviour, which involves several failure mechanisms that occur altogether, such as fibre breakage, kinking and pull-out, matrix cracking, delamination and fibre-matrix debonding.

The development and certification of composite structures is still based on the so-called Building Block Approach (BBA) [3–8], which consists in a pyramid of levels, going from coupon size up to full-scale tests. At the lowest level of the pyramid, tests are carried out on coupons under uniaxial loading, allowing to characterise the materials and obtain design allowables [3, 9]. Testing becomes more complex for the higher levels of the pyramid, where structural details are tested, until the highest level, where the full component is tested. However, these tests are commonly limited to uniaxial loading [3].

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13 Composite structures are assembled by bolts, therefore, the presence of holes or cut-outs, which lead  
14 to complex stress concentration and a strength reduction, is unavoidable [6, 10]. Commonly, the strength  
15 reduction of holes is determined by carrying out open hole tests, at the lowest levels of the pyramid [10–14].  
16 Nonetheless, open hole tests are limited to small coupons under uniaxial loading and thus, may not be repre-  
17 sentative of composite structures subjected to complex multiaxial loading. Moreover, open hole specimens  
18 commonly fail catastrophically, while in a larger structure, the crack propagates more progressively [10].  
19 This is an important fact, since aircraft manufacturers must certify their structure is safe under static loads  
20 with a large crack that could occur due to an exceptional event [6].

21 In order to accurately design CFRP components, it is relevant to test specimens that are representative  
22 of the real counterparts, and under complex loading, similar to the loads encountered for instance in an  
23 aircraft under service. There are few testing rigs in the world that are able to test structural elements  
24 (i.e. specimens at the middle level or at the top of the pyramid) under complex loading [3, 10]. Basically  
25 two types of these machines exist. In the first type, loading is applied to the specimen directly from the  
26 actuators, with the downside that many actuators are needed to generate compression or shear. In the  
27 second type of machine, the specimen is part of a larger structure (usually with a box shape), which is  
28 loaded by actuators [3, 15, 16]. This allows to generate combined tension/bending/torsion loading, which  
29 is more representative of the multiaxial loading found in aeronautical parts when in service. The drawback  
30 of these tests is that evaluating the forces supported by the specimen is more difficult than in traditional  
31 universal testing machines.

32 Almost uniquely in the world, the VERTEX testing rig of the Institut Clément Ader (Toulouse, France)  
33 is one of the few machines able to test large composite specimens (at the intermediate scale of the test  
34 pyramid). Hence, the machine is capable of testing, for instance, specimens representative of fuselage  
35 sections under multiaxial loading, at moderate cost. The details and validation of this rig were presented  
36 in Serra *et al.* [3, 6]. Recently, Grotto *et al.* [10] used the VERTEX machine for testing thin flat CFRP  
37 thermoplastic specimens (558 x 536 mm<sup>2</sup>) with a large, sharp central notch of 100 mm, under combined  
38 loadings of tension, shear and internal pressure. The results showed that pressure led to an earlier failure  
39 initiation for shear tests, but not for tension. Shear loading always led to earlier failure, regardless of the  
40 presence of combined pressure or not. These results therefore allow to get a more representative overview  
41 of the presence of a large notch, than the traditional open hole test.

42 Due to the large amount of experimental tests required to certify composite structures, and the com-  
43 plexity involved in testing composite parts under combined loading, the literature is continuously work-  
44 ing towards developing numerical models with enough predictive capabilities, able to replace real exper-  
45 imental tests [7]. Nowadays, several models are available in the literature developed at different scales:  
46 macromechanical models [17, 18], mesomechanical models [8, 12, 19–25], and micromechanical [26–29].  
47 Macromechanical models assume an homogeneous material, meaning that the interaction between plies  
48 cannot be captured and thus, they are severely limited. On the other extreme, micromechanical models  
49 physically take into account the presence of the fibre and matrix and their interaction, being more realistic.

50 Unfortunately, prohibitive computational requirements are needed to simulate even small specimens. For  
51 this reason, mesomechanical models stand as the best compromise, since these can capture delamination,  
52 while fibre breakage and matrix cracking can be modelled by means of intraply damage variables.

53 Mesomechanical models can be categorised according to their level of discretisation [12]: from mod-  
54 els fully based on continuum damage mechanics (without including cohesive interfaces), to models fully  
55 discretised (including interface elements to capture fibre breakage, delamination and matrix cracking). For  
56 example, Maimí *et al.* [19, 20] developed a continuum damage model able to capture the damage onset  
57 and evolution of composite materials. A more advanced 3D version of this approach, including plasticity,  
58 was recently presented by Cózar *et al.* [24, 25]. These models are fully continuum, excluding the use of  
59 interface elements. Chen *et al.* [13] proposed a smeared crack model, which used continuum mechanics  
60 to model fibre and matrix failure, combined with cohesive interfaces to capture delamination. Bouvet *et*  
61 *al.* [30] originally developed the Discrete Ply Model (DPM), which was refined in subsequent studies [12].  
62 In this approach, solid elements (including a damage variable) are used to capture fibre breakage, while  
63 interface elements are employed to capture matrix cracking and delamination.

64 With the objective of simulating damage progression, but with lower computational efforts, other ap-  
65 proaches such as the Equivalent Single-Layer (ESL) or the Layer-Wise (LW) have also been developed  
66 [31, 32]. ESL models assume uniform kinematics through all the thickness, with the stiffness matrix of  
67 each layer being homogenised. In contrast, LW models take into account different sets of variables for  
68 each layer, with a displacement continuity being imposed at the layer interfaces. With this context, Trom-  
69 bini *et al.* [32] recently presented a Hashin-based orthotropic damage model, linked with higher-order  
70 one-dimensional elements, capable of capturing both the ultimate load and the crack propagation.

71 Nowadays, current available numerical models have been well proven under different loading conditions  
72 and have been employed to reproduce different tests at the lower levels of the pyramid. However, to the  
73 authors' best knowledge, few studies exist presenting damage simulations performed at the higher levels of  
74 the pyramid, especially, under multiaxial loading. For example, Serra *et al.* [33] used the DPM to reproduce  
75 experiments on large notched coupons, although these were limited to pure tension tests. Later, Serra *et al.*  
76 [34] used again the DPM to simulate medium velocity impacts and complex loadings after impact on large  
77 composite panels. Good correlation between the DPM and experiments were found.

78 As a follow up from previous research [3, 6, 10, 12, 33], in this work the DPM is employed to reproduce  
79 intermediate-scale experimental tests on thermoplastic carbon notched samples tested in the VERTEX rig  
80 under combined loading. While previous work already showed the capabilities of the DPM to reproduce  
81 experiments on large notched coupons [33, 34], simulations were limited to pure tensile tests [33], and to  
82 unnotched panels [34] and thus, this paper goes one step forward. The aim and originality of the study is to  
83 demonstrate the capabilities of the numerical model to capture the failure mechanisms of notched specimens  
84 of higher levels of the pyramid of tests under multiaxial loading. Moreover, the model attempts to reproduce  
85 not only the strength found in these tests, but also the crack propagation (failure pattern) and the deformed  
86 shape. Another highlight of this work is that the tests show early buckling and development of post-buckling

87 during almost the entire tests. The results obtained show that shear, tension and combined tests were  
88 successfully reproduced in terms of strength and failure pattern, proving that accurate virtual testing is not  
89 only limited to the lower levels of the pyramid, and that the DPM approach is robust. The paper is organised  
90 as follows. First, a summary of the experimental testing campaign and the finite element approach are  
91 described. After that, the results and discussion are presented for the three cases analysed and eventually,  
92 some conclusions are drawn. All the data shown in this study is normalised due to confidentiality. It is  
93 worth noting that this paper will focus on the numerical side (i.e. to reproduce the experiments), rather than  
94 analysing the experimental results, since this was performed in another paper [10].

## 95 2. Materials and methods

96 This section presents the materials, experimental testing campaign and the finite element models that  
97 were developed in this work.

### 98 2.1. Experimental campaign

99 The experimental testing campaign was carried out by using the VERTEX testing machine of the Insti-  
100 tute Clement Ader (Toulouse, France), which is able to perform multiaxial tests [3, 6]. The same specimens  
101 presented and analysed in Grotto *et al.* [10] are here considered again. The specimen consists on a  $558 \times 536$   
102  $\text{mm}^2$  planar plate with 128 holes, that are used to bolt the specimen to the VERTEX machine. Thus, the  
103 actual ‘free area’ of the specimen during testing is about  $400 \times 400 \text{ mm}^2$ . The stacking sequence cannot be  
104 revealed due to confidentiality, but we note that the specimens are quasi-isotropic, with the same number of  
105 plies oriented at  $0^\circ$ ,  $90^\circ$ ,  $+45^\circ$  and  $-45^\circ$ . The material consists in an aeronautical thermoplastic carbon fibre  
106 reinforced polymer, with a total of 8 plies. The specimens have a centre-notch 100 mm long with an end  
107 notch radius of 1 mm, see Fig. 1.

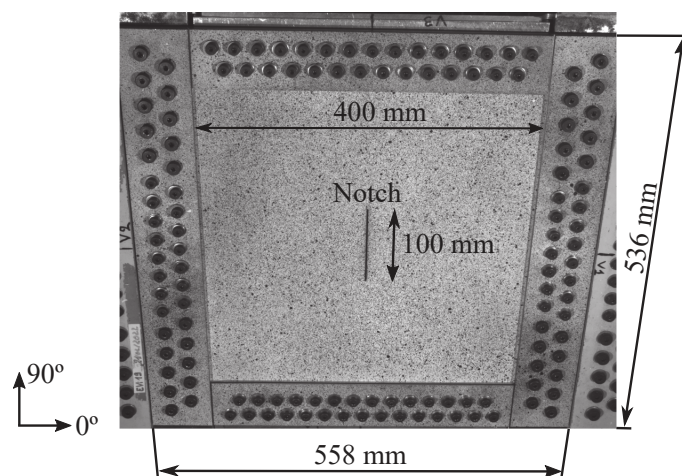


Figure 1: Geometry and dimensions of the notched specimens tested in the VERTEX machine.

108 To manufacture the plates, the consecutive plies were stacked on to another and held together by pressing  
109 a soldering iron on the current top ply [10]. The material was then cured at high pressure and temperature

110 (above 300 °C) following the manufacturer’s guidelines. For more details of the manufacturing process, the  
 111 reader is referred to [10].

112 As stated, the VERTEX test rig is used to carry out the experimental campaign, see Fig. 2. The test  
 113 bench consists in a tubular box with four actuators. The specimen is bolted at the central part and in the  
 114 upper face. The four jacks are used to obtain the desired loading conditions. Jacks 1 and 2 (see Fig. 2a) push  
 115 or pull symmetrically the box, causing it to bend. Thus, with these conditions, the specimen is subjected  
 116 to either tension or compression (Fig. 2c). On the other hand, jacks 3 and 4 generate torsional loading in  
 117 the central box, and thus, loading the specimen in shear (Fig. 2c). In addition, an air-pressurised rubber  
 118 bladder can be included in the central box to subject the specimen under pressure, although this was not  
 119 performed in this paper. The four jacks can be controlled independently to obtain any loading combination:  
 120 tension/compression + shear + pressure. In total, three different tests are considered in this study: a) tension,  
 121 b) shear and c) combined tension and shear. After bolting the specimens to the bench, loading was slowly  
 122 applied until the crack propagation was significantly long and the specimen failed. Two specimens were  
 123 tested for each case. In addition to this, two optical cameras are located on top of the specimen, which are  
 124 used for performing Digital Image Correlation (DIC), while an infrared camera is employed to detect and  
 125 follow the crack length, see Fig. 2b.

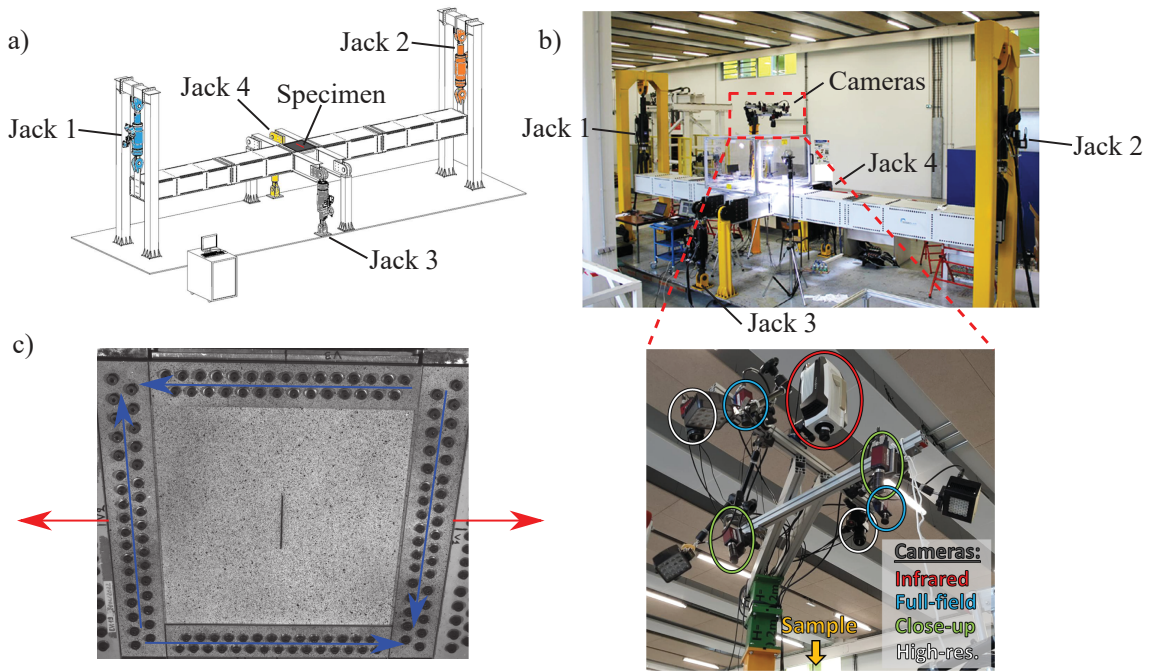


Figure 2: VERTEX testing rig. a) Scheme of the VERTEX machine, b) photo of the real machine, including also the cameras for monitoring, and c) representation of the loading conditions obtained in the specimen.

126 To perform DIC, a random black speckle pattern was painted at the outer surface of the free region of  
 127 the specimen (about  $400 \times 400 \text{ mm}^2$  of area), and pictures were taken by using the full-field optical cameras  
 128 with a frequency of 2 frames per second. The commercial software VIC-3D 7, with a local subset method  
 129 (subset=29 px, step=7 px, filter=15 px, 1 px = 0.28 mm) [10], was used to obtain the displacements based

130 on the pictures.

131 Due to the complexity of the VERTEX bench, a classical load-displacement or stress-strain curve cannot  
132 be obtained for the tests. Therefore, the same approach carried out previously [10] is employed to obtain  
133 fluxes and strains representative of the loading conditions from the DIC data. Fluxes are computed based  
134 on the calculation of the first and second derivatives of the out-of-plane and in-plane displacement, using  
135 classical laminate theory, with a 5 mm step between neighbour point values. For each frame available during  
136 the test, the longitudinal flux ( $N_{xx}$ ) is computed as the average value contained in the boxes illustrated in  
137 Fig. 3a, while the shear flux ( $N_{xy}$ ) is obtained as the average of the four boxes defined in Fig. 3b. Notice  
138 that the boxes are located close to the borders of the specimen and far away from the notch, so that these  
139 can be representative of the loading of the specimen. In addition, for the tensile test, only the flux  $N_{xx}$  has  
140 a significant value (since this corresponds with the applied load), while the shear test mainly has  $N_{xy}$  flux.  
141 The combined shear plus tension case has a significant amount of both fluxes. Moment fluxes were not  
142 analysed since these can be neglected for these tests [10]. Moreover, the DIC data was also employed to  
143 compute global strains. The longitudinal global strain,  $\epsilon_{xx}$ , is computed as

$$\epsilon_{xx} = \frac{U_R - U_L}{X_R - X_L} \quad (1)$$

144 where  $U_R$  and  $U_L$  are the average longitudinal displacements (x direction) of the right and left boxes, re-  
145 spectively, while  $X_R - X_L$  is the horizontal distance between both boxes in mm, see Fig. 3a. Likewise, the  
146 global shear strain,  $\epsilon_{xy}$ , is computed as

$$\epsilon_{xy} = \frac{U_T - U_B}{2(Y_T - Y_B)} + \frac{V_R - V_L}{2(X_R - X_L)} \quad (2)$$

147 where  $V_R$  and  $V_L$  are the average transverse displacements (y direction) of the right and left boxes, respec-  
148 tively,  $U_T$  and  $U_B$  are the average longitudinal displacements (x direction) of the top and bottom boxes,  
149 respectively, while  $Y_T - Y_B$  is the vertical distance between both boxes in mm, see Fig. 3b. Therefore, for  
150 the tensile test, the  $N_{xx} - \epsilon_{xx}$  curve is obtained, while for the shear and the combined test, both  $N_{xx} - \epsilon_{xx}$   
151 and  $N_{xy} - \epsilon_{xy}$  curves are analysed as explained later.

152 The infrared cameras are used to monitor and obtain the crack length along the test. The cameras were  
153 set up to monitor a window of  $320 \times 256$  px<sup>2</sup> with a frequency of 100 FPS, which is a low resolution, but  
154 enough to detect failure signals and follow the crack with detail. As a consequence of the different thermal  
155 emissivity and local surface orientations, all the involved components (sample, tabs, notch, bolts, etc.) can  
156 be fully distinguished. During testing, a local increase in temperature of 1°C indicates fibre failure [33].  
157 Other failure modes, such as matrix cracking or delamination, produce much smaller thermal increase (few  
158 tenths of a degree) and are more difficult to observe. Hence, the infrared measurement allows to detect fibre  
159 breakage through the entire specimen thickness, something that is not possible with DIC. During the test,  
160 as the crack starts to propagate, heat dissipation becomes clearly visible, which allows to locate the crack  
161 tip and even to see the shape of the crack. As in previous work [10, 35], the crack front is assumed to be  
162 located at the centre of the heat spot, since the width of the spot is attributed to heat diffusion and not to  
163 diffused damage [35]. Therefore, the crack length is computed as the distance between the centre of the

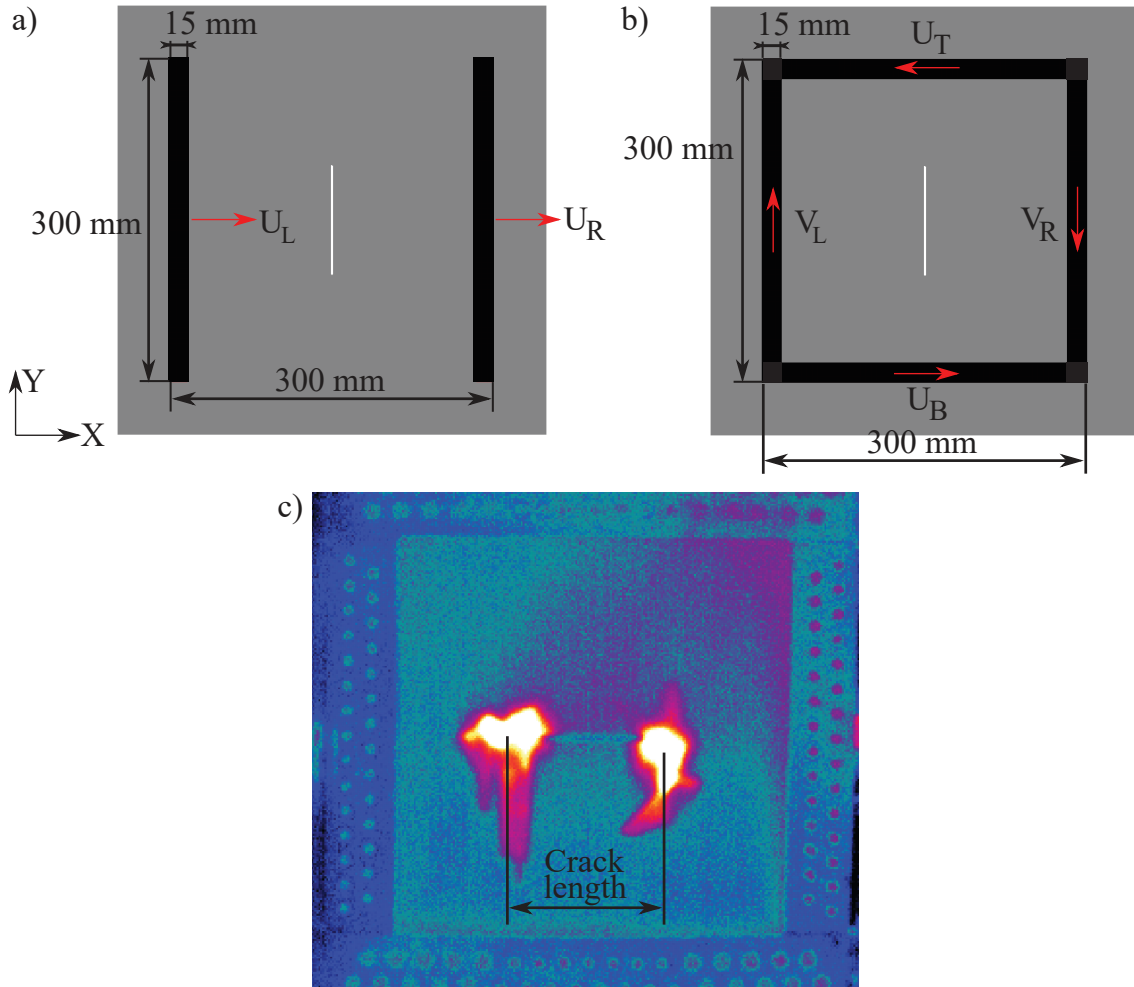


Figure 3: Post-processing of the experimental results. a) Definition of boxes to obtain the longitudinal flux and strain, b) boxes used to compute the shear flux and strain and c) infrared frame showing the approach to compute the crack length.

164 heat at the two sides of the notch, see Fig. 3c.

## 165 2.2. Finite element model

166 This section presents the Finite Element (FE) model that was developed for reproducing the experimen-  
 167 tal campaign presented in Section 2.1, carried out in the multiaxial VERTEX test bench (Fig. 2).

168 The commercial finite element software Abaqus/explicit 2018 [36] has been employed to carry out  
 169 the simulations. In total, three different models have been developed to reproduce the following tests:  
 170 a) tension, b) shear and c) combined tension and shear. The model is identical for the three cases, with  
 171 only the boundary conditions being different accordingly to the desired loading conditions. In order to  
 172 model the progressive failure of the composite material, the Discrete Ply Model (DPM) approach has been  
 173 employed [12, 30, 37]. While this method has been greatly described elsewhere [12, 30, 37], the basics of  
 174 the methodology are here briefly presented for the reader's convenience.

175 Fig. 4 shows a schematic representation of the DPM approach. The DPM is able to predict the three  
 176 main failure mechanisms that occur in composites: intra-ply fibre failure, intra-ply matrix cracking and

177 inter-ply delamination. One of the main innovative concepts of the DPM is the use of a specific mesh set  
 178 up, consisting in a combination of 3D solid elements and zero-thickness interface (cohesive) elements. The  
 179 objective of the 3D volume elements is to capture fibre breakage, while the interface elements are meant to  
 180 capture matrix cracking and delamination. The mesh is oriented with the fibre orientation, which allows to  
 181 capture accurately matrix cracking. Therefore, the mesh set up has 4 nodes at each point (see Fig. 4). In this  
 182 way, 2 of them allow to model the matrix cracking of the upper ply; the 2 others allow to capture the matrix  
 183 cracking of the lower ply and the 2 pairs of nodes are linked together by delamination elements. Thus, a  
 184 natural coupling between delamination and matrix cracking is established. The downside of this approach is  
 185 that it requires a complex mesh (with coincident nodes) at the interfaces between the cohesive elements and  
 186 the 3D elements. In addition, the use of an oriented mesh increases even more the complexity for creating  
 187 it. Unfortunately, the generation of such mesh is too complex to be generated in Abaqus directly. For this  
 188 reason, an in-house Fortran routine is used to generate the desired mesh, which is afterwards imported into  
 189 Abaqus. Notice that one element through-the-thickness of each ply is used.

190 Compared with traditional standard models, e.g. Abaqus built-in Hashin damage model, the DPM is  
 191 fully 3D, not being limited to plane stress elements, such as shell or continuum shell elements, as the Hashin  
 192 model available in Abaqus. Moreover, splitting and delamination are more accurately captured thanks to  
 193 the specific mesh set up.

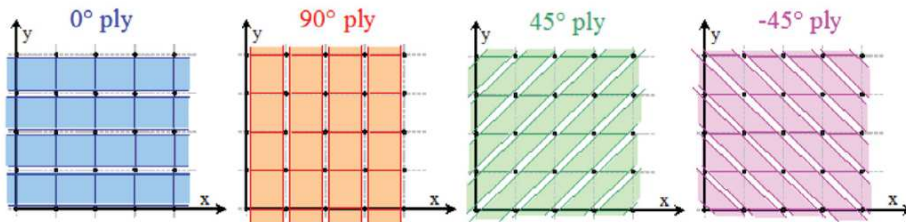
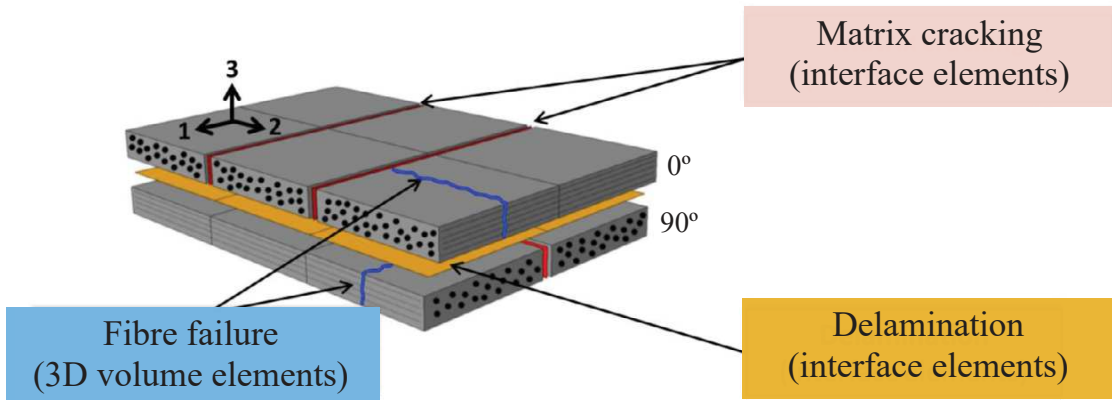


Figure 4: Schematic representation of the discrete ply model approach, showing the different type of elements, interfaces used and mesh set up [6].

194 Fibre breakage is accounted for by the volume elements (Fig. 4). In order to model the progressive  
 195 failure, a continuum damage mechanics approach is used. Thus, longitudinal failure is initiated when the

196 strain in the fibre direction reaches the longitudinal failure strain of the ply. Then, the stiffness of the  
197 volume element is gradually reduced until the critical fracture toughness has been dissipated, essentially  
198 following a linear softening law. Abaqus C3D8 elements were used (an eight node, 3D linear element with  
199 full integration), in order to have an accurate bending behaviour with only one element through the ply  
200 thickness. To ensure that the correct amount of energy is dissipated for each element, a communication  
201 law between the 8 integration points is used. Mesh independence is ensured by regularising the dissipated  
202 energy with respect to the characteristic element length, so that constant energy is released per unit area  
203 independently of the element length.

204 Matrix cracking is captured by means of the interface elements normal to the transversal direction (Fig.  
205 4). Hashin failure criterion [38] is evaluated in the neighbouring volume elements. If the Hashin matrix  
206 failure criterion is met in either of the neighbouring solid elements failure is assumed to occur. Then, a clas-  
207 sical linear cohesive law is used in order to degrade the penalty stiffness of the interface element according  
208 to the corresponding critical fracture toughness. Once all energy is dissipated, the penalty stiffness of the  
209 interface (initially  $10^6$  MPa/mm) is set equal to zero to simulate the generation of a transverse crack.

210 Similar to matrix cracking, delamination is modelled using the cohesive element interfaces between  
211 two consecutive plies of different orientation (Fig. 4). Damage of the delamination elements is driven  
212 by a classical linear cohesive law that depends on the mode I and mode II strengths as well as the frac-  
213 ture toughnesses. Linear softening is employed. The DPM is implemented by using a vumat subroutine  
214 in Abaqus/explicit. In total, the model only needs 13 material properties: 5 elastic constants, transverse  
215 and shear strengths, tensile and compressive longitudinal failure strains, the longitudinal fracture tough-  
216 ness in tension and compression, and the mode I and mode II fracture toughnesses. All properties were  
217 measured by following the appropriate test standards [39–44], except for the longitudinal tensile fracture  
218 toughness, which was adjusted numerically. The material properties values used cannot be revealed due to  
219 confidentiality. For further details of the DPM, the reader is referred to [12, 30, 37].

220 Fig. 5 presents a picture of the full FE model geometry including also the mesh. All the dimensions  
221 match the experimental ones. The stacking sequence cannot be revealed due to confidentiality. The spec-  
222 imens have a centre notch of 1 mm radius and 100 mm length, see Fig. 5. Modelling the entire specimen  
223 dimensions using the DPM approach would lead to millions of elements and a prohibitive computational  
224 time. Therefore, the specimen plate was split up into two regions. The first region, of dimensions  $200 \times 60$   
225  $\text{mm}^2$ , includes the notch and is modelled with the DPM (i.e., it contains 3D solid elements and interface  
226 elements). The in-plane mesh size used in this region is about twice the ply thickness for the volume and  
227 interface elements. This dimension is motivated by the fact that experimental observations show that, com-  
228 monly, two matrix cracks are separated by a distance ranging from 1.5 to 2 times the ply thickness [45].  
229 The validity of using this mesh size was also explored in Serra *et al.* [12]. In addition, all plies are modelled  
230 with one element per ply thickness, as it is commonly done in the literature. The use of fully integrated  
231 elements allows to capture well the stress through-the-thickness of the plies with a single element.

232 The remaining of the plate, corresponding to region 2, contains Abaqus continuum shell elements SC8R

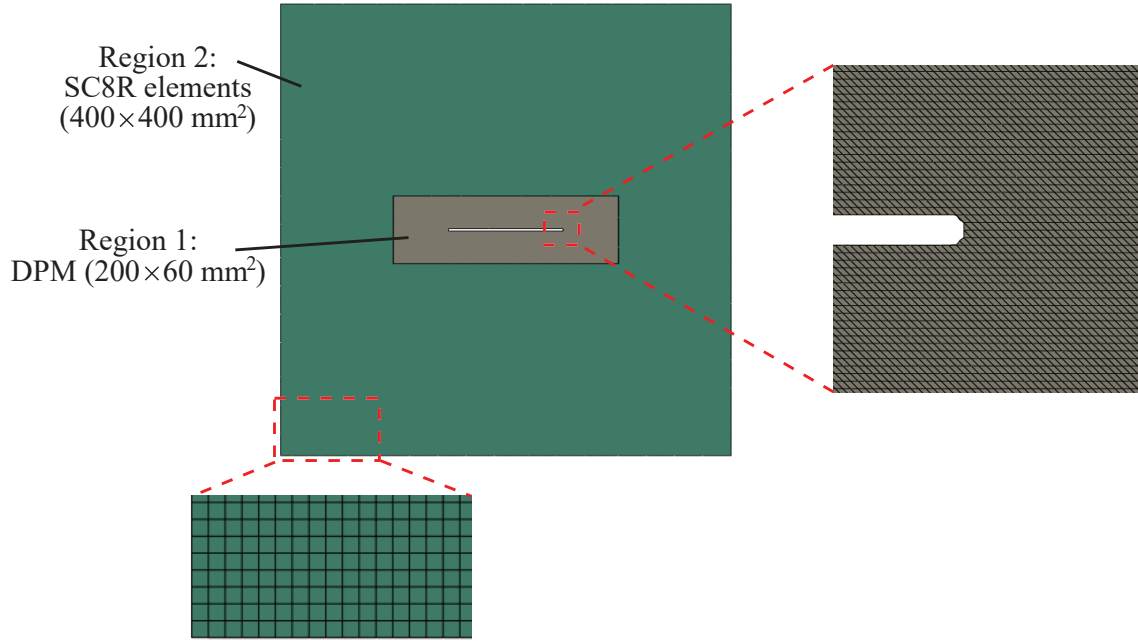


Figure 5: Full FE model of the tested specimens, with the two regions used for modelling and a zoomed view of the mesh in both regions.

233 (eight node continuum shell elements with reduced integration). These kind of elements have displacement  
 234 degrees of freedom like solid elements, but their kinematic formulation is similar to that of shell elements  
 235 [36]. In this region, a coarse mesh size of 5 mm is used, together with a single element through the entire  
 236 laminate thickness. The composite layup feature of Abaqus, which is based on classical laminate theory, is  
 237 used to account for the stacking sequence in this region. In this area no damage is modelled, being elastic  
 238 for the entire simulation. Thanks to this approach, we model damage where it is needed (close to the notch)  
 239 while far from it, the computational requirements are reduced by using the SC8R elements. Tie constraints  
 240 are employed to merge both regions. In total, the models have 1091064 elements and 1545480 nodes.

241 Due to the complex loading imposed by the VERTEX test rig, especially in the shear and in the com-  
 242 bined (tension plus shear) cases, boundary conditions well representative of the tests have to be imposed  
 243 in the FE model. To do so, DIC was used in the experimental campaign to obtain the displacement fields  
 244 during the tests (see Section 2.1 for all details). These fields are imposed in the model as displacement  
 245 boundary conditions, allowing to faithfully apply the same loading conditions as occurred in the real tests.  
 246 To properly do this, the same strategy used in previous work [3, 6] was employed. Four squares of nodes  
 247 are selected where the displacements are imposed, see Fig. 6. The three displacement components ( $x$ ,  $y$   
 248 and  $z$ ), obtained by DIC, are imposed on the outer nodes, forming a  $300 \times 300 \text{ mm}^2$  square, see Fig. 6.  
 249 Then, in order to be able to capture well the rotations, an out-of-plane displacement ( $U_z$ ) is imposed on the  
 250 remaining inner 3 rows of nodes (Fig. 6). The boundary conditions are imposed node by node, and degree  
 251 of freedom by degree of freedom. Notice that the only difference between the three models (tension, shear  
 252 and combined tension plus shear), is the displacement values applied in these nodes. It is worth mentioning

253 that before starting the test, some pretension is applied into the specimen due to the bolts that are used  
 254 to screw the specimen into the vertex test rig (Fig. 1). The effect of the pretension in the model is also  
 255 accounted for since the DIC displacements were started to be recorded before bolting the specimen.

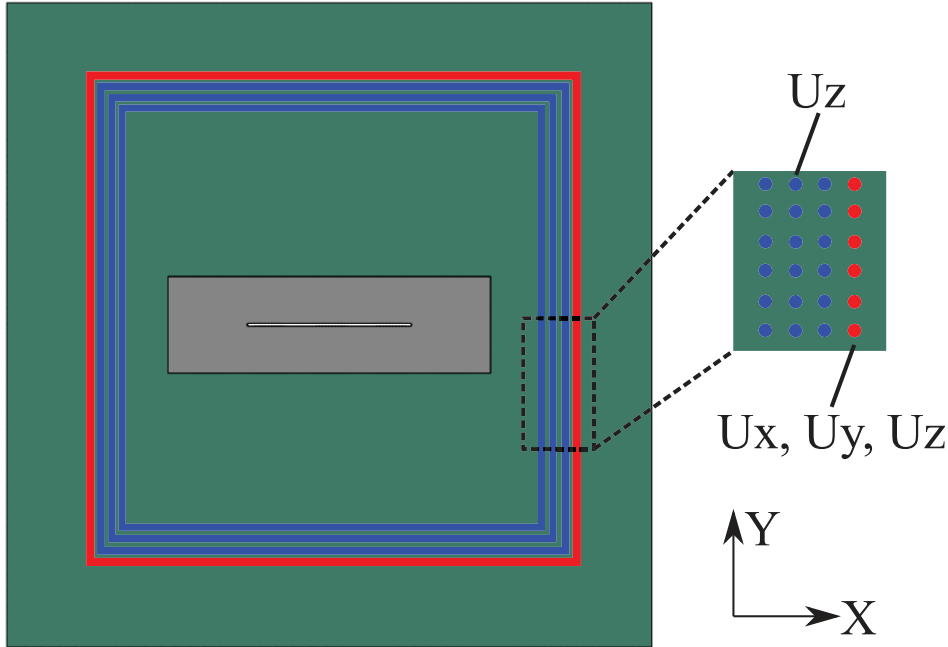


Figure 6: Boundary conditions applied into the FE model extracted from DIC. All displacements are imposed in the outer nodes (in red), and only the out-of-plane displacement to the inner nodes (coloured blue).

256 Explicit time integration was used to avoid convergence issues. The total loading time for each simulated  
 257 test was adjusted to be as short as possible, but still long enough to maintain the kinetic energy as low as  
 258 possible (at least equal or lower than 10% of the internal energy for most of the simulation) to ensure quasi-  
 259 static loading conditions. Similarly, mass scaling was used to have a reasonable stable time increment, but  
 260 without significantly affecting the kinetic energy. After several attempts, the mass was adjusted to have a  
 261 stable time increment of  $1 \cdot 10^{-8}$  s, while the total loading time was 0.075 s, 0.112 s, and 0.120 s for the  
 262 tension, shear and combined tests, respectively. This combination was found to be the most optimum one  
 263 for each particular test.

264 Since damage progression is quite significant before reaching final failure, element distortion becomes  
 265 a classical challenge to be managed. After several trial and error explorations, the following approach was  
 266 implemented. When the longitudinal damage of a volume element becomes equal to or higher than 0.999,  
 267 and this element has a strain component higher than 100%, it is removed from the model. This approach  
 268 guarantees that deletion is only performed when the element starts to be severely distorted, and only when  
 269 it sustains no significant stiffness. Cohesive elements were not removed regardless of their damage or  
 270 distortion since these were not found to lead to errors. Alternative approaches, such as using Abaqus built-  
 271 in distortion control were also explored but were less efficient. However, despite of this strategy and as  
 272 it will be commented later, it was impossible to simulate some of the tests entirely due to the (inevitable)  
 273 distortion issues.

274 Several data is extracted from the simulation and compared with the experimental tests in order to  
 275 validate the numerical model and demonstrate the model capabilities. The flux – strain curve is extracted  
 276 from the model and compared with the experimental one. To do so, the fluxes and global strains are  
 277 computed in the model in the same locations as in the experiments, following the same approach described  
 278 in Section 2.1. Besides this, the crack length along the simulation is extracted and compared with the  
 279 experiment. To do so, the crack length is computed simply by taking the maximum distance up to where  
 280 fibre damage is equal to or larger than 0.99, see Fig. 7. Finally, the displacement fields and the failure  
 281 pattern are also compared between the models and the experiments to corroborate that the displacements,  
 282 deformed shape and failure pattern predicted correlate well.

## Fibre damage

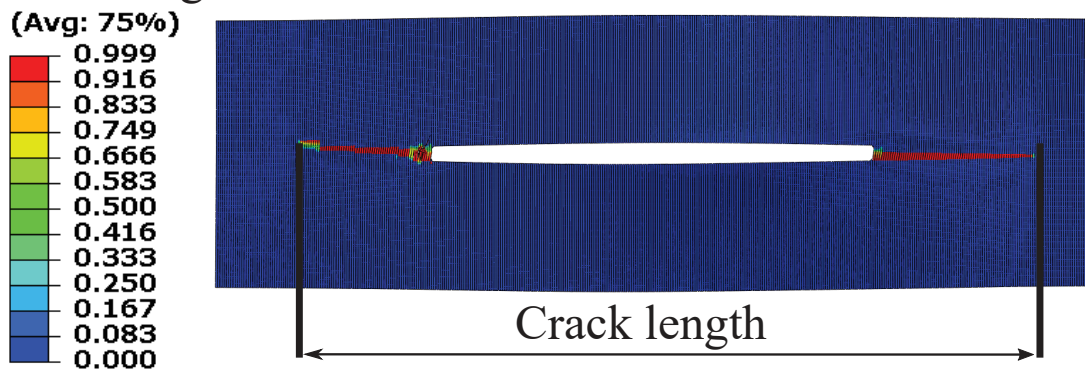


Figure 7: Methodology used to obtain the crack length in the simulations.

283 The models were run by using the high performance computing resources of CALMIP (Toulouse), using  
 284 72 CPUs, taking approximately 67 hours, 104 hours and 73 hours, for the tension, shear and combined cases,  
 285 respectively.

### 286 3. Results and discussion

287 This section presents all the results from this work. First, we show a comparison between the flux -  
 288 strain curve for each test. Secondly, we analyse the crack growth between the model and experiments as  
 289 well as the failure mechanisms. Finally, we compare the displacements and deformed shape. Please note  
 290 that some results are normalised due to confidentiality. Nonetheless, the same normalisation coefficient was  
 291 used in all cases so that all results can be directly comparable.

#### 292 3.1. Tension

293 Fig. 8 shows the longitudinal flux as a function of the longitudinal strain (plotted as continuous curves)  
 294 as well as the crack length as a function of the strains (dashed curves). Notice that two experimental curves  
 295 are shown to analyse the scatter.

296 The longitudinal flux curve of both experiment and numerical model shows a linear response until  
 297 approximately a strain of 0.5%, when a plateau appears until the end of the test. Overall, the stiffness in

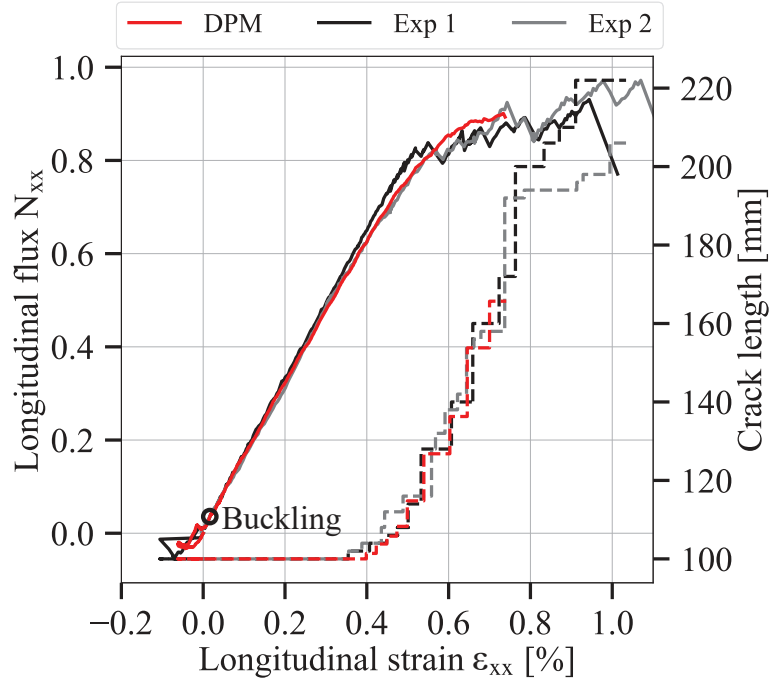


Figure 8: Tension specimen longitudinal flux – strain and crack length – strain predicted by the DPM and compared with the experimental measurements. The right Y axis indicates the crack length, while the left axis indicates the flux. Dashed curves correspond to the crack length, and continuous curves to the flux. The flux is normalised by the maximum experimental value of all tested specimens.

298 tension is well captured by the DPM compared with the experiments. However, the non-linear behaviour  
 299 starts slightly before in the DPM, although the difference is not significant. While the experimental curves  
 300 reach a strain of about 1% (when the tests were stopped), the numerical one only reaches a strain of about  
 301 0.7%. It is worth clarifying that final failure in the model does not occur at this point. Instead, the model  
 302 stopped due to excessive distortion, and consequently it was not possible to simulate further from that.  
 303 Modelling beyond this point is quite challenging, not only because of (inevitable) distortion issues, but also  
 304 because at that point the region with damage is very extent, as will be analysed later. To simulate farther  
 305 from this point, a bigger DPM region needs to be created, which would largely increase the computational  
 306 time. In any case, to that extent, the agreement between model and experiments is remarkable, with the  
 307 DPM capturing quite well the plateau and stiffness during the non-linear region. It should be noted that the  
 308 curves do not start at zero strain and flux, this is caused by the pretension of the specimen into the VERTEX  
 309 test rig. This pretension is also reasonably captured by the DPM. It is worth noting that the progressive  
 310 failure of the specimen is mainly related to the thermoplastic matrix employed. Similar tests carried out in  
 311 thermoset matrices presented more brittle failures [10]. In addition, buckling occurred very early in the test  
 312 (around 0.02% of applied strain, see black circle in Fig. 8), as will be further analysed later.

313 Regarding the crack length, the model is again in excellent agreement with the experiments. Crack  
 314 propagation starts at a strain of 0.4%. Soon after, when the crack length reaches a value of 110 mm (i.e.,  
 315 the crack has grown about 5 mm in each side), the presence of the crack starts to be noticeable in the  
 316 macroscopic response, and thus, the non-linear behaviour starts. While this comparison shows that the  
 317 crack growth is well captured, it gives no indication about the shape of the crack or the failure pattern, and

318 whether the DPM is capturing it or not. For this reason, Fig. 9 presents a comparison of the failure pattern  
 319 between the model and the specimen ‘exp 1’, highlighting also the crack shape, when the model stopped  
 320 (i.e., around a strain of 0.7%). To ease the validation and better show the failure pattern, in the model all  
 321 elements with damage equal to or larger than 0.99 are removed. Please notice that we included a picture  
 322 taken by the DIC cameras and a photo from the infrared one. Overall, the failure pattern from the model  
 323 resembles very well the experiments: the model captures the same 45° matrix cracks expanding from the  
 324 initial notch as in the experiments (Fig. 9a and b). Further to this, the model shows that fibre damage in the  
 325 central 0° ply expanded parallel to the initial notch, see Fig. 9c, which makes sense considering the tensile  
 326 loading conditions. Delamination between the 0°/90° interface follows a similar pattern (Fig. 9d). Notice  
 327 that notch propagation in the model is limited by the dimensions of the DPM (region 1 in Fig. 5).

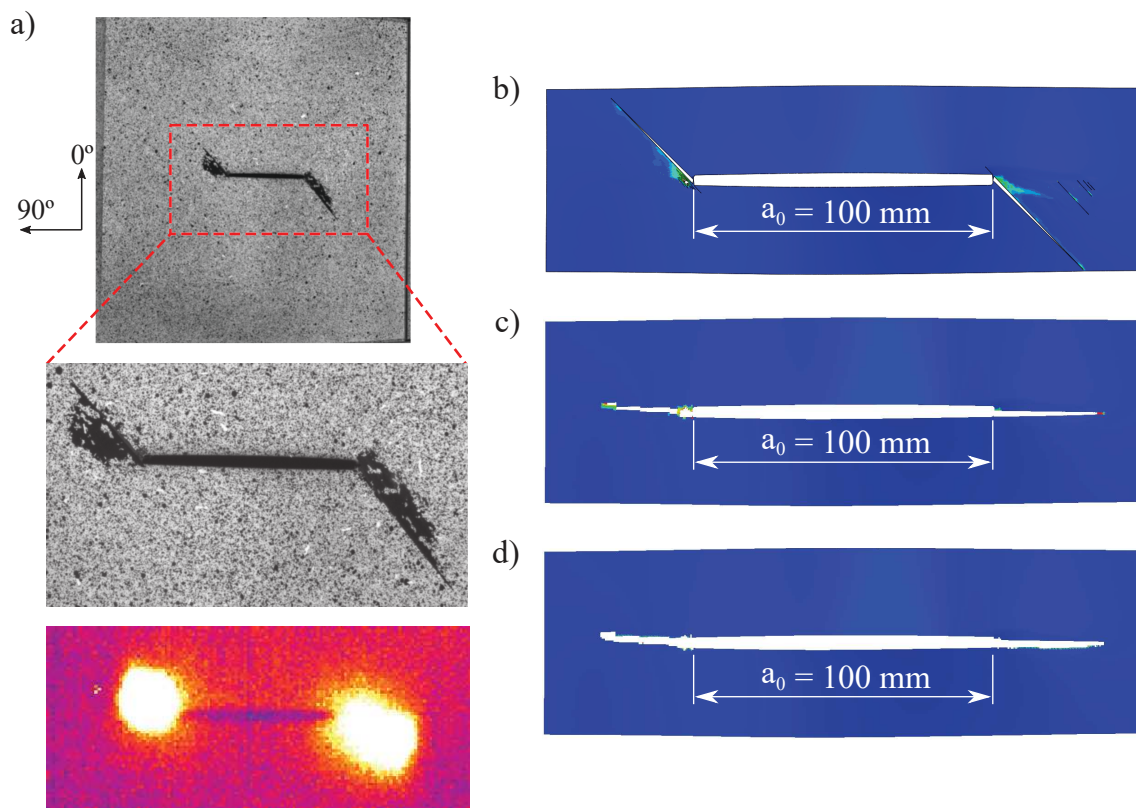


Figure 9: Tension specimen ‘exp 1’ failure pattern comparison with the DPM: a) experimental pictures, b) DPM 45° outside ply matrix cracking, c) DPM central 0° ply fibre breakage and d) DPM 0°/90° interface delamination.

328 The failure pattern along the simulation predicted by the numerical model is further illustrated in Fig.  
 329 10. Similarly to the observations in Serra *et al.* [33], the 0° fibre fracture and 0°/90° interface delamination  
 330 propagated parallel to the notch (perpendicular to the loading direction) and did so progressively. Matrix  
 331 cracking in the 90° ply also propagated continuously mainly parallel to the notch, although damage was less  
 332 straight, following a kind of ‘butterfly wings’ type evolution [33], thus, being quite different to the damage  
 333 seen in the outer 45° ply.

334 The out-of-plane displacement of the simulations was also compared with the DIC of specimen ‘exp

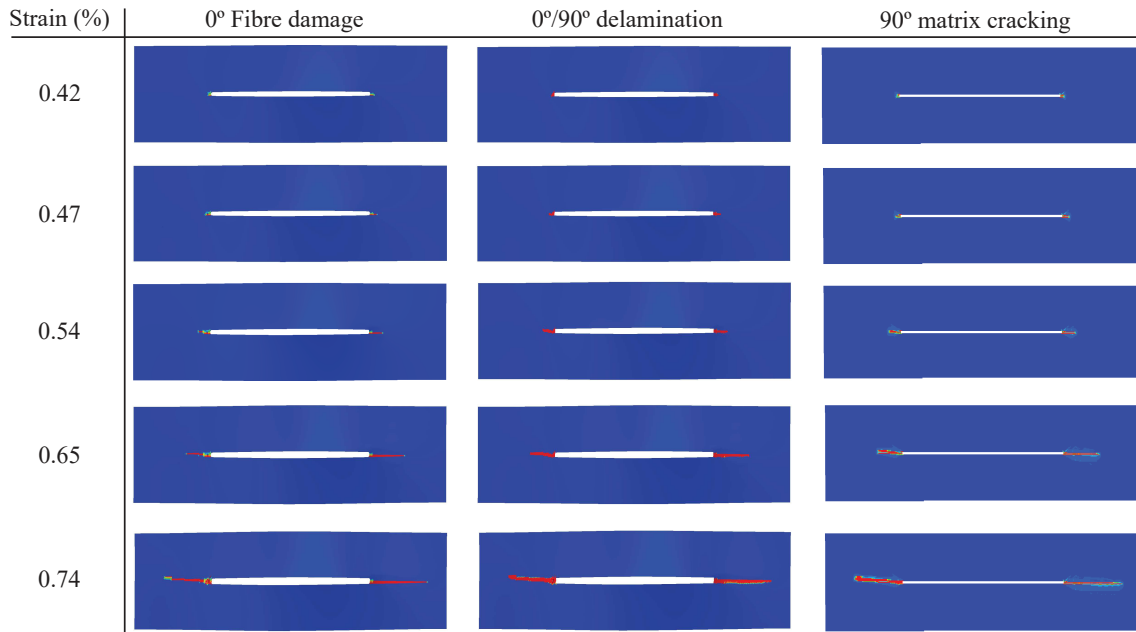


Figure 10: Numerical failure pattern predicted for the tensile specimen. Longitudinal damage is shown for the central 0° ply, delamination between the 0°/90° interface and matrix cracking for the 90° ply.

335 1', in order to validate the deformed shape and the application of the boundary conditions representing the  
336 VERTEX rig. Fig. 11 shows this comparison at the start of the test (preload), towards the middle (strain  
337 of 0.35%) and when the simulation was stopped (0.74% of strain). Results show the presence of buckling  
338 before starting the test, leading to a large displacement (about 7 mm) next to the notch. This is caused by  
339 the pretension of the specimen to the test rig, which constrains the specimen causing it to buckle before any  
340 jack related loading is applied [10]. Surprisingly, buckling occurred again very early after starting to load  
341 the specimen (around 0.02% of applied strain, see Fig. 8), as can be seen with the other two displacement  
342 plots at 0.35% and 0.74% of longitudinal strain (Fig. 11). This tension buckling occurs because the flanks of  
343 the central test rig box bend towards the centre, generating transverse compression, which leads to buckling  
344 of the specimen. Consequently, this tension test is in reality a biaxial longitudinal tension plus transverse  
345 compression test, although the longitudinal contribution is the main one [10].

346 The numerical model captures well the out-of-plane displacement (and thus the deformed shape), at the  
347 beginning and through the full test. There are small differences in the absolute values between both cases,  
348 but this mainly occurs in the edges, where the DIC fails to work correctly. As a consequence, the DPM  
349 captured well the physics of the full tension test, including the post-buckling behaviour.

### 350 3.2. Shear

351 Fig. 12 illustrates the shear flux as a function of the shear strain, the longitudinal flux as a function of  
352 the longitudinal strain (both plotted as continuous curves), and the crack length as a function of the shear  
353 strain (dashed curves). Although the test is meant to be pure shear, there is actually some tension loading  
354 during the test, which is the reason why the two curves are illustrated [3, 46]. This additional tension is

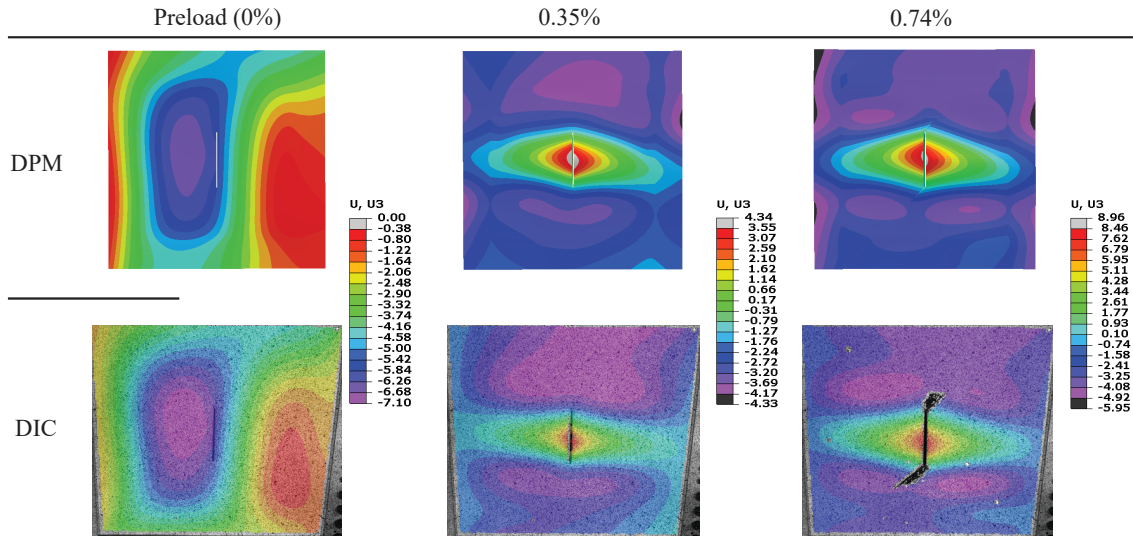


Figure 11: Comparison of the out-of-plane displacement (in mm) between the tensile specimen ‘exp 1’ and the numerical prediction at three different instants through the test (longitudinal strain indicated).

355 linked to the principle of post-buckling in shear. The saturation of compression stress due to shear creates  
 356 an induced tension stress, which is usually referred to as the ‘diagonal tension’ theory [47–50].

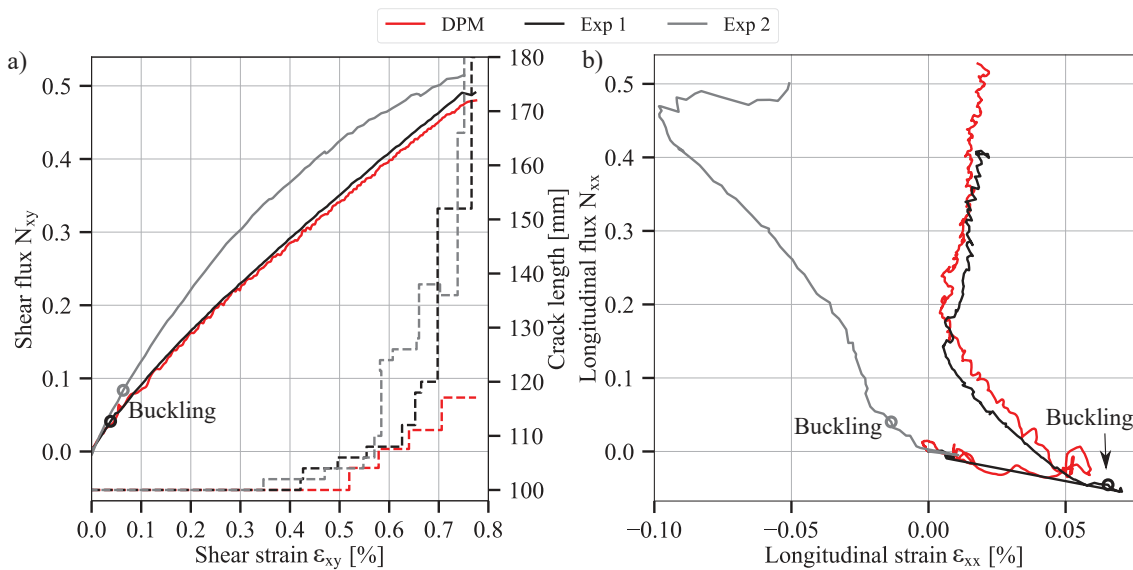


Figure 12: Shear specimen DPM predictions compared with the experimental data. a) shear flux and crack length as a function of the shear strain, and b) longitudinal flux – strain curve. The right Y axis indicates the crack length, while the left axis indicates the flux. Dashed curves correspond to the crack length, and continuous curves to the flux. The fluxes are normalised by the maximum experimental value of all tested specimens.

357 The DPM captures quite well both the shear flux and longitudinal flux curves (especially the shear one),  
 358 following the same stiffness and behaviour. There is better agreement with ‘exp 1’ than ‘exp 2’, which  
 359 can be attributed to the fact that the boundary conditions applied into the model to perform the simulation  
 360 were taken from this specimen. The shear response is very non-linear, especially for ‘exp 2’. Although

361 an initial stiffness can be identified, a non-linear response becomes clear very early in the test (around a  
362 0.05% of shear strain). This response is attributed to the apparition of buckling, as indicated by the grey  
363 and black circles. Essentially, buckling happened after the preload, before any jack related loading was  
364 applied, as it occurred with the tension specimens. However, another buckling mode was again triggered  
365 around 0.05% of shear strain, i.e., nearly at the beginning of the test, especially, specimen 'exp 1' buckled  
366 almost immediately after loading. This buckle can be more easily identified with the longitudinal flux -  
367 strain curve response. Initially, the longitudinal flux is negative and keeps increasing until a strain of 0.07%  
368 for 'exp 1' or a strain of 0.01% for 'exp 2'. After these points, a snap-through characteristic behaviour can  
369 be identified, attributed to buckling (particularly with 'exp 1'). The DPM captures very well the buckling  
370 point, especially compared with 'exp 1' and all the post-buckling behaviour.

371 The results of this paper, with the presence of early buckling and an important post-buckling are quite  
372 uncommon. As a difference from classical coupon or biaxial tests, the specimens tested here are more  
373 representative of the loadings of larger structures, such as a fuselage in service. Therefore, this is one of  
374 the main highlights of this study. Despite of the complexities involved, the model is again able to capture  
375 reasonably well the physics of the problem.

376 Crack propagation starts slightly later in the DPM (shear strain of 0.5%, compared with a shear strain of  
377 0.35 - 0.42% in the tests). However, the crack growth is in reasonable agreement with the two experimental  
378 measurements along the test, especially taking into account the inherent variability. The final value is,  
379 however, quite underestimated by the DPM when the test was stopped. Notice that when the crack starts  
380 to propagate no clear effect is observed on the stiffness of the specimen, contrary to what was seen under  
381 tension (see Section 3.1), without any plateau. The experimental test was stopped due to the fact that failure  
382 occurred at the corner of the specimen where it was clamped with the test bench, instead of failing at the  
383 notch. Although this crack developing at the corner did not merge with the central notch, it was decided to  
384 stop the test since this was not the desired failure mode. For this reason, no load drops are seen in the flux -  
385 strain curves. In this case, we note that we were able to model the full test.

386 As stated earlier, although the test is meant to be pure shear, there is actually some tension loading during  
387 the test. To better highlight this coupling, Fig. 13 presents the shear flux as a function of the longitudinal  
388 flux. Before buckling, the shear loading gives approximately pure shear (this is especially the case for 'exp  
389 2', and in the DPM that is a more ideal case). Nonetheless, after buckling, additional loading imposes about  
390 the same amount of both shear and tensile fluxes. Again, this is related to the 'diagonal tension' theory  
391 [47-50]. This coupling is also well captured by the model. More insight on this tension-shear coupling of  
392 the VERTEX test rig can be found in [46].

393 Fig. 14 shows the failure pattern at the end of the test predicted by the model and compared with the  
394 specimen 'exp 1'. Like in the tensile case, the failure pattern given by the model resembles reasonably well  
395 the experimental observations. In both cases, we can notice that the crack extended mostly in a diagonal  
396 way, with a slight angle, see Fig. 14a and b. The crack length is small, especially when compared with  
397 the one seen in tension. Fibre damage mainly appeared in the -45° plies (Fig. 14c), being nearly inexistent

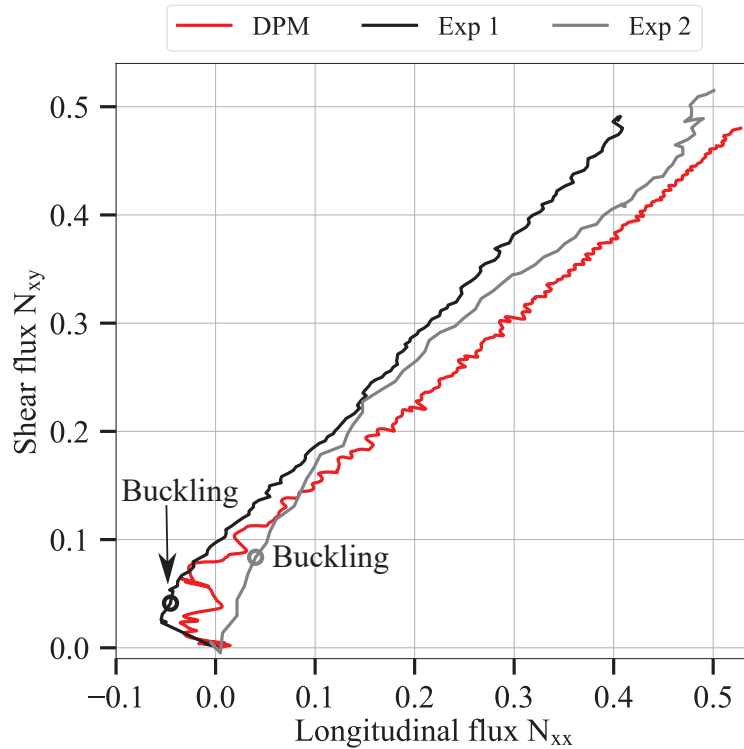


Figure 13: Shear flux as a function of the longitudinal flux for the shear test. The fluxes are normalised by the maximum experimental value of all tested specimens.

398 in the other plies when the simulation was stopped. Delamination between the  $0^\circ/90^\circ$  interface (Fig. 14d)  
 399 shows a different pattern compared to what was seen before in tension: damage extended both outwards  
 400 and inwards from the crack, clearly caused by the shear loading.

401 The failure pattern through the simulation is more extensively detailed in Fig. 15. Fibre damage and  
 402 matrix cracking are shown for the  $-45^\circ$  ply, since this was the ply that had larger longitudinal and transverse  
 403 damage though the simulation. In both cases, damage slowly grows from the notch with a  $45^\circ$  angle, quite  
 404 differently to what was observed with the tension case in Section 3.1. On the other hand, the  $0^\circ/90^\circ$  interface  
 405 delamination propagates inwards and outwards of the notch as indicated before, and this progression was  
 406 very continuous. Overall, the failure mechanisms and crack propagation are more complex than for the  
 407 tension case as expected.

408 Fig. 16 presents the out-of-plane displacement of the simulations compared with the DIC of specimen  
 409 ‘exp 1’ at three different instants through the tests (after preloading the specimen, towards the middle  
 410 and at the end). As commented with the tensile specimen in Section 3.1, results show buckling right  
 411 after performing the pretension [10]. In fact, after preloading, the deformed shape and the displacement  
 412 magnitudes are in-line to the ones seen with the tensile case, which shows good repeatability. As commented  
 413 before, just after starting the loading, the specimen buckled again, as shown for the other two test instants.  
 414 The DPM correlates well with the experiments through the entire test, although the maximum values are  
 415 slightly larger for the numerical model, just like it occurred for the tensile case. In any case, the field  
 416 distribution and deformed shape is in remarkable agreement again.

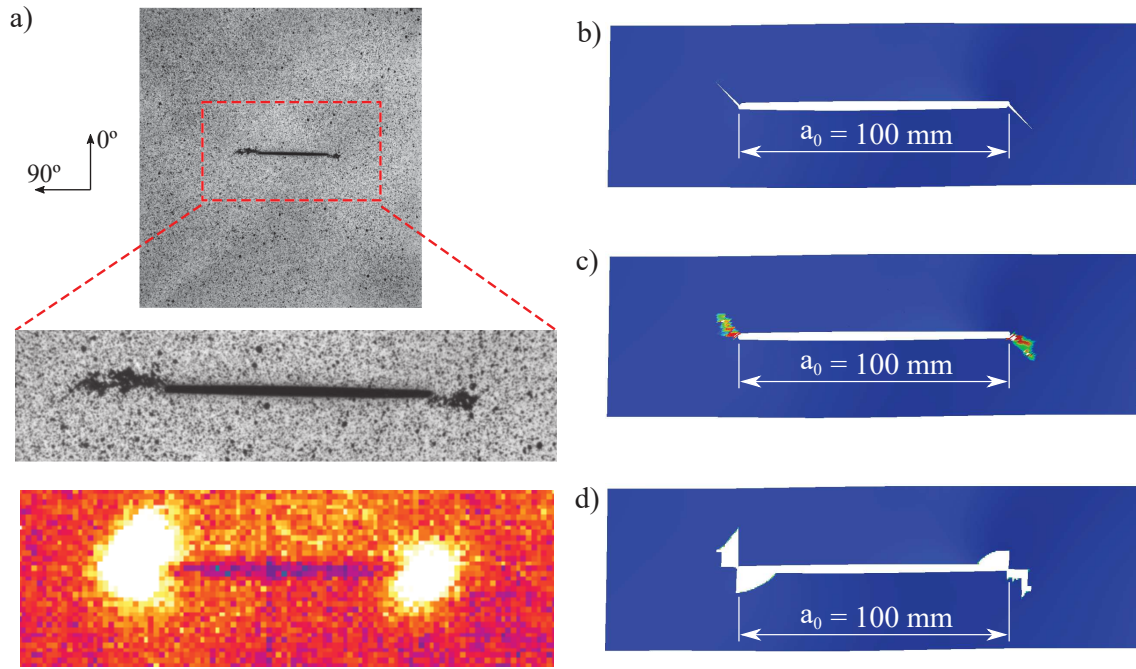


Figure 14: Shear specimen 'exp 1' failure pattern comparison with the DPM: a) experimental pictures, b) DPM 45° outside ply matrix cracking, c) DPM -45° ply fibre breakage and d) DPM 0°/90° interface delamination. In the model all elements with damage equal to or larger than 0.99 are removed.

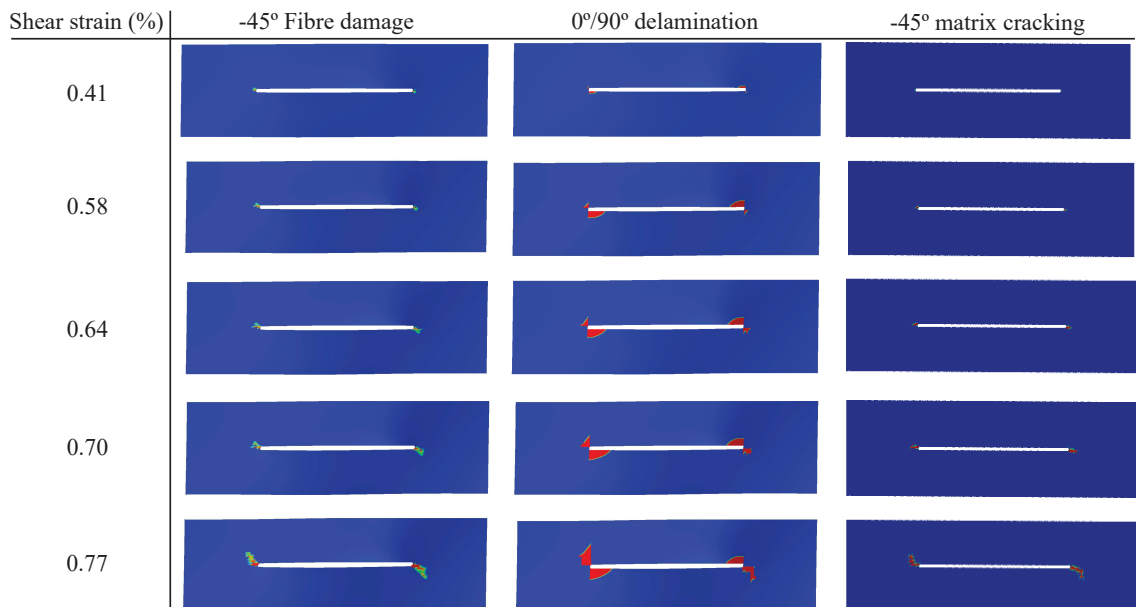


Figure 15: Numerical failure pattern predicted for the shear specimen. Longitudinal damage is shown for the -45 ply, delamination between the 0°/90° interface and matrix cracking for the -45 ply.

### 417 3.3. Combined tension and shear

418 Fig. 17 shows the longitudinal flux as a function of the longitudinal strain, the shear flux as a function of  
 419 the shear strain (both plotted as continuous curves), and the crack length as a function of the corresponding  
 420 strain (dashed curves). Notice that two experimental specimens are presented as in previous tests.

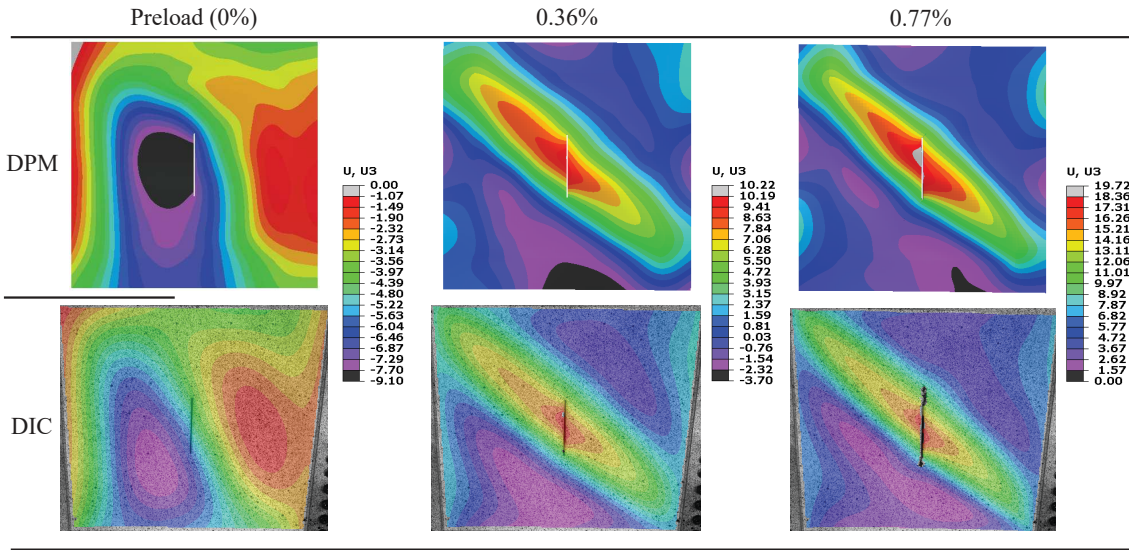


Figure 16: Comparison of the out-of-plane displacement (in mm) between the shear specimen 'exp 1' and the numerical prediction at three different instants through the test (shear strain indicated).

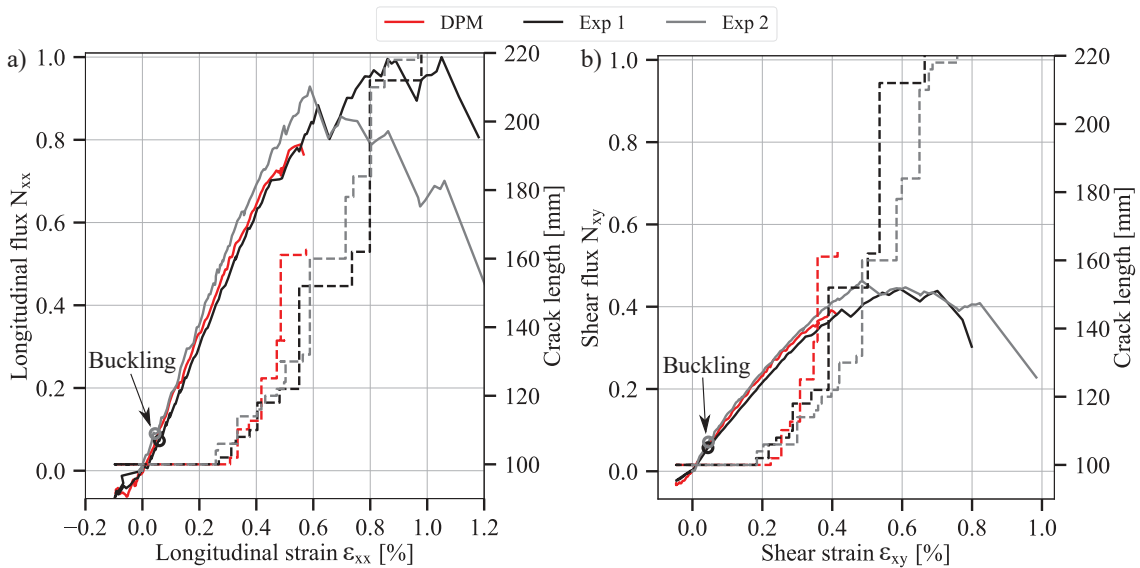


Figure 17: Combined shear and tension specimen DPM predictions compared with the experimental data. a) Longitudinal flux and crack length as a function of the longitudinal strain, and b) shear flux and crack length as a function of the shear strain. The right Y axis indicates the crack length, while the left axis indicates the flux. Dashed curves correspond to the crack length, and continuous curves to the flux. The fluxes are normalised by the maximum experimental value of all tested specimens.

421 Overall, the shear and longitudinal curves present a similar behaviour. Firstly, negative strains and fluxes  
 422 are obtained, which are caused by the preload. After that, the behaviour is mostly linear until significant  
 423 non-linearities become evident at about a longitudinal strain of 0.3% (or a shear strain of about 0.35%). For  
 424 larger strains a plateau follows up, with some load drops, very similar to the behaviour encountered with  
 425 the pure tensile specimen. Although it is hard to identify in the fluxes, buckling also occurred similarly to  
 426 the shear specimen. First, buckling happened again after preloading the sample. After, a second buckling  
 427 mode was again triggered early in the test, when the longitudinal strain was around 0.05% (or a shear strain

428 of about 0.04%), see the circular points in Fig. 17. The DPM captures reasonably well the experimental  
429 behaviour both in tension and shear. However, the numerical model stopped at a longitudinal strain of  
430 0.58% due to distortion issues, and it was impossible to model what happens afterwards. Hence, the authors  
431 were unable to simulate beyond that point and check whether the full experimental curve was reproducible.  
432 Nonetheless, the behaviour up to the simulated point is in reasonable agreement with the experiments.

433 Crack propagation starts at about the same strain for the numerical model and the two experimental  
434 coupons (0.3% and 0.2% for tensile and shear strain, respectively). The crack keeps growing linearly until  
435 a longitudinal strain of about 0.3% and a shear strain of 0.35% - 0.5%, when a large increase suddenly  
436 occurs. This response is very well predicted by the DPM. After this, the model stopped and we could not  
437 model any further. However, to this point the crack length is already 160 mm, which means that a large  
438 crack propagation has been simulated with accuracy, even the experimental magnitude is the same at this  
439 instant of the test. As explained in Section 3.1, modelling further from this point is very challenging since  
440 it requires detecting and removing distorted elements before they lead to instabilities and increasing even  
441 more the DPM size (region 1 in Fig. 5), which would lead to unfeasible computational times (the CPU  
442 time for this model was already 73 hours with 72 cpus). In line with the shear and tension specimens, when  
443 the crack starts propagating no substantial effect is seen in the flux curves. Load drops become clearly  
444 visible when the crack length is already about 130 mm, and no load drops occur until the crack is more than  
445 160 mm. Again, this is well captured by the DPM. This behaviour highlights well that this thermoplastic  
446 material is very damage tolerant, even under complex loading.

447 Overall, both the longitudinal and shear strains have similar magnitudes, which confirms that the test  
448 is a combination of both loading types as desired. To better observe this, Fig. 18 shows the shear flux  
449 as a function of the longitudinal flux, for the present combined case and also for the shear and tension  
450 specimens for direct comparison. As it can be seen, there is about twice longitudinal flux than shear flux  
451 in the combined case (Fig. 18c), which indicates that the VERTEX bench imposes more tension than  
452 shear loading. Comparing all cases, the shear test (Fig. 18b) is the one that shows more shear flux, which  
453 corresponds with the desired loading conditions. On the other hand, the tension test (Fig. 18a) shows nearly  
454 no shear flux compared with the other 2 cases, which again agrees well with the desired loading of that test.  
455 Next we analyse the failure pattern of the combined specimen.

456 Fig. 19 illustrates the failure pattern when the simulation was stopped (i.e. at a longitudinal strain of  
457 0.58%) compared with specimen 'exp 1'. In-line with the other tests, the failure pattern predicted correlates  
458 well with the experiments, and in general, it is quite similar to the one seen in the tension test (see Fig.  
459 9). The damage in the outer ply shows that the crack expanded following a 45° angle, see Fig. 19a and b.  
460 Again, at this analysed point, the crack length is quite large (160 mm), and thus, much larger than for the  
461 shear case, and more in-line with the crack length seen in the tensile case. In addition, fibre damage in the  
462 0° and -45° plies grew mostly parallel to the notch, but with a slight angle, thus, being a combination of  
463 the damage pattern seen for the 'pure' loading cases. Finally, the delamination in the 0°/90° interface (Fig.  
464 19e) shows a crack parallel from the notch with a slight angle, nearly identical to the tension case (and very

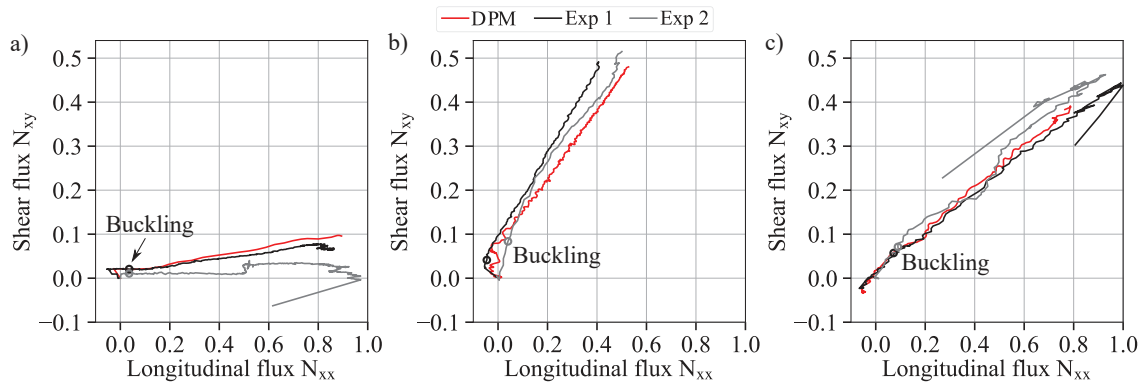


Figure 18: Shear flux as a function of the longitudinal flux. a) For the tension specimen, b) for the shear case and c) for the combined test. The fluxes are normalised by the maximum experimental value of all tested specimens.

465 different from the shear one). Taking into account that the failure pattern of this combined specimen seems  
 466 to be more similar to the tension than to the shear one, this is consistent with the fact that this specimen is  
 467 subjected to a larger amount of tensile strain than shear strain (Fig. 18).

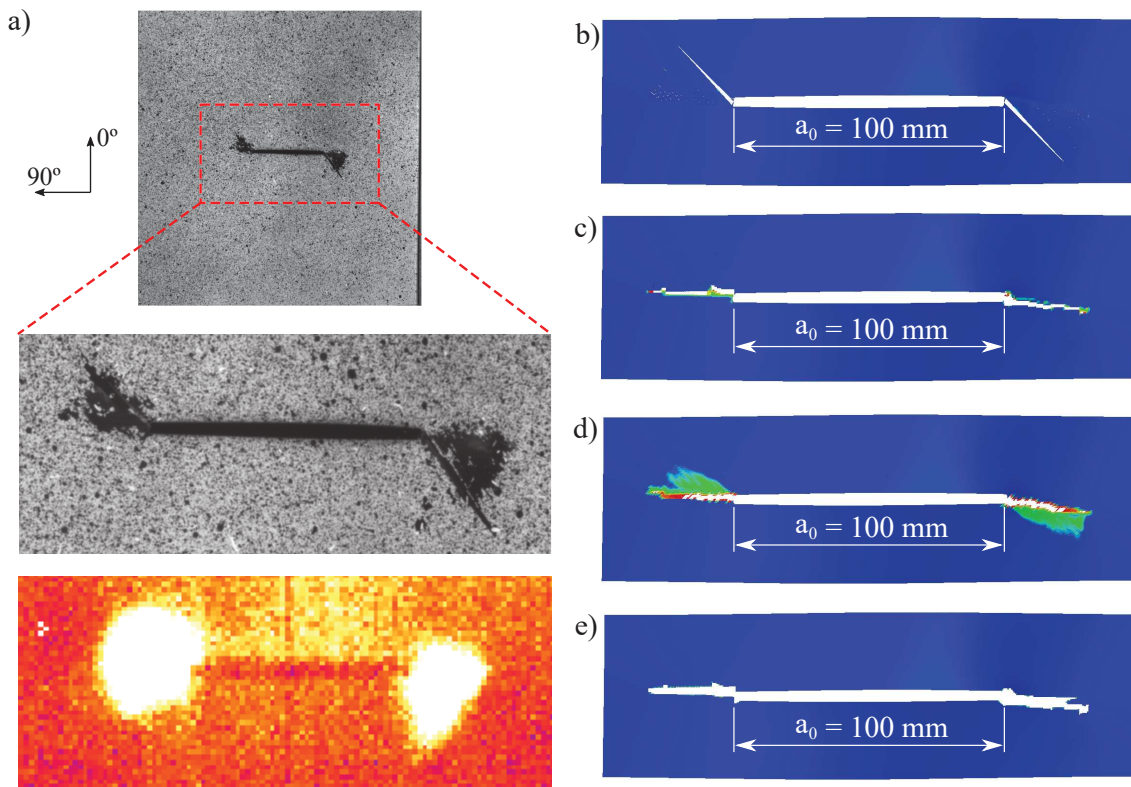


Figure 19: Combined shear and tension specimen 'exp 1' failure pattern comparison with DPM: a) experimental picture, b) DPM 45° outside ply matrix cracking, c) DPM 0° central ply fibre breakage, d) DPM -45° ply fibre breakage and e) DPM 0°/90° interface delamination. In the model all elements with damage equal to or larger than 0.99 are removed.

468 Next, we present the progression of the damage predicted by the model, in the same plies that were  
 469 analysed for the tension and shear specimens. Fig. 20 presents the fibre breakage failure progression in  
 470 the -45° and 0° plies as well as the 0°/90° interface delamination, whereas Fig. 21 shows the progression

471 of matrix cracking in the  $-45^\circ$  and  $90^\circ$  plies. The fibre damage in the  $-45^\circ$  and  $0^\circ$  plies is very similar,  
 472 growing slowly and smoothly from the notch with a slight angle. Both look reasonably similar to the shear  
 473 and tension specimens, highlighting well the combination of both loading conditions. Likewise, the  $0^\circ/90^\circ$   
 474 interface delamination grows progressively with a slight angle from the notch, as it occurred with the tension  
 475 specimen (Fig. 10), but differently to what was observed with the shear case (Fig. 15). In line with this,  
 476 matrix cracking in the  $-45^\circ$  and  $90^\circ$  plies looks very similar, growing progressively from the notch with a  
 477 slight angle, looking nearly identical to the observations from the tensile specimen (Fig. 10).

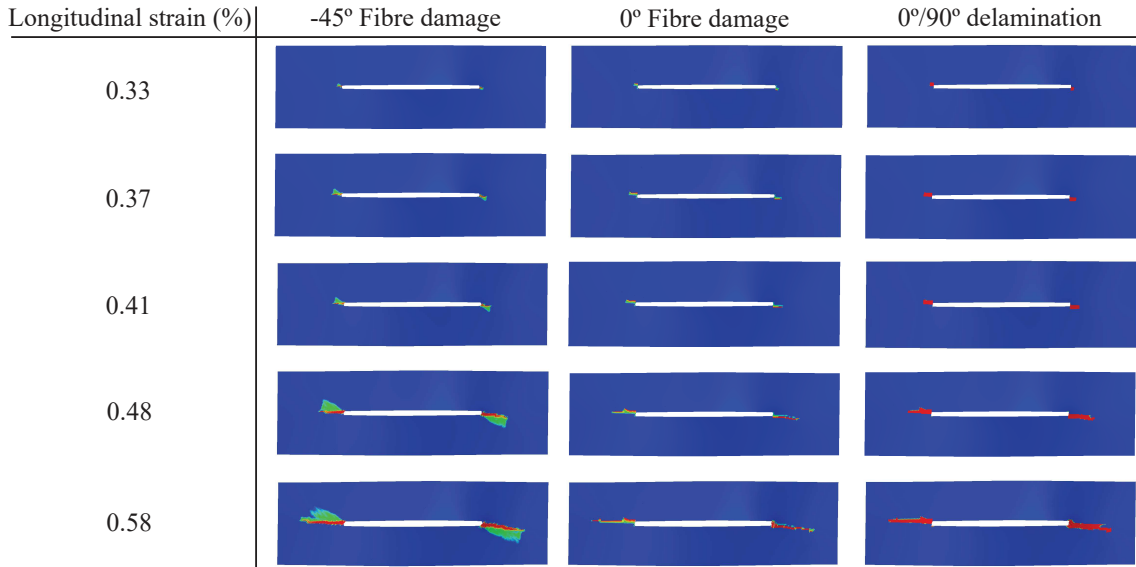


Figure 20: Fibre damage in the  $-45^\circ$  ply,  $0^\circ$  ply, and delamination between the  $0^\circ/90^\circ$  interface predicted for the combined loading specimen.

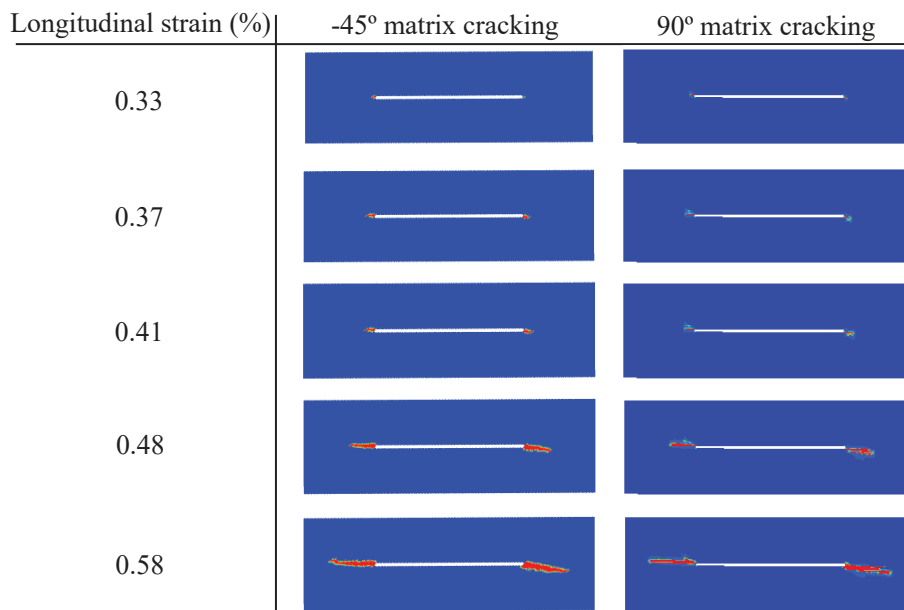


Figure 21: Matrix cracking in the  $-45^\circ$  and  $90^\circ$  plies predicted for the combined loading specimen.

478 Fig. 22 shows a comparison between the out-of-plane displacement predicted by the DPM compared  
 479 with the experimental DIC measurements of specimen ‘exp 1’ at three different instants through the tests  
 480 (after preloading the specimen, towards the middle and at the end). Like the previous tension and shear  
 481 specimens (Sections 3.1 and 3.2), buckling developed after preloading, which is again well captured by the  
 482 DPM. Early after the test starts and some loading is applied, a second buckling mode arises, leading with  
 483 the shape shown with a strain of 0.29% and 0.58%. The shape of the buckle is somewhere in-between the  
 484 one observed for the tension and shear specimens (see Figs. 11 and 16). The numerical results correlate  
 485 well with the experimental measurements, in terms of deformed shape and magnitude, capturing well the  
 486 early buckling and post-buckling behaviour. Again, we note that there are some differences in the maximum  
 487 values, but in general the agreement is remarkable.

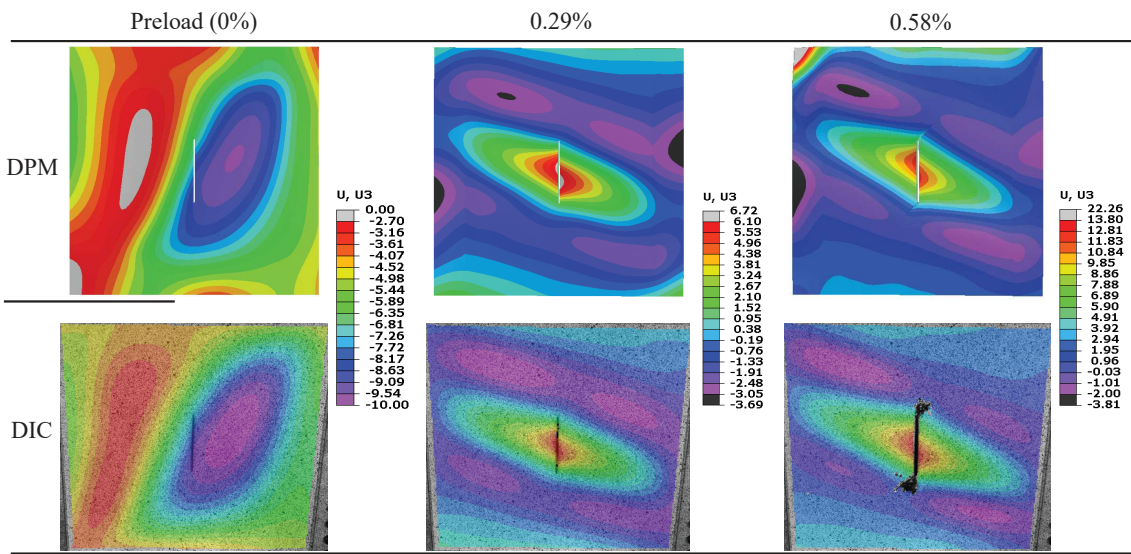


Figure 22: Comparison of the out-of-plane displacement (in mm) between the combined specimen ‘exp 1’ and the numerical prediction at three different instants through the test (longitudinal strain indicated).

488 To sum up the comparison between the numerical predictions of the three specimens compared with the  
 489 experiments, we highlight that the model is in good agreement with the experiments in many areas. Firstly,  
 490 the flux - strain response is very well captured, even the significant non-linearities and buckling found in the  
 491 tests are well predicted. Secondly, crack propagation prediction presents an excellent agreement between  
 492 the model and experiments, not only in magnitude, but also in terms of crack shape. Finally, the comparison  
 493 with DIC highlights two things. On the one hand, it validates the methodology used to extrapolate the  
 494 loading conditions from the VERTEX test rig to the model and, on the other hand, it also highlights the  
 495 capabilities of the DPM to capture correctly the deformed shape, despite of the complexities near the notch.

496 While numerical models reproducing experimental data with accuracy are very common, for instance  
 497 [8, 12, 19–21, 25], this paper goes one step beyond in the literature. Models are commonly validated and  
 498 proven against experiments performed in small specimens under uniaxial loading. Nonetheless, in this work  
 499 we modelled intermediate-scale specimens ( $400 \times 400 \text{ mm}^2$ ) with a 100 mm notch, which are uncommon  
 500 in the literature, since very few test rigs are capable of testing such specimens. In addition, we tested and

501 modelled specimens under different loading conditions: tension, shear and a combination of both. Again,  
502 while simulations on notched, open-hole or filled-hole specimens under uniaxial tension or compression are  
503 very common [7, 8, 33], to the authors' best knowledge, there is a lack of numerical validations performed  
504 on specimens under multiaxial loading as carried out in this paper. Moreover, the tests performed in this  
505 work presented the presence of early buckling (particularly for shear, and for combined tension plus shear  
506 loading) and the development of an important post-buckling behaviour for most of the test. Again, this is  
507 quite uncommon in the literature, and the numerical results presented were able to capture this buckling.  
508 Further to this, DIC and infrared measurements were employed to corroborate the predictions of the crack  
509 propagation and failure pattern. Results demonstrate that virtual testing can also be used accurately at higher  
510 levels of the pyramid under complex loading to decrease the amount of experimental tests needed to certify  
511 composite structures. The DPM has been proven to be a robust approach to predict failure of composites at  
512 the intermediate-scale and under complex loading.

#### 513 **4. Conclusions**

514 In this paper, a finite element model was developed to reproduce experimental tests on large notched  
515 carbon fibre reinforced thermoplastic laminates under tension, shear and combined loading. The numerical  
516 model makes use of the Discrete Ply Model (DPM) approach, which is able to capture fibre breakage, matrix  
517 cracking and delamination by means of combining 3D volume elements and cohesive interfaces. The fluxes  
518 as a function of the strain, the crack propagation, the failure pattern, and the predicted displacements and  
519 deformed shape were compared with the experimental data.

520 The results obtained show that the DPM is capable of predicting accurately the flux-strain curves of  
521 the tested notched panels for all loading conditions, even under multiaxial (tension plus shear) loading.  
522 Likewise, the crack length along the test predicted by the model correlated well against the experimental  
523 measurements obtained by infrared cameras. In addition, the crack shape and failure pattern was also  
524 reasonably captured by the model. The DPM was also able to predict accurately the displacements and  
525 deformed shape during the test, even near to the notch, as well as the buckling modes. Results from this  
526 work demonstrate the capabilities of advanced numerical models, such as the DPM, to predict accurately  
527 the response and failure of not only small coupons under uniaxial loading, but also intermediate-scale  
528 specimens (more representative of real aeronautical components) under multiaxial loading.

529 Future work will explore the development of more complex models including the VERTEX test rig in  
530 the model, which could allow to perform even more realistic simulations, and reduce the need to perform  
531 experimental tests. In addition, other multiaxial tests could be explored, for instance, including internal  
532 pressure and non-proportional loadings, since these may have an important effect on the buckling mode and  
533 on the crack propagation.

534 **CRedit authorship contribution statement**

535 **José M. Guerrero:** Conceptualization, Methodology, Validation, Formal analysis, Investigation, Writ-  
536 ing - original draft, Writing - review & editing. **Christophe Bouvet:** Conceptualization, Methodology,  
537 Validation, Formal analysis, Investigation, Writing - review & editing, Supervision. **John-Eric Dufour:**  
538 Conceptualization, Methodology, Validation, Formal analysis, Investigation, Writing - review & editing,  
539 Supervision. **Joël Serra:** Conceptualization, Methodology, Validation, Formal analysis, Investigation,  
540 Writing - review & editing, Supervision.

541 **Declaration of competing interest**

542 The authors declare that they have no known competing financial interests or personal relationships that  
543 could have appeared to influence the work reported in this paper.

544 **Data availability**

545 The raw/processed data required to reproduce these findings cannot be shared at this time due to legal  
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