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Point-wise evaluation of the growth driving direction for arbitrarily shaped delamination fronts using cohesive elements

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Abstract

The identification of the delamination propagation direction in three-dimensional structures with arbitrarily shaped fronts is needed in many applications. In the cohesive element framework, the propagation direction may be computed as the normal direction to a numerical damage isoline. The damage isoline tracking requires to exchange information between neighboring elements, thus post-processing global data, which is computationally expensive. This work presents a novel approach for the evaluation of the growth driving direction, only using local element information. The method can be directly implemented in a user-defined element subroutine and be evaluated at the execution time of the analysis. The presented formulation and its implementation in the commercial Finite Element code Abaqus is validated by comparison to the damage isoline shape rendering using global information.

Keywords:

Delamination growth, Cohesive zone model, Finite element analysis

1. Introduction

Long fiber-reinforced polymers are layered materials produced by stacking plies which contain continuous fibers in different orientations. Fibers supply stiffness and strength to the material in the laminate plane. Although laminated composite structures are designed so that the highest stresses are in the fiber directions, out-of-plane stresses may also occur at many types of geometric discontinuities

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6 such as ply drops, skin-stiffener terminations, intersections, sandwich panels, free edges, holes, cut-
7 outs, flanges, bonded and bolted joints or impacted zones. These load cases may damage the interface
8 between plies, causing the failure mechanism called delamination. Delamination is considered the most
9 detrimental failure mechanism in laminated composite structures because it occurs at relatively low
10 load levels but still entails significant reduction of the structure's load carrying capacity. To address
11 this problem without recouring to impractical safe-life designs, damage-tolerant approaches are used.
12 In that event, Finite Element (FE) analysis is an indispensable tool to predict delamination growth in
13 complex laminated structures subjected to both static and fatigue loading.

14 The virtual crack closure technique (VCCT) is one of the most widely used FE techniques [1].
15 However, its application to realistic three-dimensional geometries with arbitrarily shaped crack front
16 requires a continuous adaptive meshing technique in order to get a smooth front that fits with the
17 instantaneous crack front curvature [2–4]. Alternative methods, that allow the use of stationary meshes,
18 consist of tracing a smooth virtual front around the stepped front [5–7]. These techniques require the
19 use of algorithms to determine the normal direction to the virtual delamination front using global
20 information (or 18-noded elements as in [5]). This direction is used to compute the virtually closed
21 area and to define a local coordinate system that enables to calculate the energy release rate components
22 according to it.

23 An alternative to VCCT, is the cohesive zone model (CZM), firstly developed by Dugdale [8] and
24 Barrenblatt [9]. In contrast with the VCCT approach, the application of the CZM is not limited to
25 Linear Elastic Fracture Mechanics (LEFM). Indeed, it accounts for a large fracture process zone ahead
26 of the crack tip where the material undergoes stiffness degradation until complete decohesion. This
27 nonlinear material behavior is lumped into a surface, the cohesive zone, modeled by cohesive elements.
28 Under static loading conditions, no crack tip tracking algorithm is required as long as the assumptions
29 of identical fracture toughnesses for shear mode openings and independence of fracture toughness
30 with propagation direction with respect to fiber orientation are made [10–17]. However, some of the
31 existing methods for the simulation of fatigue-driven delamination using the CZM approach do require

32 the identification of the propagation direction for its three-dimensional implementation [18–22], even
33 making the same assumptions as in the static formulation. To the authors knowledge, the existing
34 formulations to estimate the direction of crack propagation using CZM are nonlocal and, thus, require
35 additional post-processing. In practice, these algorithms are computationally inefficient for the analysis
36 of large structures.

37 Another and more recent approach presented by Van der Meer et al. [23] uses the level set method
38 to describe the crack front location. Like the VCCT, it is a fracture mechanics approach. Furthermore,
39 its variant for large process zone simulation [24] makes use of a stiffness degrading damage variable
40 that allows a band of damaged material with predefined width. Conversely to most of the existing
41 CZM formulations, the damage variable is not a function of the local properties but it is defined by
42 the distance to the crack front, where the crack front is defined as the line that separates the damage
43 process zone and the completely damaged interface.

44 In this work, a local algorithm to determine the growth driving direction in CZM is presented. It
45 can be evaluated at any point within the cohesive zone at the same time the damage state is being
46 computed. Therefore, it can be used to enhance the cohesive element formulation under static loading,
47 preserving the local nature of the formulation. Moreover, it is an efficient alternative to the existing
48 nonlocal propagation direction algorithms used in the methods for fatigue simulation.

49 The concept of growth driving direction applied to cohesive elements is presented in 2.1. Three
50 different criteria for the growth driving direction identification are defined in Section 2.2. The formu-
51 lation according to the first criterion is developed in Section 2.3. The formulation for the other two
52 criteria is given in Appendix B. The three growth driving direction criteria are implemented for the
53 particular case of the CZM presented in [15, 17], which is summarized in Appendix A. However, it
54 is worth to mention that the same criteria could be applied to any other CZM formulation. Sections
55 3 and 4 present the results from the application of the formulation to three one-element case studies
56 under different loading conditions and a real three-dimensional composite structure, respectively. The
57 work closes by discussing the obtained results and with the conclusions.

58 2. Determination of the growth driving direction

59 In the framework of LEFM, the propagation direction is assumed to be the normal direction to
60 the crack front, where the crack front is the line separating the uncracked and cracked parts (see
61 Figure 1.a). In contrast to LEFM, the CZM technique accounts for a band of damaged interface of
62 variable length, called the fracture process zone, FPZ (light grey band in Figure 1.b). Therefore, the
63 propagation direction, understood as the normal to the crack front line, can not be defined in the
64 CZM framework. In this work, the concept of “growth driving direction” is introduced for CZM as the
65 analogous to the propagation direction. It is assumed to be normal to a given damage isoline and can
66 be calculated at any point within the FPZ. This definition follows naturally from the LEFM definition
67 and provides the exact same result in the limiting case where the length of the fracture process zone
68 goes to zero.

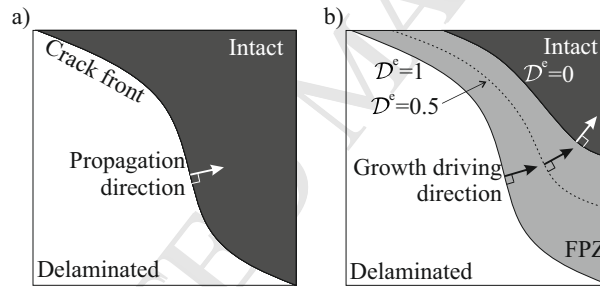


Figure 1: a) The propagation direction is assumed to be the normal direction to the crack front in the LEFM framework. b) The growth driving direction is assumed to be the normal direction to a damage isoline in the CZM framework. The energy-based damage variable, \mathcal{D}^e , is defined in Appendix A.

69 2.1. Growth driving direction using cohesive elements

70 Consider a laminated structure undergoing a delamination crack restricted to propagate in the
71 interface between two adjacent plies. The degradation process of the material ahead of the crack tip
72 is modeled in this work using the bilinear CZM formulation developed by Turon et al. in [15, 17].
73 As detailed in Appendix A, the process of the degradation of the interface properties is governed by
74 an energy-based damage variable, \mathcal{D}^e , defined in Equation (A.16) as the ratio between the specific
75 dissipated energy, ω_d , and the fracture toughness, \mathcal{G}_c . Thus, \mathcal{D}^e is a scalar quantity that measures the

76 degree of crack development: when \mathcal{D}^e equals 0, the degradation process is yet to start, while, when
 77 \mathcal{D}^e equals 1, the crack is completely developed. The total specific work, ω_{tot} , corresponding to a given
 78 state of damage is the sum of the specific dissipated energy, ω_d , and the specific elastic energy, ω_e .

79 To ensure the proper energy dissipation under mixed-mode conditions, a one-dimensional cohesive
 80 law relates the equivalent mixed-mode traction, μ , to the equivalent mixed-mode displacement jump,
 81 λ . Such constitutive law is formed by an initial elastic region, before damage initiation, and a softening
 82 region. When the area under the one-dimensional traction-displacement jump curve is equal to the
 83 fracture toughness, \mathcal{G}_c , a new crack surface is formed. The Benzeggagh-Kenane criterion [25] is used
 84 to define the mixed-mode displacement jumps at which the onset of damage, λ_o , and propagation, λ_c ,
 85 occur. A sketch of the equivalent one dimensional bilinear law is represented in Figure 2 for a given
 86 mode-mixity, B .

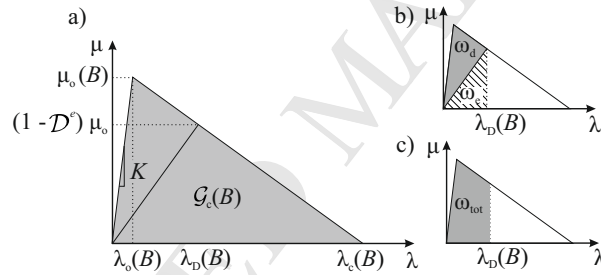


Figure 2: Equivalent one-dimensional cohesive law for a given mode-mixity, B . The shadowed area in a) represents the fracture toughness, \mathcal{G}_c , in b), the specific dissipated energy, ω_d , and the specific elastic energy, ω_e , and in c), the total specific work, ω_{tot} , for a given state of damage.

87 Complying with the cohesive element definition, the interfacial tractions and displacement jumps
 88 are evaluated at the interfacial deformed midsurface, \bar{S} , and determined by its local orientation. Thus,
 89 the normal and tangential traction components, acting on a unit deformed interfacial midsurface area,
 90 are conjugated to the normal and tangential displacement jumps across the material discontinuity. For
 91 the analysis of delamination propagation in three-dimensional structures, the interfacial midsurface
 92 is defined by the Cartesian coordinates \bar{x}_i , with $i = 1, 2, 3$. The local Cartesian coordinate system
 93 located on the deformed midsurface is defined by two tangential unit vectors, \hat{e}_1 and \hat{e}_2 , and a normal
 94 unit vector, \hat{e}_3 . Assuming that the crack propagation is confined to the interface, the vector defining

95 the growth driving direction must belong to the plane spanned by the tangential vectors \hat{e}_1 and \hat{e}_2 at
 96 the point \bar{p}_i where the direction is evaluated. Thus, the three-dimensional problem, can be solved in a
 97 two-dimensional space defined by the local Cartesian coordinates (e_1, e_2) , where e_l , with $l = 1, 2$, are
 98 the coordinates spanned by the unit vectors \hat{e}_l .

99 Then, for any given distribution of $\mathcal{D}^e(e_1, e_2)$, the growth driving direction at any point on the
 100 midsurface is assumed normal to the damage isolines, following the discussion related to Figure 1, i.e.
 101 is given by the negative of the gradient vector:

$$-\nabla \mathcal{D}^e(e_1, e_2) \quad (1)$$

102 2.2. Growth driving direction criteria

103 The growth driving direction at any point \bar{p}_i , contained in \bar{S} , is defined in this work as the one that
 104 provides the largest rate of decrease of \mathcal{D}^e . This is the direction of the negative gradient of \mathcal{D}^e , defined
 105 in the local Cartesian coordinate system (e_1, e_2) with origin at \bar{p}_i (see Equation (1)). However, polar
 106 coordinates are most appropriate when looking for a direction from a pole (See Figure 3). Thus, the
 107 growth driving direction can be found by identifying the angle φ that minimizes the slope of \mathcal{D}^e with
 108 respect to the radial coordinate, ρ :

$$\min_{\varphi} \frac{\partial \mathcal{D}^e}{\partial \rho} \quad (2)$$

109 Considering the energy-based damage, \mathcal{D}^e , dependent on both the mode mixity, B , and the mixed-
 110 mode displacement jump, λ , and by application of the chain rule, the angle φ that minimizes Equation
 111 (2) can be found by solving:

$$\frac{\partial}{\partial \varphi} \frac{\partial \mathcal{D}^e(B, \lambda)}{\partial \rho} = \frac{\partial}{\partial \varphi} \left(\frac{\partial \mathcal{D}^e}{\partial B} \frac{\partial B}{\partial \rho} + \frac{\partial \mathcal{D}^e}{\partial \lambda} \frac{\partial \lambda}{\partial \rho} \right) = 0 \quad (3)$$

112 and by checking its convexity:

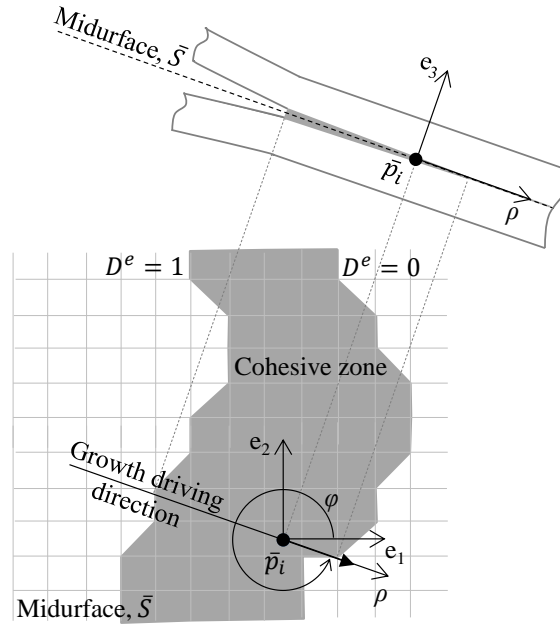


Figure 3: The growth driving direction evaluated at point \bar{p}_i is embedded in the tangential plane spanned by the local Cartesian coordinates e_1 and e_2 .

$$\frac{\partial^2}{\partial \varphi^2} \frac{\partial \mathcal{D}^e(B, \lambda)}{\partial \rho} = \frac{\partial^2}{\partial \varphi^2} \left(\frac{\partial \mathcal{D}^e}{\partial B} \frac{\partial B}{\partial \rho} + \frac{\partial \mathcal{D}^e}{\partial \lambda} \frac{\partial \lambda}{\partial \rho} \right) > 0 \quad (4)$$

113 However, equations (3) and (4) are equal to zero in the elastic regime ($\lambda \in [0, \lambda_o]$), since the energy
 114 based damage variable, \mathcal{D}^e , is also equal to zero (see Equation (A.16)). In order to compute the growth
 115 driving direction before the initiation of the degradation process, another criterion, based on the ratio
 116 between the total specific work, ω_{tot} and the fracture toughness, \mathcal{G}_c , can be formulated such that the
 117 growth driving direction can be found by solving:

$$\min_{\varphi} \frac{\partial \left(\frac{\omega_{tot}}{\mathcal{G}_c}(B, \lambda) \right)}{\partial \rho} \quad (5)$$

118 Note that, similarly to the energy-based damage, \mathcal{D}^e , the ratio between the total specific work
 119 and the fracture toughness, $\frac{\omega_{tot}}{\mathcal{G}_c}$, is dependent on both the mode mixity, B , and the mixed-mode
 120 displacement jump, λ .

121 Finally, for the sake of simplicity, a third criterion, which is also active before damage initiation,

122 can be formulated only taking into account the mixed-mode displacement jump field, λ :

$$\min_{\varphi} \frac{\partial \lambda}{\partial \rho} \quad (6)$$

123 The general expressions to solve for each of the criteria are listed in Table B.5.

124 In summary, three different criteria are presented depending on the quantity being analyzed: the
 125 energy-based damage, \mathcal{D}^e , (Criterion 1), the total specific work over the fracture toughness, $\frac{\omega_{tot}}{\mathcal{G}_c}$ (Cri-
 126 terion 2), and the mixed-mode displacement jump, λ , (Criterion 3). The evolution of these quantities
 127 along the growth driving direction are sketched in Figure 4 for an interface opened under pure mode
 128 I conditions. The three criteria are listed in Table 1 and presented in the following.

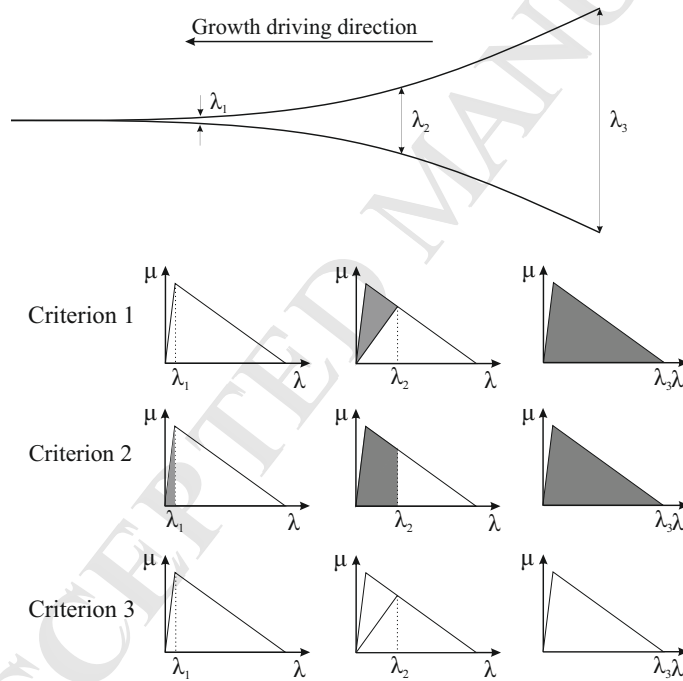


Figure 4: Quantities being minimized in each criterion for a pure mode I opened interface.

129 Criterion 1. The growth driving direction is defined by the negative gradient of the energy-based
 130 damage variable, \mathcal{D}^e . This is equivalent to computing the negative gradient of the ratio between the
 131 specific dissipated energy, ω_d (see Figure 2.b), and the fracture toughness, \mathcal{G}_c . Since Criterion 1 is
 132 based on the energy-based damage distribution, \mathcal{D}^e , it is only active once the degradation process is

| Criterion ID | Function to solve | Nomenclature | Approach | Limitations |
|--------------|--|--|--------------|--|
| 1 | $-\nabla \mathcal{D}^e$ | \mathcal{D}^e : Energy-based damage | Energy-based | Not active in elastic regime |
| 2 | $-\nabla \frac{\omega_{tot}}{\mathcal{G}_c}$ | ω_{tot} : total specific work \mathcal{G}_c : fracture toughness | Energy-based | May depend on the specific elastic energy in CZM |
| 3 | $-\nabla \lambda$ | λ : mixed-mode opening displacement | Geometrical | Independent of interface properties |

Table 1: Summary of the criteria to determine the growth driving direction.

133 already initiated. Moreover, Criterion 1 is an energy-based approach that depends on the kinematics
 134 and the constitutive law of the cohesive element. Since the cohesive law is usually mode-dependent,
 135 an uneven distribution of mode-mixity, B , can affect the gradient vector.

136 Criterion 2. The growth driving direction is defined by the negative gradient of the ratio between
 137 the total specific work, ω_{tot} (see Figure 2.c), and the fracture toughness, \mathcal{G}_c . Thus, both the specific
 138 dissipated energy, ω_d and the specific elastic energy, ω_e , are included in the computation of Criterion 2.
 139 Since, as soon as two initially coinciding points separate from each other some elastic energy is stored,
 140 Criterion 2 is active before any energy dissipation due to fracture takes place. Moreover, this approach
 141 depends on both the kinematics and the constitutive law of the cohesive element and, therefore, can
 142 be affected by the variation in mode-mixity, B , with the direction.

143 It is worth to mention that, with the constitutive model used in this work, presented in Appendix
 144 A.2, criteria 1 and 2 lead to the same growth driving direction results. However, since both the
 145 conservative and non-conservative work are computed in Criterion 2, in contrast to Criterion 1, in
 146 which only the non-conservative work is quantified, both criteria might provide different results when
 147 using other CZ formulations that allow the definition of mode-dependent penalty stiffness, K [26].

148 Criterion 3. The growth driving direction is defined by the negative gradient of the mixed-mode
 149 displacement jump, λ . This is a pure geometrical approach, since the only governing parameter is the
 150 mixed-mode displacement jump. Thus, the solution only depends on the kinematics of the cohesive
 151 element. Indeed, changes in the cohesive law due to variation in mode-mixity, B , with direction are

152 not affecting Criterion 3.

153 *2.3. Formulation of Criterion 1 for the identification of the growth driving direction*

154 A complete description of the derivation of Criterion 1 is presented in this section. Moreover,
155 the formulation for the evaluation of the growth driving direction using criteria 2 and 3 is given in
156 Appendix B.

157 It can be seen, from equations (3) and (4), that, in order to find the growth driving direction using
158 Criterion 1, the radial slope of the energy-based damage, $\frac{\partial \mathcal{D}^e}{\partial \rho}$, must be minimized as a function of the
159 angle φ . Each of the terms in equations (3) and (4) are derived in the following.

160 The derivative of the energy-based damage with respect to the mode mixity, $\frac{\partial \mathcal{D}^e}{\partial B}$, and the derivative
161 of the energy-based damage with respect to the mixed-mode displacement jump, $\frac{\partial \mathcal{D}^e}{\partial \lambda}$, are scalar factors
162 that depend on the parameters defining the CZM. The expression for $\frac{\partial \mathcal{D}^e}{\partial B}$ obtained after the particular
163 application to the CZM from [15, 17] is:

$$\frac{\partial \mathcal{D}^e}{\partial B} = \frac{\eta (\mathcal{G}_{IIc} - \mathcal{G}_{Ic}) B^{(\eta-1)} \lambda}{K \lambda_c \lambda_o (\lambda_o - \lambda_c)} = F_B \quad (7)$$

164 and the expression for $\frac{\partial \mathcal{D}^e}{\partial \lambda}$ reads:

$$\frac{\partial \mathcal{D}^e}{\partial \lambda} = \frac{1}{\lambda_c - \lambda_o} = F_\lambda \quad (8)$$

165 Furthermore, the radial slope of the mixed-mode displacement jump, $\frac{\partial \lambda}{\partial \rho}$, in equations (3) and (4)
166 is addressed in the following. Taking into account the dependency of the mixed-mode displacement
167 jump, λ (Equation (A.7)), on the normal and tangential displacement jumps, arranged in vector δ_i ,
168 and by application of the chain rule, the following expression is obtained:

$$\frac{\partial \lambda}{\partial \rho} = \frac{\partial \lambda}{\partial \delta_j} \frac{\partial \delta_j}{\partial \rho} \quad (9)$$

169 The first term in the right hand side of Equation (9) reads:

$$\frac{\partial \lambda}{\partial \delta_j} = \left\{ \frac{\delta_1}{\lambda}, \frac{\delta_2}{\lambda}, \frac{\langle \delta_3 \rangle}{\lambda} \right\}^T = A_j \quad (10)$$

170 and the second term in the right hand side of Equation (9) is the derivative of the displacement jumps,
171 δ_j , with respect to the radial coordinate, ρ , which is obtained as follows:

$$\frac{\partial \delta_j}{\partial \rho} = \frac{\partial \Theta_{ji}}{\partial \rho} M_{im} Q_m + \Theta_{ji} \frac{\partial M_{im}}{\partial \rho} Q_m \quad (11)$$

172 where Θ_{ji} is the rotation matrix that relates the global to the local Cartesian coordinate system and
173 M_{im} is the transformation matrix that relates the global displacement jump with the nodal global
174 displacement, Q_m (see Appendix A).

175 The derivative of the rotation matrix, Θ_{ji} , with respect to the radial coordinate, ρ , can be approx-
176 imated to zero, by assuming that the curvature of the interface within the element domain is small.
177 Moreover, its derivation leads to a complex expression that would increase the difficulty of the formu-
178 lation and its further implementation into FE without a substantial improvement in the accuracy of
179 the solution. For the sake of simplicity, in the following it is assumed that $\frac{\partial \Theta_{ji}}{\partial \rho} = 0$. Therefore, only
180 the second summand in the right hand side of Equation (11) is addressed.

181 The derivative of the transformation matrix, M_{im} , with respect to the local polar coordinate, ρ , is
182 obtained by successive application of the chain rule:

$$\frac{\partial M_{im}}{\partial \rho} = \frac{\partial M_{im}}{\partial \eta_\alpha} \frac{\partial \eta_\alpha}{\partial e_l} \frac{\partial e_l}{\partial \rho} \quad (12)$$

183 The first partial derivative in the right hand side of Equation (12) is the variation of the transfor-
184 mation matrix, M_{im} , with the isoparametric coordinates of the cohesive element formulation, η_α (see
185 Appendix A):

$$\frac{\partial M_{im}}{\partial \eta_\alpha} = \left[-\frac{\partial N_{ik}}{\partial \eta_\alpha}, \frac{\partial N_{ik}}{\partial \eta_\alpha} \right] = E_{im\alpha} \quad (13)$$

186 where N_{ik} is the shape function matrix and the subscript k runs from 1 to the number of degrees of
 187 freedom of each of top and bottom surface of the cohesive element. In case of an eight-noded element,
 188 $k = 1 \dots 12$.

189 The derivative $\frac{\partial \eta_\alpha}{\partial e_l}$ is the inverse matrix of the two vectors tangential to the deformed midsurface,
 190 described in Equation (A.2) and expressed in local tangential coordinates, these being:

$$\frac{\partial e_l}{\partial \eta_\alpha} = \Theta_{li} \frac{1}{2} \frac{\partial N_{ik}}{\partial \eta_\alpha} (C_k^+ + C_k^- + Q_k^+ + Q_k^-) = \Theta_{li} J_{i\alpha} \quad (14)$$

191 where $J_{i\alpha}$ is the Jacobian matrix defined in Equation (A.26). Thus, let matrix $G_{\alpha l}$ be defined as:

$$G_{\alpha l} = (\Theta_{li} J_{i\alpha})^{-1} = \begin{bmatrix} \frac{\partial \eta_1}{\partial e_1} & \frac{\partial \eta_2}{\partial e_1} \\ \frac{\partial \eta_1}{\partial e_2} & \frac{\partial \eta_2}{\partial e_2} \end{bmatrix} \quad (15)$$

192 Using the following transformation relation:

$$\begin{bmatrix} e_1 \\ e_2 \end{bmatrix} = \begin{bmatrix} \rho \cos(\varphi) \\ \rho \sin(\varphi) \end{bmatrix} \quad (16)$$

193 the derivative of the local Cartesian coordinates, e_l , with respect to the radial coordinate, ρ , reads:

$$\frac{\partial e_l}{\partial \rho} = \begin{bmatrix} \cos(\varphi) \\ \sin(\varphi) \end{bmatrix} \quad (17)$$

194 Then, the slope of the mixed-mode displacement jump, λ , with respect to the radial coordinate, ρ ,
 195 is obtained using equations (10)-(17) in Equation (9):

$$\frac{\partial \lambda}{\partial \rho} = A_j \Theta_{ji} E_{im\alpha} (G_{\alpha 1} (\cos \varphi) + G_{\alpha 2} (\sin \varphi)) Q_m \quad (18)$$

196 The same procedure can be applied to find the radial slope of the mode mixity, $\frac{\partial B}{\partial \rho}$, in equations
 197 (3) and (4). Taking into account the dependency of the mode mixity, B , defined in Equation (A.10),

198 on the displacement jumps, δ_j , the radial slope $\frac{\partial B}{\partial \rho}$ is obtained by applying the chain rule as:

$$\frac{\partial B}{\partial \rho} = \frac{\partial B}{\partial \delta_j} \frac{\partial \delta_j}{\partial \rho} \quad (19)$$

199 where the derivative of the mode mixity, B , with respect to the displacement jumps, δ_j , reads:

$$\frac{\partial B}{\partial \delta_j} = \left\{ \frac{2\delta_1 \langle \delta_3 \rangle^2}{\lambda^4}, \frac{2\delta_2 \langle \delta_3 \rangle^2}{\lambda^4}, -\frac{2\delta_s^2 \langle \delta_3 \rangle}{\lambda^4} \right\}^T = O_j \quad (20)$$

200 and $\frac{\partial \delta_j}{\partial \rho}$ is developed through equations (11)-(17). Hence, the radial slope $\frac{\partial B}{\partial \rho}$ is given by:

$$\frac{\partial B}{\partial \rho} = O_j \Theta_{ji} E_{im\alpha} (G_{\alpha 1} (\cos \varphi) + G_{\alpha 2} (\sin \varphi)) Q_m \quad (21)$$

201 Finally, let matrix V_α be:

$$V_\alpha = F_B O_j \Theta_{ji} E_{im\alpha} Q_m \quad (22)$$

202 and matrix W_α be:

$$W_\alpha = F_\lambda A_j \Theta_{ji} E_{im\alpha} Q_m \quad (23)$$

203 then, the growth driving direction according to Criterion 1 is found using equations (18) and (21)-(23)

204 in Equation (3), solving for the angular coordinate, φ :

$$\varphi = \text{atan} \left(-\frac{(V_1 + W_1) G_{11} + (V_2 + W_2) G_{21}}{(V_1 + W_1) G_{12} + (V_2 + W_2) G_{22}} \right) \quad (24)$$

205 and fulfilling the condition for convexity (Equation (4)):

$$(V_\alpha + W_\alpha) (G_{\alpha 1} (-\cos \varphi) + G_{\alpha 2} (-\sin \varphi)) > 0 \quad (25)$$

206 Once φ is identified, the transformation of the global Cartesian coordinates, X_i , into the local

207 Cartesian coordinates that are located on the midsurface and oriented according to the growth driving
208 direction is done by means of the following rotation matrix:

$$R_{ri} = T_{rj} \Theta_{ji} \quad (26)$$

209 where T_{rj} is:

$$T_{rj} = \begin{bmatrix} \cos \varphi & -\sin \varphi & 0 \\ \sin \varphi & \cos \varphi & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (27)$$

210 As shown, all the information necessary to evaluate Criterion 1 (and also criteria 2 and 3, as
211 demonstrated in Appendix B) are the global nodal coordinates, C_m and displacements Q_m . Using the
212 cohesive element formulation in [15, 17], this information is available at the element level and, thus,
213 the presented growth driving direction algorithms can be implemented into a user-defined element
214 subroutine and evaluated at any point in the cohesive zone without any additional post-processing or
215 non-local information.

216 3. One-element validation examples

217 The following one-element studies serve to validate the formulation of the growth driving direction
218 criteria presented in Section 2. The proposed method has been implemented in a MATLAB program.
219 The eight-noded cohesive element used is illustrated in Figure 5. The kinematics and constitutive law
220 associated to the element are detailed in Appendix A. Newton-Cotes integration scheme is used, with
221 2x2 integration points located at the midsurface vertexes. The undeformed element is 0.1 mm wide,
222 0.1 mm long and has zero thickness. The cohesive properties are listed in Table 2. Three different
223 loading cases (A, B and C) have been analyzed. The applied nodal displacement is listed in Table 3 for
224 each case. The growth driving direction is calculated at a point $\bar{\mathbf{p}}(\eta_1, \eta_2)$ located on the midsurface,
225 with natural coordinates $(-0.5, -0.5)$. The results of the angle φ obtained in each case are listed in

| Interface properties | | |
|----------------------|------|-------------------|
| \mathcal{G}_{Ic} | 0.3 | N/mm |
| \mathcal{G}_{IIc} | 0.7 | N/mm |
| τ_{Ic} | 50 | MPa |
| τ_{IIc} | 76.4 | MPa |
| η | 2 | - |
| K | 1E5 | N/mm ³ |

Table 2: Cohesive law properties used in the one-element case studies.

| Case ID | Loading conditions | Nodal displacements (mm) | φ at point \bar{p} (deg) | | |
|---------|---|--|------------------------------------|-------------|-------------|
| | | | Criterion 1 | Criterion 2 | Criterion 3 |
| A | Pure mode I B constant | $u_3^5 = 0.005$ $u_3^6 = 0.005$ $u_3^7 = 0.01$ $u_3^8 = 0.01$ | 270.0 | 270.0 | 270.0 |
| B | Mixed mode I-shear B constant | $u_1^5 = u_2^5 = u_3^5 = 0.001$ $u_1^6 = u_2^6 = u_3^6 = 0.002$ $u_1^7 = u_2^7 = u_3^7 = 0.003$ $u_1^8 = u_2^8 = u_3^8 = 0.002$ | 225.3 | 225.3 | 225.3 |
| C | Mixed mode I-shear same λ at nodes | $u_1^5 = \sqrt{2} \cdot 0.008$ $u_1^6 = u_3^6 = 0.008$ $u_3^7 = \sqrt{2} \cdot 0.008$ $u_1^8 = u_3^8 = 0.008$ | 225.0 | 225.0 | 45.0 |

Table 3: Loading conditions and growth driving direction results at point \bar{p} from the one-element case studies

226 Table 3 for the three criteria.

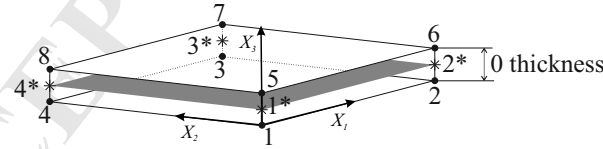


Figure 5: Sketch of the undeformed cohesive element. The nodes are represented as black dots and numbered from 1 to 8 and the integration points are represented as asterisks and numbered from 1* to 4*.

227 Case A is a pure mode I-opened element. The distribution of the mixed-mode displacement jump,
 228 λ , along the element midsurface is projected on the deformed element midsurface in Figure 6, where
 229 the point \bar{p} is highlighted in white. Integration points 1 and 2 have the lowest λ value, while points
 230 3 and 4 are the most opened. As illustrated, the growth driving direction according to Criterion 3

231 is determined by the greatest rate of decrease of λ . The other quantities being analyzed in criteria 1
 232 and 2, \mathcal{D}^e and $\frac{\omega_{tot}}{\mathcal{G}_c}$ respectively, are represented in Figure 7, as well as the mode-mixity, B . Like the
 233 B -distribution along the element midsurface is constant, the growth driving direction is only defined
 234 by the direction that minimizes the slope of the mixed-mode displacement jump. Therefore, in Case
 235 A only, the kinematics of the element governs the growth driving direction, independently of which
 236 criteria is used.

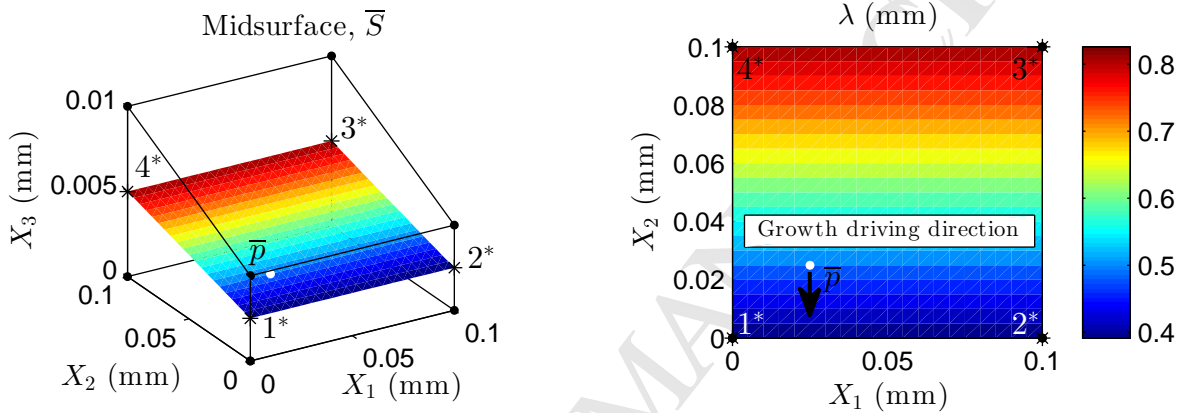


Figure 6: Mixed-mode displacement jump distribution at the element midsurface for Case A loading conditions. The growth driving direction is analyzed at point \bar{p} , indicated with a white circle, and the result is listed in Table 3.

237 On the other hand, in Case B, the element is opened under constant mixed mode I-shear opening
 238 conditions (See Figure 8). In this case, λ linearly increases along the midsurface diagonal direction,
 239 from integration point 1 to integration point 3. However, B is constant and, thus, also the constitutive
 240 law associated to it. Again, in Case B, the growth driving direction is only defined by the direction
 241 that minimizes the slope of the mixed-mode displacement jump, λ . Therefore, it is governed by the
 242 kinematics of the cohesive element and there is agreement between the three criteria.

243 Finally, in Case C, all the integration points have the same λ -value, although the mode-mixity, B ,
 244 changes from 0 to 1 along the midsurface diagonal direction (See Figure 9). At integration point 1, only
 245 shear sliding displacement is applied, while at the opposite corner, at integration point 3, there is only
 246 mode I opening. At the integration points 2 and 4, there is 50% mixed-mode opening. On the other

247 hand, λ is lower at the center part of the element midsurface than at the corners and its distribution
 248 is determined by the interpolation functions. Criterion 3 is only affected by the λ -interpolation and
 249 results in the direction that points to the center of the element. Furthermore, due to the uneven B -
 250 distribution, the constitutive law is not constant. With the cohesive properties used in these studies,
 251 the direction of steepest negative slopes of \mathcal{D}^e and $\frac{\omega_{tot}}{\mathcal{G}_c}$ coincides with the direction that maximizes
 252 the rate of increase of B . Note that, when evaluated at point $\bar{\mathbf{p}}$, this is the direction of largest slope
 253 of λ . Therefore, Criterion 3 and criteria 1 and 2 point to opposite directions.

254 In addition, the slopes $\frac{\Delta \mathcal{D}^e}{\Delta \rho}$, $\frac{\Delta(\omega_{tot}/\mathcal{G}_c)}{\Delta \rho}$ and $\frac{\Delta \lambda}{\Delta \rho}$ have been numerically evaluated using a central
 255 difference at every 1 degree at point $\bar{\mathbf{p}}$ under Case C loading conditions using a perturbation size for
 256 the radius of 0.001 mm. Thus, the slope of any quantity f has been calculated as:

$$\frac{\Delta f}{\Delta \rho} = \frac{f(0.001, \varphi) - f(-0.001, \varphi)}{2 \cdot 0.001} \quad (28)$$

257 The resulting slopes are represented in Figure 10. The disagreement between Criterion 3 and
 258 criteria 1 and 2 can be observed. For Criterion 3, the angle φ that minimizes $\frac{\Delta \lambda}{\Delta \rho}$ is 45 degrees, while
 259 for criteria 1 and 2, the angle that minimizes $\frac{\Delta \mathcal{D}^e}{\Delta \rho}$ and $\frac{\Delta(\omega_{tot}/\mathcal{G}_c)}{\Delta \rho}$, respectively, amounts 225 degrees.
 260 Note that these results are in agreement with the results obtained by implementing the formulation
 261 developed in Section 2.

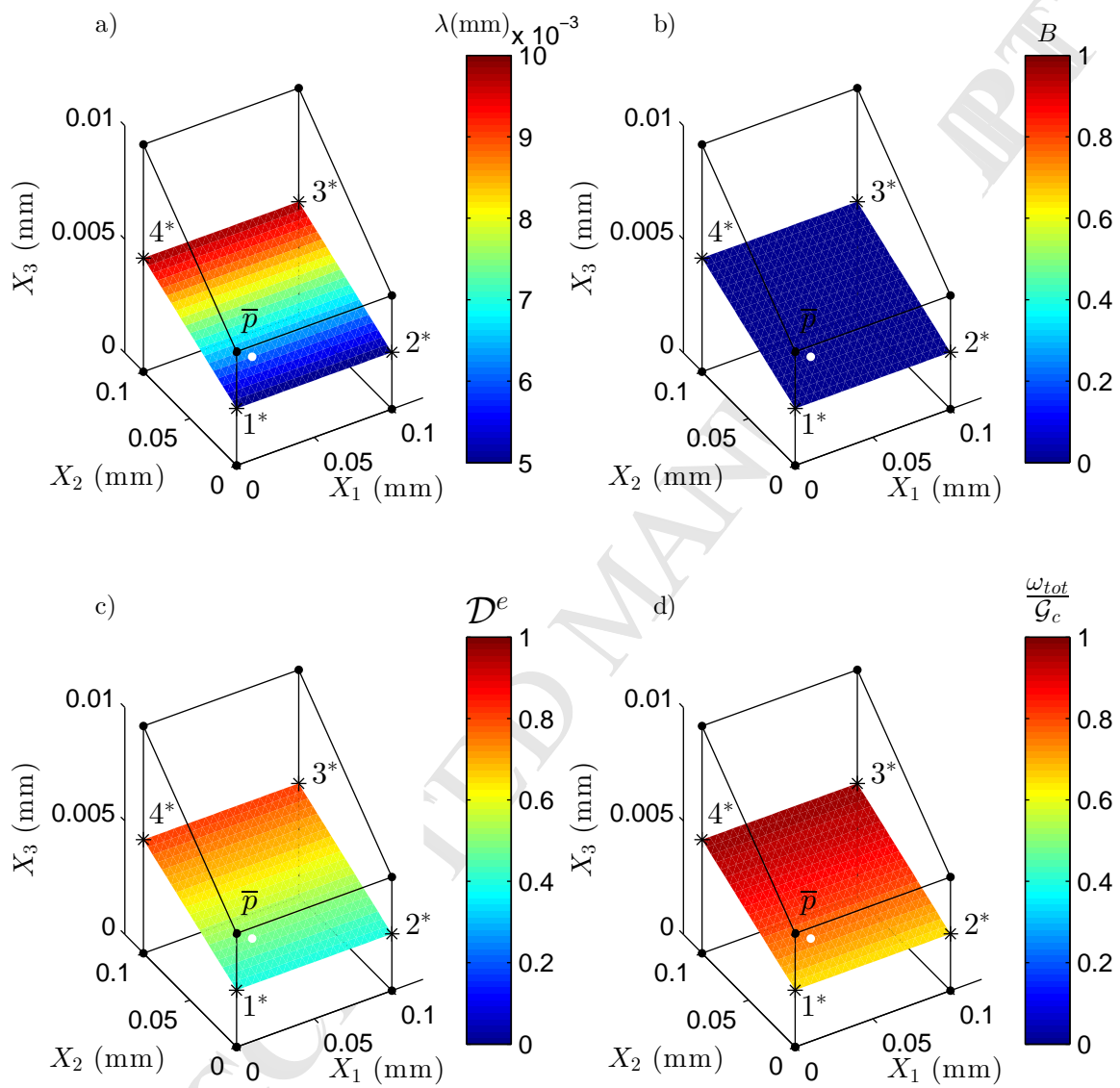


Figure 7: a) Mixed-mode displacement jump, λ , b) mode-mixity, B , c) energy-based damage, \mathcal{D}^e , and d) total specific work over the fracture toughness, $\frac{\omega_{tot}}{\mathcal{G}_c}$, distributions at the element midsurface for Case A loading conditions. The point \bar{p} , where the growth driving direction is analyzed, is indicated with a white circle.

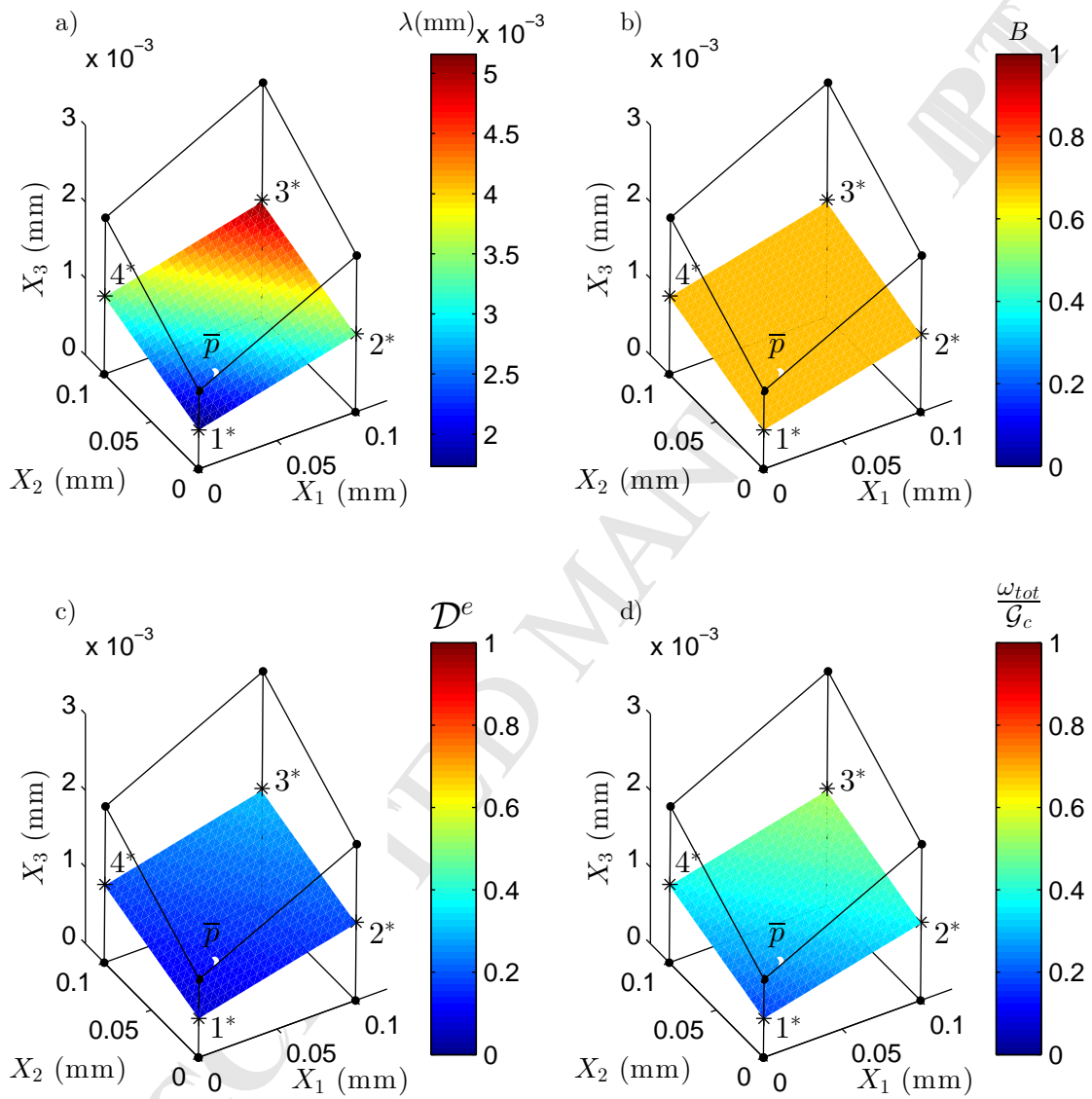


Figure 8: a) Mixed-mode displacement jump, λ , b) mode-mixity, B , c) energy-based damage, \mathcal{D}^e , and d) total specific work over the fracture toughness, $\frac{\omega_{tot}}{\mathcal{G}_c}$, distributions at the element midsurface for Case B loading conditions. The point \bar{p} , where the growth driving direction is analyzed, is indicated with a white circle.

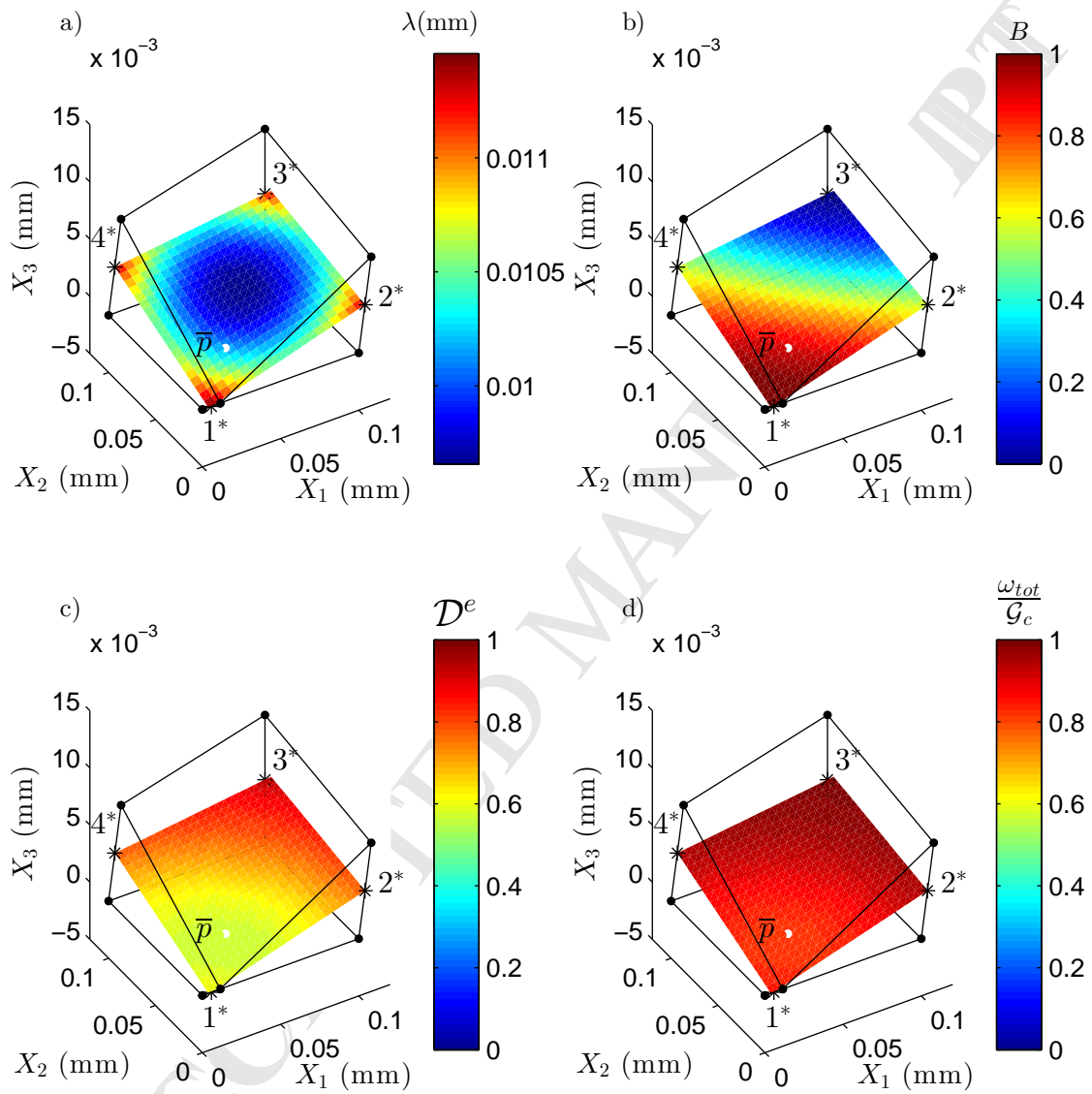


Figure 9: a) Mixed-mode displacement jump, λ , b) mode-mixity, B , c) energy-based damage, \mathcal{D}^e , and d) total specific work over the fracture toughness, $\frac{\omega_{tot}}{\mathcal{G}_c}$, distributions at the element midsurface for Case C loading conditions. The point \bar{p} , where the growth driving direction is analyzed, is indicated with a white circle.

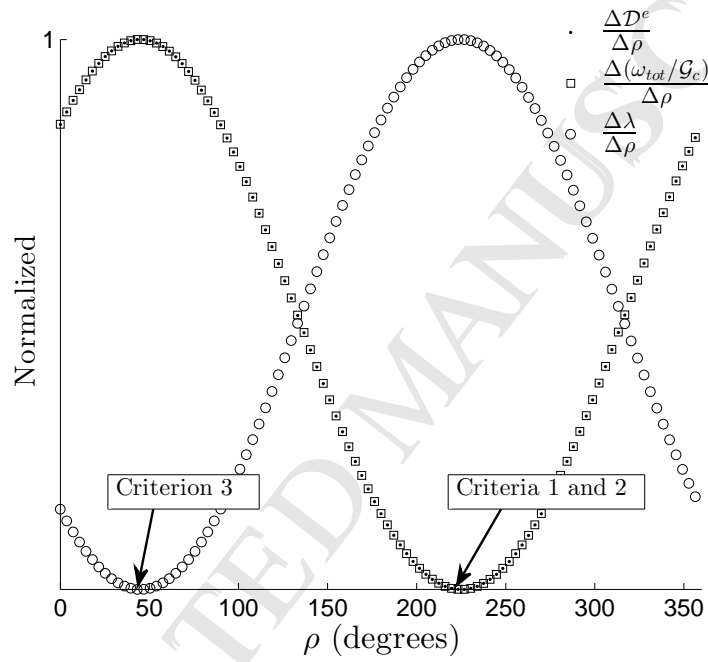


Figure 10: Slopes in the radial direction, ρ , of the energy-based damage, \mathcal{D}^e , the total specific work over the fracture toughness, $\frac{\omega_{tot}}{\mathcal{G}_c}$, and the mixed-mode displacement jump, λ , as a function of the angle φ evaluated at point \bar{p} for Case C loading conditions. The slopes have been calculated using a central difference with a perturbation for the radius of 0.001 mm. The values $\frac{\Delta \mathcal{D}^e}{\Delta \rho}$, $\frac{\Delta(\omega_{tot}/\mathcal{G}_c)}{\Delta \rho}$ and $\frac{\Delta \lambda}{\Delta \rho}$ have been normalized by their maximum value.

262 **4. Three-Dimensional application**

263 To exemplify the applicability of the presented formulation, a three-dimensional model with a non-
 264 straight crack front is used. The test configuration is a End-Loaded Split (ELS) test on a symmetric
 265 run-out specimen with a midplane initial defect. A Teflon insert acts as an initial straight delami-
 266 nation (see Figure 11). Moreover, the middle width of the specimen is stiffened by bonding CFRP
 267 reinforcements on the upper and lower faces. During propagation the crack front shape changes when
 268 it approaches the reinforced region. The formulation presented in Section 2 can be used to evaluate the
 269 growth driving criteria at any given loading state during the quasi-static simulation. To this end, the
 270 method in [15, 17] has been enhanced with the growth driving direction calculation and implemented in
 271 Abaqus [27] as a UEL subroutine. The user-defined cohesive elements that model the middle interface
 272 are 0.2 mm x 0.5 mm. The laminate and interface properties used in the simulation are listed in Table
 273 4.

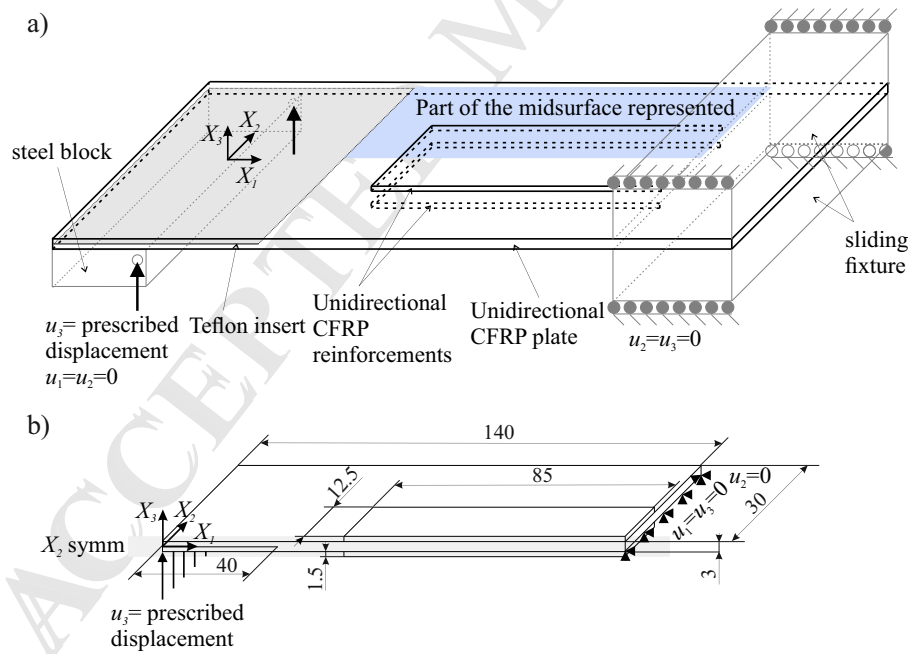


Figure 11: a) Sketch of the partially reinforced ELS specimen. The grey-shaded area represents the Teflon insert. The blue-shaded area is the area represented in figures 12.b, 13 and 18. b) Simplified model for FE simulation and dimensions (units in mm).

274 The historical evolution of the 0.5-valued damage isoline is plotted in Figure 12.a. The energy-

| Laminate properties | | | Interface properties | | |
|---|-------|-----|----------------------|-------|-------------------|
| E_{11} : Longitudinal Young's modulus | 154 | GPa | \mathcal{G}_{Ic} | 0.3 | N/mm |
| $E_{22} = E_{33}$: Transversal Young's modulus | 8.5 | GPa | \mathcal{G}_{IIc} | 3 | N/mm |
| $G_{12} = G_{13}$: Shear modulus in the longitudinal planes | 4.2 | GPa | τ_{Ic} | 10 | MPa |
| G_{23} : Shear modulus in the transversal plane | 3.036 | GPa | τ_{IIc} | 31.62 | MPa |
| $\mu_{12} = \mu_{13}$: Poison's coefficient in the longitudinal planes | 0.35 | - | η | 2 | - |
| μ_{23} : Poison's coefficient in the transversal plane | 0.4 | - | K | 1E5 | N/mm ³ |

Table 4: Laminate and interface properties used in the simulation study of Section 4. The nomenclature of the interface properties is defined in Appendix A.

275 based damage, \mathcal{D}^e , distribution is projected on the deformed midsurface, in Figure 12.c, for a prescribed
276 displacement of 32.55 mm. Only the blue-shadowed area in Figure 11 is represented. The crack growth
277 direction is evaluated at each integration point within the FPZ using criteria 1, 2 and 3, and represented
278 in Figure 13. Note that criteria 1 (Figure 13.a) and 2 (Figure 13.b) are coincident except from at the
279 elastic region, where no results from Criterion 1 can be obtained. By comparison of figures 13.b and
280 13.c, it can be observed that Criterion 3 only differs from criteria 1 and 2 at a region located at the
281 upper left part of the cohesive zone ($X_1 < 85$ mm and $X_2 > 10$ mm). Indeed, the mode-mixity, B , is
282 constant and equal to 1 in the entire cohesive zone, except for this region, where it locally decreases to
283 0.6 (see Figure 13.d). As demonstrated in Section 3, under constant B conditions, the growth driving
284 direction is only governed by the kinematics of the cohesive elements. Therefore, evaluating any of the
285 three criteria results in the same growth driving direction solution. On the other hand, only criteria 1
286 and 2 are affected by changes in the mode-dependent constitutive law, leading to different results, if
287 compared to Criterion 3, at the region where the mode-mixity, B , varies.

288 In addition, four damage isolines have been traced. The damage isolines are constructed by con-
289 necting integration points with the same damage value. The first damage isoline, represented in Figure
290 14.a, is the line connecting the completely damaged integration points adjacent to the damage process
291 zone. At each point on the damage isoline, the geometrical normal direction has been approximated
292 by the normal to the slope of a second degree polynomial expression fitted to five consecutive points
293 represented in white in Figure 14.a): the current point and the two preceding and the two succeeding
294 points. Therefore, the approximated normal direction is computed by post-processing global informa-

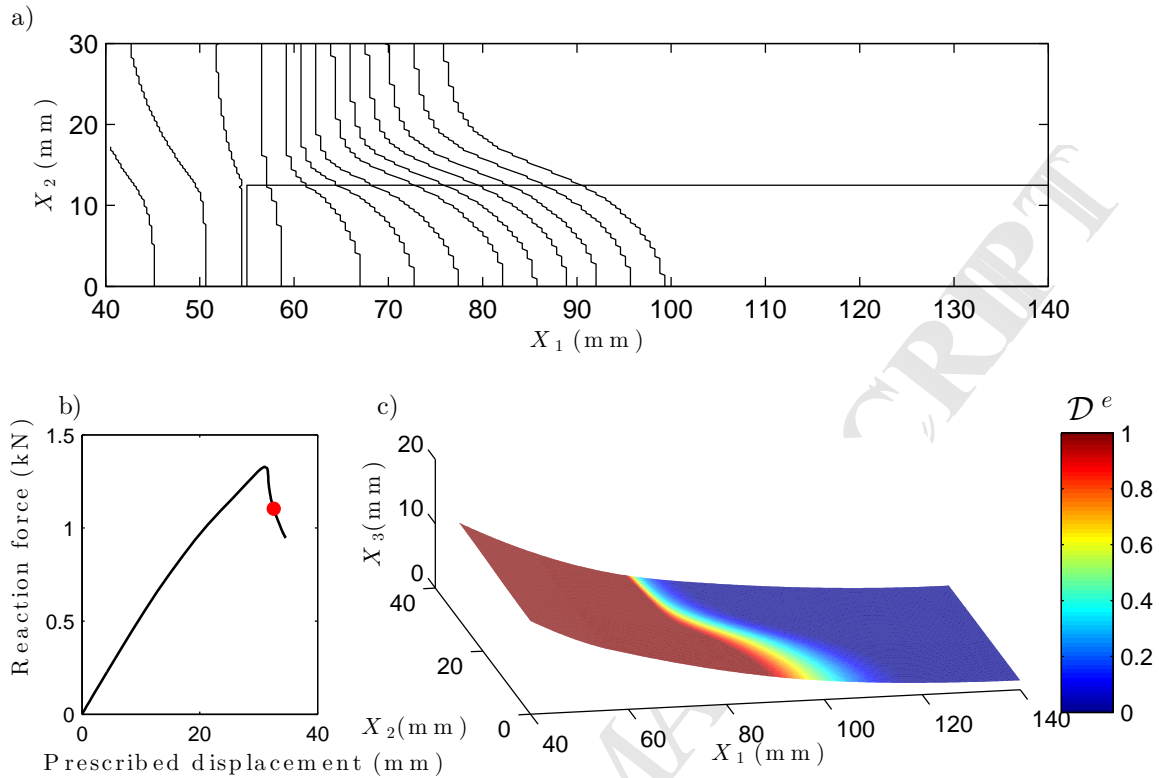


Figure 12: a) Historical evolution of the 0.5-valued damage isoline. b) Reaction force vs prescribed displacement curve with the current loading state highlighted in red. c) Energy-based damage projected on the deformed midsurface.

tion and it is heavily affected by the discretization and the choice of the fitting function. The results are compared to the local growth driving direction criteria developed in Section 2 in Figure 14.b. The same analysis is done with a 0.5-valued damage isoline (Figure 15), a 0.1-valued damage isoline (Figure 16) and the line connecting the undamaged integration points adjacent to the damage process zone (Figure 17). Note that, although for comparison purposes the growth driving direction is evaluated in a discrete manner at the same points where the approximated normal direction is computed, it is a continuous field that can be evaluated at any point, as shown in Figure 13.

Finally, three different FE models with element sizes 0.5 x 0.2 mm, 1 x 1.25 mm and 2.5 x 2.5 mm (see Figure 18) are used to compare the element size effect on both the approximated normal direction to the 1-valued damage isoline, evaluated by using global information, and the predicted growth driving direction using Criterion 1, evaluated point-wise at the element level. The results are

306 obtained using the information of the points on the 1-valued damage isoline traced in Figure 19 for
307 the three meshes. The direction obtained along the damage isoline using both methods is plotted in
308 Figure 20.

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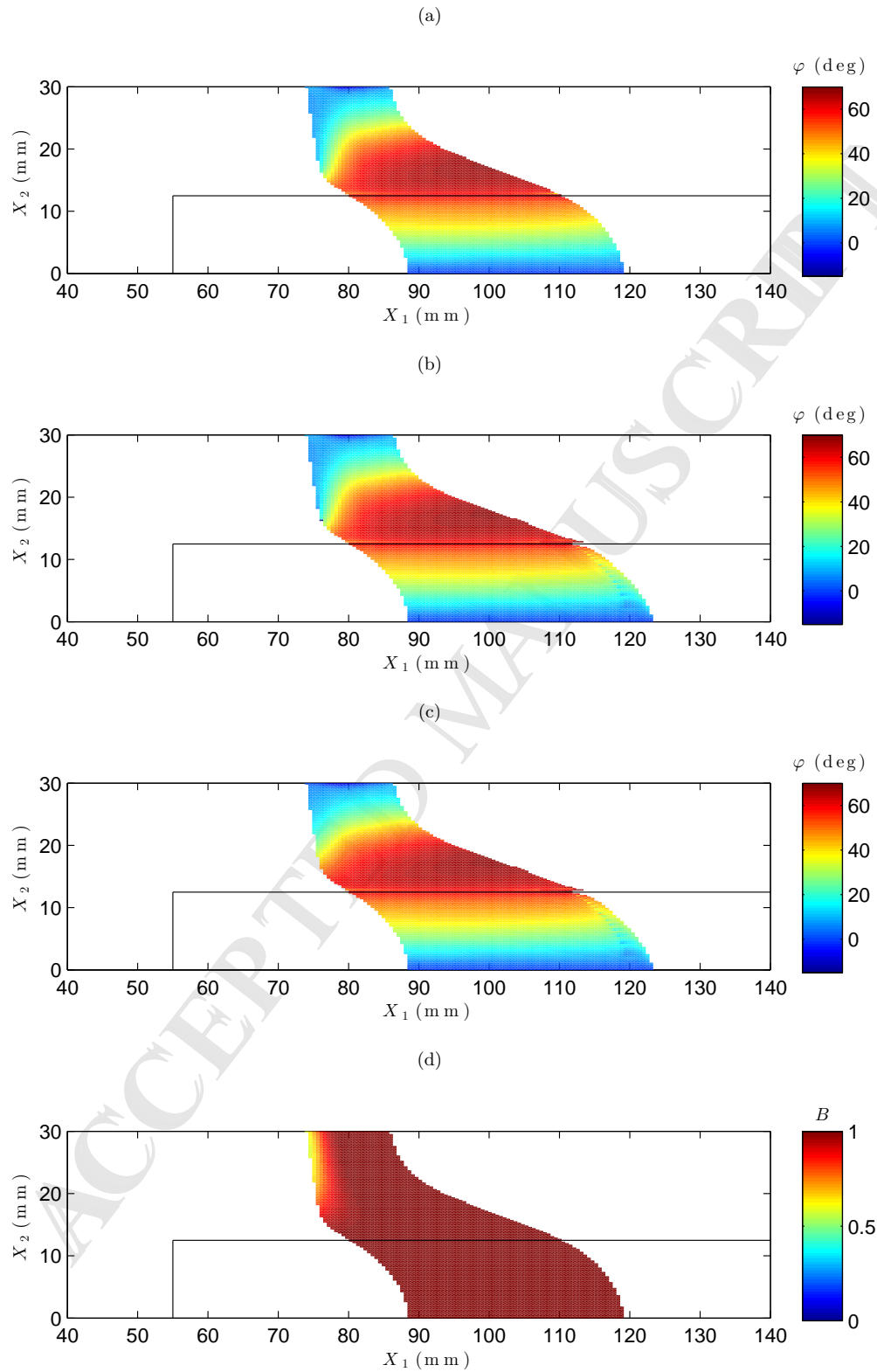


Figure 13: a) Growth driving direction resulting from the evaluation of Criterion 1. b) Growth driving direction resulting from the evaluation of Criterion 2. c) Growth driving direction resulting from the evaluation of Criterion 3. d) Mode mixity, B . The black line marks the reinforcements.

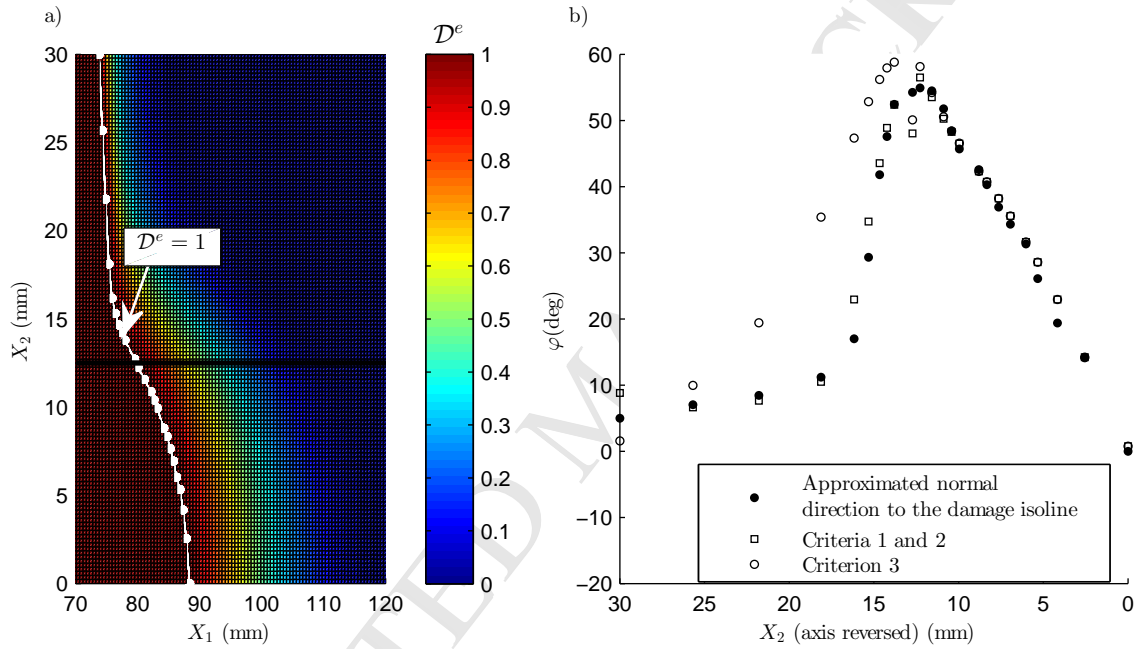


Figure 14: a) Energy-based damage, \mathcal{D}^e , distribution along the cohesive zone. The points forming the 1-valued damage isoline are highlighted in white. The thick black solid line marks the reinforcements border. b) Comparison of the angle φ obtained at the 1-valued damage front by computing the normal direction using global information and by locally evaluating the growth driving direction criteria. Criteria 1 and 2 are represented by the same marker because they lead to identical growth driving direction results.

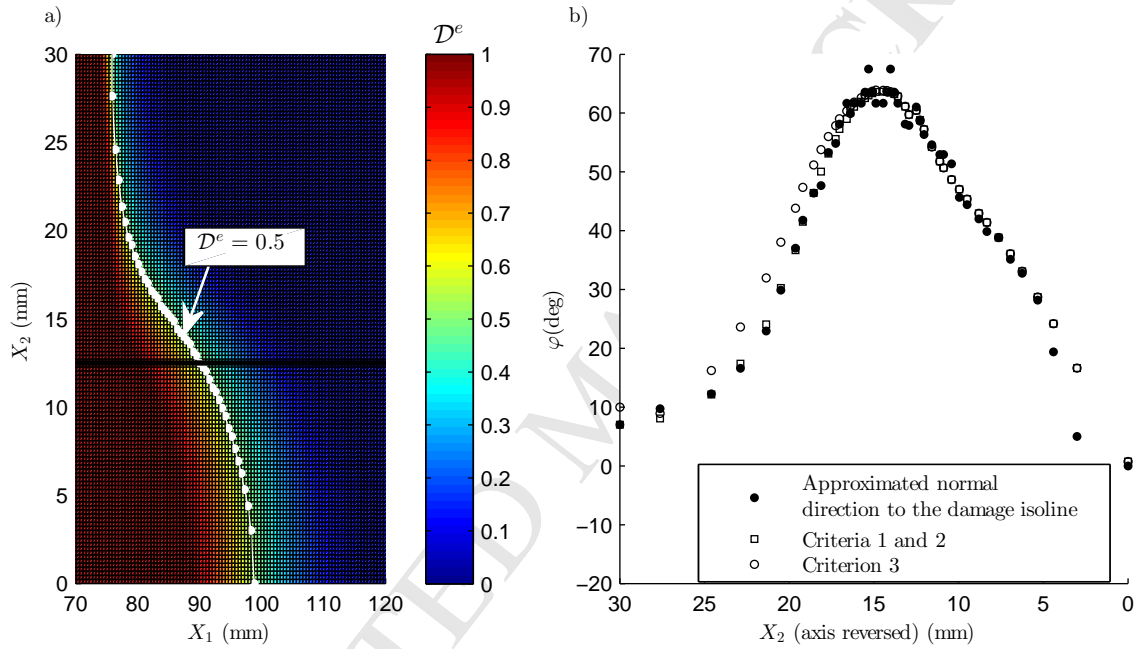


Figure 15: a) Energy-based damage, \mathcal{D}^e , distribution along the cohesive zone. The points forming the 0.5-valued damage isoline are highlighted in white. The thick black solid line marks the reinforcements border. b) Comparison of the angle φ obtained at the 0.5-valued damage front by computing the normal direction using global information and by locally evaluating the growth driving direction criteria. Criteria 1 and 2 are represented by the same marker because they lead to identical growth driving direction results.

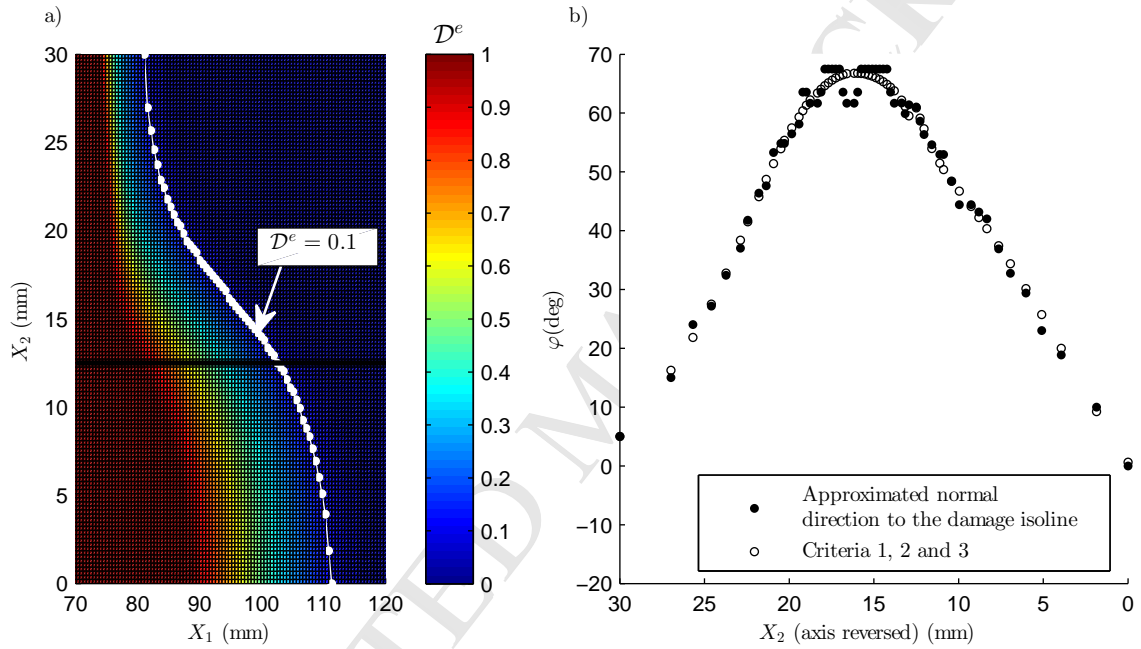


Figure 16: a) Energy-based damage, \mathcal{D}^e , distribution along the cohesive zone. The points forming the 0.1-valued damage isoline are highlighted in white. The thick black solid line marks the reinforcements border. b) Comparison of the angle φ obtained at the 0.1-valued damage front by computing the normal direction using global information and by locally evaluating the growth driving direction criteria. Criteria 1, 2 and 3 are represented by the same marker because they lead to identical growth driving direction results.

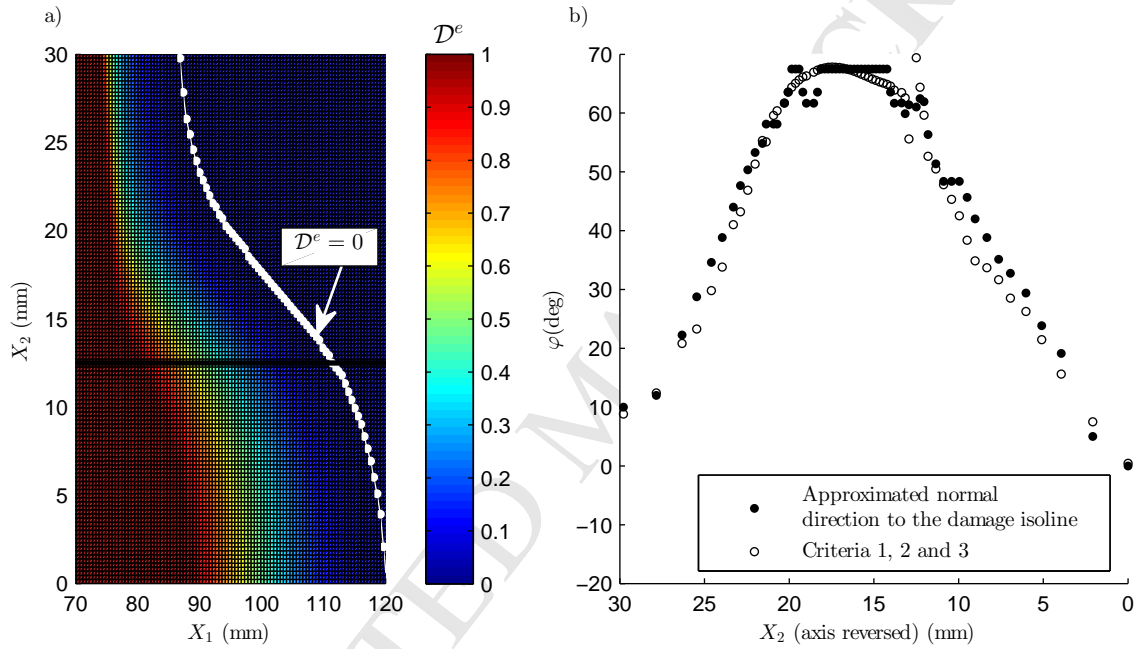


Figure 17: a) Energy-based damage, \mathcal{D}^e , distribution along the cohesive zone. The points forming the 0-valued damage isoline are highlighted in white. The thick black solid line marks the reinforcements border. b) Comparison of the angle φ obtained at the 0-valued damage front by computing the normal direction using global information and by locally evaluating the growth driving direction criteria. Criteria 1, 2 and 3 are represented by the same marker because they lead to identical growth driving direction results.

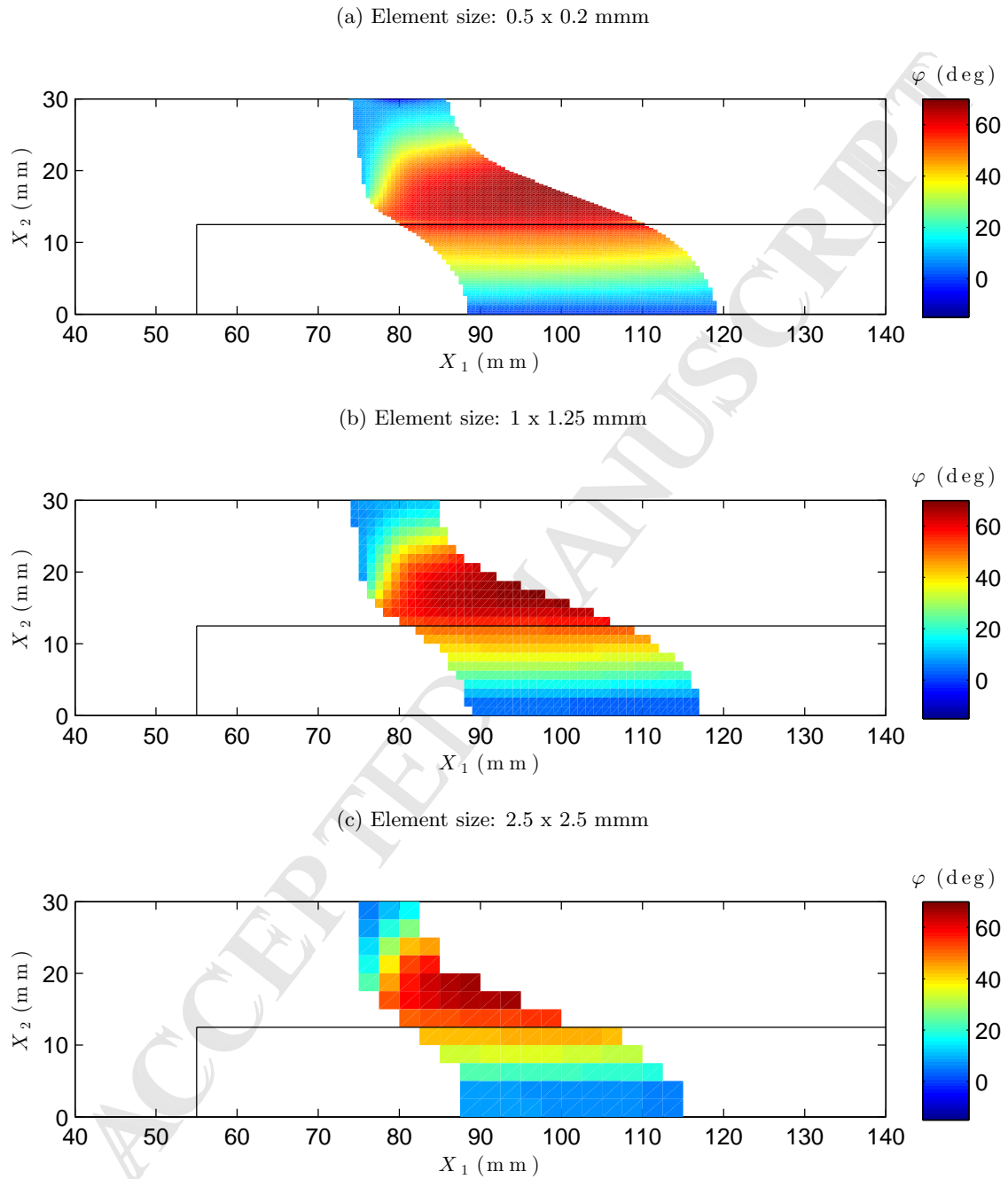


Figure 18: Growth driving direction resulting from the evaluation of Criterion 1 using three different element sizes.

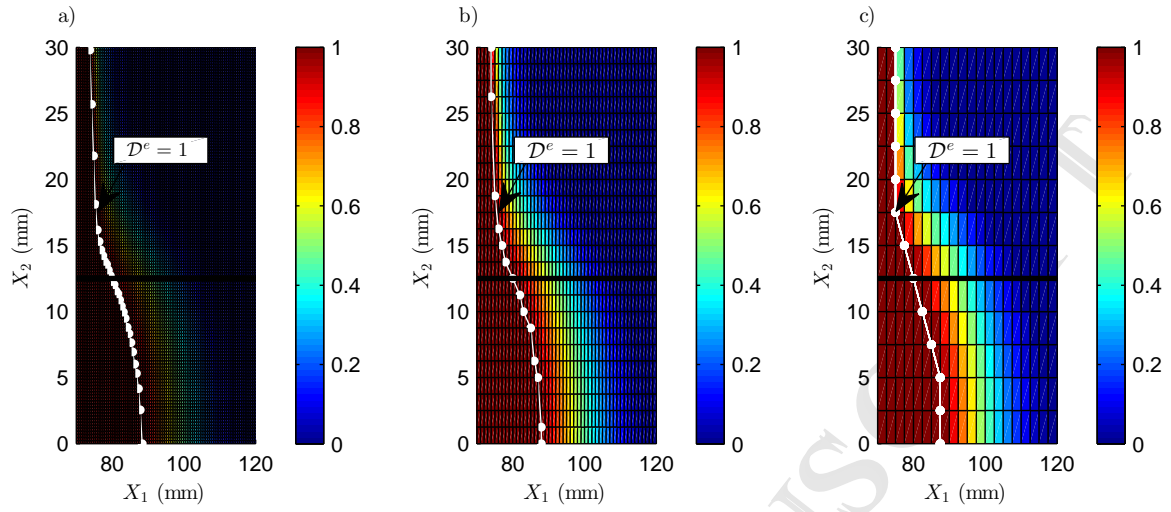


Figure 19: 1-valued damage fronts using different element sizes: a) 0.2 x 0.5 mm. b) 1 x 1.25 mm. c) 2.5 x 2.5 mm.

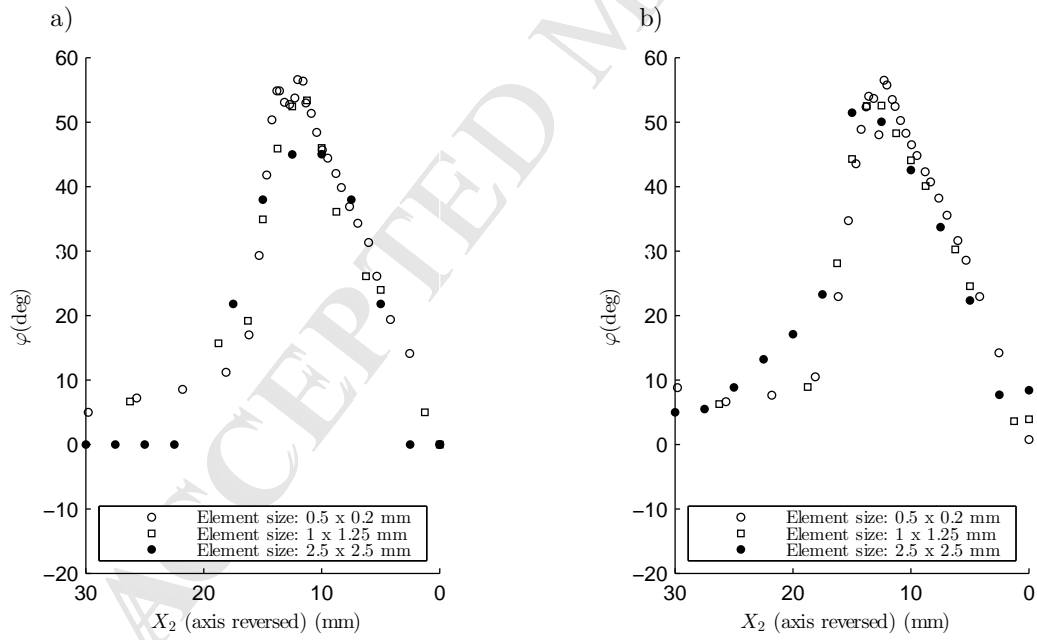


Figure 20: Comparison of the angle φ obtained at the 1-valued damage isoline using three different element sizes by a) computing the normal direction to the crack front using global information and b) evaluating Criterion 1.

309 **5. Discussion**

310 Three different growth driving direction criteria have been proposed as element-level algorithms,
311 that can be evaluated at any point within the cohesive zone. Criteria 1 and 2 are energetically-based
312 formulations that account for both the kinematics and the constitutive law of the interface element.
313 On the other hand, Criterion 3 is a geometrical approach, which only accounts for the kinematics of
314 the interface element. Therefore, when the mode-mixity, B , is not constant, criteria 1 and 2 are the
315 most appropriate. Moreover, Criterion 2 computes the rate of decrease of both the specific elastic
316 energy, ω_e , and the dissipated energy, ω_d , normalized to the fracture toughness, \mathcal{G}_c . On the contrary,
317 Criterion 1 only computes the rate of decrease of the dissipated energy, ω_d , normalized to the fracture
318 toughness, \mathcal{G}_c , which is equivalent to computing the rate of decrease of the energy-based damage, \mathcal{D}^e .
319 On this basis, Criterion 1 is not active before damage initiation, while Criterion 2 can be computed
320 as soon as some separation between two initially coinciding points at the interface occurs. The three
321 criteria have been presented for completeness, since they can be developed for other CZM formulations
322 following the methodology described in Section 2.3. With the CZM used in this work, criteria 1 and 2
323 lead to the same growth driving direction solution at the damaged region. However, different results
324 may be obtained if a mode-dependent penalty-stiffness is used, which could render the specific elastic
325 energy of Criterion 2 dependent on growth driving direction.

326 The implementation of the formulation for the proposed growth driving direction criteria has been
327 validated with one-element case studies in Section 3. The distribution of the quantities being ana-
328 lyzed have been projected on the element midsurface for visual verification (see figures 7-9 for different
329 loading cases). In addition, the slopes of such quantities have been numerically evaluated at different
330 orientations around a given evaluation point under Case C loading conditions (Figure 10). The orien-
331 tation that results in lowest slopes coincides with the angle of growth driving direction predicted by
332 each criteria, respectively.

333 Finally, the capabilities of the presented formulation are demonstrated in Section 4 using a three-
334 dimensional run-out specimen loaded under ELS test conditions (Figure 11). The crack front propa-

335 gates with non-straight shape due to the reinforcements bonded at the middle width of the specimen
336 Figure 12. The growth driving direction criteria are evaluated at all the integration points within
337 the cohesive zone for a given loading state with large deformations (Figure 13). The results from
338 the three criteria differ only at those regions where the mode-mixity, B , is not constant, as already
339 demonstrated in Section 3. Moreover, the resulting crack growth driving direction is compared with
340 the geometrical normal direction of four different damage isolines computed by post-processing global
341 information (figures 14-17). Both results are in good agreement, although the agreement is higher
342 between the geometrical normal direction to the damage isolines derived from global information and
343 the results from criteria 1 and 2, than from Criterion 3, specially at the non-constant mode-mixity,
344 B , region. It is noteworthy that the global description of the damage isoline is highly dependent on
345 the methodology used to compute it, mainly the number of points taken into account and its fitting.
346 Therefore, in a FE framework, the computation of the approximated normal direction to the damage
347 isoline using global information may, in some cases, misrepresent the actual normal direction. Indeed,
348 the local computation of the negative gradient of the energy-based damage, \mathcal{D}^e , by means of Criterion
349 1 is the exact normal to the damage isolines. The fitting of the points forming the damage isoline,
350 that leads to an approximate global description of it, is only used to validate the implementation of
351 the formulation presented. To close, the effect of the mesh size on the determination of the normal
352 direction to the 1-valued damage isoline is analyzed using both methods (Figure 20): the approximated
353 normal direction using global information and the growth driving direction obtained by evaluating Cri-
354 terion 1. The results show that the growth driving direction, evaluated locally, shows less sensitivity
355 to the element size. Indeed, the growth driving direction is a continuum field which does not explicitly
356 depend on the mesh size, but it implicitly does, due to discretization of the displacement field in the
357 FEM [28].

358 6. Conclusions

359 A novel method has been proposed for the determination of the growth driving direction for cohesive
360 zone models. The presented formulation is evaluated point-wise. Therefore, it can be implemented as
361 a part of a user-defined cohesive element subroutine and evaluated during simulation without the need
362 of any extra loop, post-processing or global information.

363 The growth driving direction is defined as the negative gradient of the energy-based damage vari-
364 able. However, other quantities can be used for the sake of simplicity. In this work, three different
365 criteria are proposed. The implementation of the formulation for the proposed criteria applied to a
366 particular CZM [15, 17] is derived and validated by using one-element analysis under different loading
367 conditions.

368 Finally, the usefulness of the method has been demonstrated via the analysis of delamination
369 propagation in a three-dimensional structure with a complex shaped crack front. The results using the
370 proposed point-wise formulation for the evaluation of the growth driving direction are in agreement
371 with the results from a global approximation of the normal direction to different damage isolines. Apart
372 from being a low computational time-consuming task, the proposed formulation has the advantage that
373 it can be evaluated at any point within the cohesive zone.

374 7. Acknowledgements

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451 **Appendix A. The cohesive element formulation**

452 The cohesive zone model from the original work of Turon et al. [15, 17] and its finite element
453 implementation are outlined in the following.

454 *Appendix A.1. Kinematics*

455 Let the delamination be understood as a strong discontinuous singular surface, S , that crosses a
456 volume of material, Ω , and divides it into two subdomains, Ω^+ and Ω^- , as shown in Figure A.21.
457 There are two surfaces that bound into S : the upper surface, S^+ , associated with Ω^+ , and the lower
458 surface, S^- , associated with Ω^- . These two surfaces, which are initially coincident with the reference
459 surface, S^0 , in the undeformed configuration, represent the crack faces. They independently translate,
460 rotate and stretch, though their motion is constrained by the constitutive law used to describe the
461 interface.

462 The reference surface, S^0 , is defined in a the three-dimensional space, as shown in Figure A.22,
463 by the global Cartesian coordinates X_i , where $i = 1, 2, 3$. Conveniently, the internal deformed middle
464 surface, \bar{S} , can be defined, through the history of deformations, as the average distance between two
465 initially coinciding points,

$$\bar{x}_i = X_i + \frac{1}{2} (u_i^+ + u_i^-) \quad (\text{A.1})$$

466 where u_i^\pm are the displacements of the two material points on S^\pm that are related to the point X_i ,
467 contained in S^0 . Hence, defining a local Cartesian coordinate system $(\hat{e}_1, \hat{e}_2, \hat{e}_3)$ on \bar{S} , the normal and
468 tangential components of the displacement jump across the material discontinuity can be expressed
469 according to the local orientation of the midsurface.

470 Let η_1 and η_2 be curvilinear coordinates located on \bar{S} , as represented in Figure A.22 (Note that the
471 isoparametric representation of the physical space is reduced to the interfacial element midsurface).
472 Then, two vectors tangential to the deformed midsurface are established as:

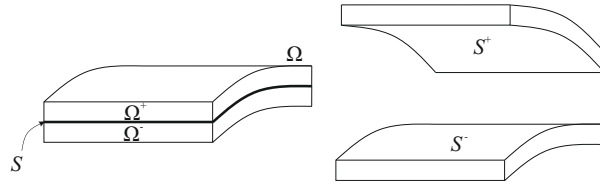


Figure A.21: Interfacial surface, S , traversing a body, Ω , and diving it into Ω^+ and Ω^- subdomains. The exploded view shows the upper S^+ and lower S^- surfaces that bound into S .

$$\mathbf{e}'_1 = \frac{\partial \bar{x}_i}{\partial \eta_1} \quad \mathbf{e}'_2 = \frac{\partial \bar{x}_i}{\partial \eta_2} \quad (\text{A.2})$$

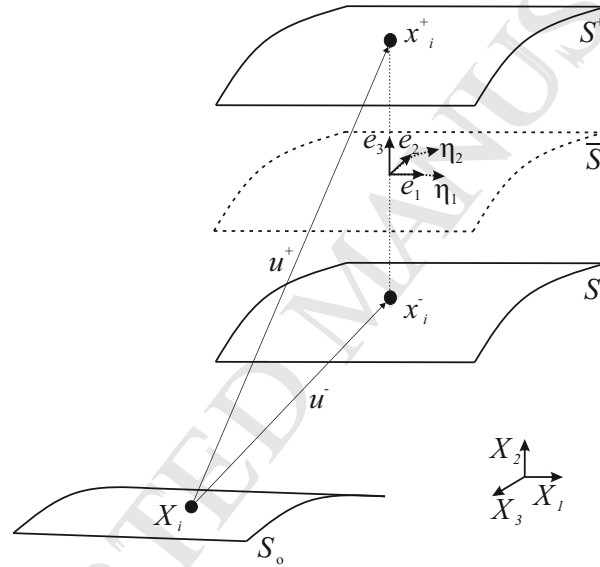


Figure A.22: Description of the deformed element midsurface, \bar{S} .

473 The direction cosines of the local Cartesian coordinate system, are the normal, $\hat{\mathbf{e}}_3$, and tangential,
474 $\hat{\mathbf{e}}_1$ and $\hat{\mathbf{e}}_2$, unit vectors to \bar{S} , and can be derived from the Equation (A.2) as follows:

$$\hat{\mathbf{e}}_1 = \frac{\mathbf{e}'_1}{|\mathbf{e}'_1|} \quad \hat{\mathbf{e}}_3 = \frac{\mathbf{e}'_1 \times \mathbf{e}'_2}{|\mathbf{e}'_1 \times \mathbf{e}'_2|} \quad \hat{\mathbf{e}}_2 = \hat{\mathbf{e}}_3 \times \hat{\mathbf{e}}_1 \quad (\text{A.3})$$

475 Finally, the displacement jump in local coordinates can be expressed in terms of the displacement
476 field:

$$\delta_j = \Theta_{ji} (u_i^+ - u_i^-), \quad i, j = 1, 2, 3 \quad (\text{A.4})$$

477 where $(u_i^+ - u_i^-)$ is the separation of two initially coinciding points at the interface in the global
 478 Cartesian coordinate system, and Θ_{ji} is the transformation tensor that relates the global to the local
 479 coordinate system,

$$\Theta = [\hat{e}_1, \hat{e}_2, \hat{e}_3]^T \quad (\text{A.5})$$

480 *Appendix A.2. Constitutive model*

481 The constitutive relation between the displacement jumps, δ_j , and the tractions between crack
 482 faces, τ_j , is defined as

$$\begin{aligned} \tau_j &= (1 - \mathcal{D}^K) K \delta_j \quad \text{for } j = 1, 2 \\ \tau_3 &= (1 - \mathcal{D}^K) K \delta_3 - \mathcal{D}^K K \langle -\delta_3 \rangle \end{aligned} \quad (\text{A.6})$$

483 where $\mathcal{D}^K \in [0, 1]$ is a scalar damage parameter reducing the initial constitutive tangent stiffness, K
 484 and $\langle \cdot \rangle$ are the Macaulay brackets defined as $\langle x \rangle = (x + |x|)$. Note that, as interpenetration of crack
 485 faces is physically prevented by contact, negative normal opening values are avoided.

486 The evolution of the stiffness degrading damage variable, \mathcal{D}^K is governed by an equivalent one-
 487 dimensional cohesive law and a damage criterion. For the formulation of this equivalent one-dimensional
 488 cohesive law, and so that different stages of the degrading process can be compared under changing
 489 mixed-mode loading conditions, a non-negative scalar displacement jump is defined:

$$\lambda = \sqrt{(\delta_I)^2 + (\delta_s)^2} \quad (\text{A.7})$$

490 where δ_I is the mode I opening, associated to the displacement jump in the normal direction to the

491 midsurface, and δ_s is the shear sliding resulting of the displacement jumps in the tangential directions
492 to the midsurface.

$$\delta_I = \langle \delta_3 \rangle, \quad \delta_s = \sqrt{(\delta_1)^2 + (\delta_2)^2} \quad (\text{A.8})$$

493 Note that the two tangential (orthogonal among each other) displacement jumps, δ_1 and δ_2 , are
494 reduced to an equivalent shear displacement jump, δ_s . It is worth to mention that this is due to the
495 incapability of the original formulation [15, 17] to distinguish into modes II and III, mainly attributed
496 to the hitherto lack of computationally-efficient crack front tracking algorithms, and not supported by
497 any physical evidence. In any event, shear opening mode is, conservatively, treated as mode II in the
498 present constitutive model.

499 The equivalent one-dimensional interface traction is related to the equivalent one-dimensional dis-
500 placement jump with

$$\mu = (1 - \mathcal{D}^K) K \lambda \quad (\text{A.9})$$

501 With increasing displacement jump, the traction increases to a peak value, μ_o , corresponding to
502 the interfacial strength, and then decreases until complete decohesion. To ensure the correct energy
503 dissipation during the process of fracture, the total area under the traction-displacement jump curve
504 is set equal to the fracture toughness, \mathcal{G}_c . Both the interfacial strength and the fracture toughness are
505 material parameters that depend on the opening mode-mixity, and, together with the penalty stiffness,
506 K , define the shape of the constitutive law.

507 The local mode-mixity, B , is defined in terms of the displacement jump as:

$$B = \frac{\delta_s^2}{\delta_I^2 + \delta_s^2} \quad (\text{A.10})$$

508 and it is equivalent to the amount of total specific work related to shear mode over the entire total

509 specific work (the reader is referred to Figure 2 for an schematic representation of the total specific
510 work of the interface).

511 The critical energy release rate, \mathcal{G}_c , for a given mode-mixity is determined using the expression
512 proposed in [25],

$$\mathcal{G}_c = \mathcal{G}_{Ic} + (\mathcal{G}_{IIc} - \mathcal{G}_{Ic}) B^\eta \quad (\text{A.11})$$

513 where subscripts I and II denote the pure modes I and II values, respectively, and η is an experi-
514 mentally determined mode interaction parameter. Similarly, the interfacial strength, μ_o , for a given
515 mode-mixity is defined as

$$\mu_o = \sqrt{(\tau_{Io})^2 + [(\tau_{IIo} - \tau_{Io})] B^\eta} \quad (\text{A.12})$$

516 In terms of the displacement jump, the onset, λ_o , and propagation, λ_c , of delamination are related
517 to the parameters of the cohesive law:

$$\lambda_o = \frac{\mu_o}{K}, \quad \lambda_c = \frac{2\mathcal{G}_c}{\mu_o} \quad (\text{A.13})$$

518 The damage criterion is formulated ensuring damage irreversibility, such that the damage variable
519 at the current time t_c determined as

$$\mathcal{D}^K = \min \left(\max \left(0, \frac{\lambda_c^t (\lambda^t - \lambda_o^t)}{\lambda^t (\lambda_c^t - \lambda_o^t)} \right), 1 \right) \quad \forall t \in [0, t_c] \quad (\text{A.14})$$

520 Thus, the mixed-mode displacement jump associated to the current damage state is

$$\lambda_{\mathcal{D}} = \frac{\lambda_o \lambda_c}{\lambda_c - \mathcal{D}^K (\lambda_c - \lambda_o)} \quad (\text{A.15})$$

521 The stiffness degrading damage variable, \mathcal{D}^K , is strongly nonlinear in terms of $\lambda_{\mathcal{D}}$. This might
522 hinder the performance of the numerical method [21]. Conversely, an energy-based damage variable,

523 which exhibits linear dependency with $\lambda_{\mathcal{D}}$, is defined in [17] and [21] as the specific dissipated energy
 524 due to fracture over the fracture toughness during degradation ($\lambda_o < \lambda_{\mathcal{D}} < \lambda_c$):

$$\left\{ \begin{array}{ll} \mathcal{D}^e = 0 & \text{for } \lambda_{\mathcal{D}} \leq \lambda_o \\ \mathcal{D}^e = \frac{\omega_d}{\mathcal{G}_c} & \text{for } \lambda_o \leq \lambda_{\mathcal{D}} \leq \lambda_c \\ \mathcal{D}^e = 1 & \text{for } \lambda_{\mathcal{D}} \geq \lambda_c \end{array} \right. \quad (\text{A.16})$$

525 where ω_d is, in terms of the displacement jump is given as:

$$\omega_d = \max \left\{ 0, \frac{1}{2} K \lambda_o \lambda_c \frac{\lambda_o - \lambda_{\mathcal{D}}}{\lambda_o - \lambda_c} \right\} \quad (\text{A.17})$$

526 Finally, the total specific work associated to the current damage state can also be determined in
 527 terms of the displacement jump:

$$\omega_{tot} = \frac{1}{2} K \lambda_o \left(\lambda_c - \frac{(\lambda_c - \lambda_{\mathcal{D}})^2}{\lambda_c - \lambda_o} \right) \quad (\text{A.18})$$

528 Note that, during crack propagation, the μ - λ relation follows the equivalent one-dimensional cohe-
 529 sive law, i.e.:

$$\lambda_{\mathcal{D}} = \lambda \quad (\text{A.19})$$

530 and that before damage initiation, the no energy is dissipated yet and the total specific work corre-
 531 sponds to the specific elastic energy:

$$\omega_{tot} = \frac{1}{2} K \lambda^2 \quad (\text{A.20})$$

532 *Appendix A.3. Finite element implementation*

533 The three dimensional crack propagation problem is discretized here using the FE method. The
 534 cohesive interface is implemented into an eight-noded zero-thickness element. This interface element

535 is compatible with three dimensional continuum elements that may form the upper and lower part of
536 the body containing the singularity.

537 The nodal coordinates of the undeformed interface element are arranged in vector \mathbf{C} in such a way
538 that:

$$\mathbf{C} = \{\mathbf{C}^-, \mathbf{C}^+\} \quad (\text{A.21})$$

539 being $\mathbf{C}_k^- = \{X_1^1, X_2^1, X_3^1, \dots, X_1^4, X_2^4, X_3^4\}^T$ and $\mathbf{C}_k^+ = \{X_1^5, X_2^5, X_3^5, \dots, X_1^8, X_2^8, X_3^8\}^T$ the global co-
540 ordinates of the nodes at the lower and upper interfaces, respectively, where X_i^n is the i -th coordinate
541 of the n -th node.

542 The nodal displacements, relative to the global coordinates, are arranged in vector \mathbf{Q} similarly to the
543 nodal coordinates, i.e. the nodal displacements of the lower interface, $\mathbf{Q}_k^- = \{u_1^1, u_2^1, u_3^1, \dots, u_1^4, u_2^4, u_3^4\}^T$,
544 are numbered first, and the nodal displacements of the upper interface, $\mathbf{Q}_k^+ = \{u_1^5, u_2^5, u_3^5, \dots, u_1^8, u_2^8, u_3^8\}^T$,
545 are numbered second,

$$\mathbf{Q} = \{\mathbf{Q}^-, \mathbf{Q}^+\} \quad (\text{A.22})$$

546 The material coordinates and the displacement field are interpolated within the domain of the
547 surface element using isoparametric bilinear shape functions,

$$\begin{aligned} L_1 &= \frac{1}{2}(1 - \eta_1)(1 - \eta_2); & L_2 &= \frac{1}{2}(1 + \eta_1)(1 - \eta_2) \\ L_3 &= \frac{1}{2}(1 + \eta_1)(1 + \eta_2); & L_4 &= \frac{1}{2}(1 - \eta_1)(1 + \eta_2) \end{aligned} \quad (\text{A.23})$$

548 organized in matrix the shape function matrix, N_{ik} , as follows:

$$N_{ik} = \begin{bmatrix} L_1 & 0 & 0 & L_2 & 0 & 0 & L_3 & 0 & 0 & L_4 & 0 & 0 \\ 0 & L_1 & 0 & 0 & L_2 & 0 & 0 & L_3 & 0 & 0 & L_4 & 0 \\ 0 & 0 & L_1 & 0 & 0 & L_2 & 0 & 0 & L_3 & 0 & 0 & L_4 \end{bmatrix} \quad (\text{A.24})$$

549 According to Equation (A.1) and making use of equations (A.21)-(A.24), the coordinates of the
550 interfacial deformed midsurface are:

$$\bar{x}_i = \frac{1}{2} N_{ik} (C_k^+ + C_k^- + Q_k^+ + Q_k^-) \quad (\text{A.25})$$

551 The tangential vectors to the interfacial midsurface at (η_1, η_2) , defined in Equation (A.2), are now
552 arranged in the Jacobian matrix,

$$\mathbf{J} = [\mathbf{e}'_1, \mathbf{e}'_2] \quad \text{where} \quad J_{i\alpha} = \frac{1}{2} \frac{\partial N_{ik}}{\partial \eta_\alpha} (C_k^+ + C_k^- + Q_k^+ + Q_k^-) \quad (\text{A.26})$$

553 where the subscript $\alpha = 1, 2$.

554 Hence, the unit vectors, $\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3$, corresponding to the direction cosines of the local Cartesian
555 coordinate system, can be derived from $J_{i\alpha}$ following equation (A.3).

556 Finally, the transformation matrix, M_{im} , computes the displacement jump in global coordinates of
557 two initially coinciding points from the nodal global displacement vector:

$$u_i^+ - u_i^- = M_{im} Q_m \quad (\text{A.27})$$

558 where subscript m runs from 1 to the number of degrees of freedom of the element ($m = 1 \dots 24$) and
559 M_{im} is defined as:

$$M_{im} = [-N_{ik} \ N_{ik}] \quad (\text{A.28})$$

560 Thus, from Equation (A.4), the displacement jump in local coordinates reads:

$$\delta_j = \Theta_{ji} M_{im} Q_m \quad (\text{A.29})$$

561 For the sake of simplicity, only the derivation of the displacement jump field is depicted above,
562 as the only field needed for the resolution of the criteria presented in section 2.2. See [15] for the
563 derivation of the interface element tangent stiffness matrix, \mathbf{K} , and internal force vector, $^{int}\mathbf{f}$ required
564 in the nonlinear solution procedure.

565 Appendix B. Development of the criteria to determine the growth driving direction

566 The formulation of the three proposed criteria in section 2.2 to determine the growth driving
567 direction is synthesized in Table B.5. The equations to solve for Criterion 1 are found by introducing
568 equations (B.2) and (B.3) in equations (B.1) and (B.4) and computing the radial slopes of the mixed-
569 mode displacement jump, $\frac{\partial\lambda}{\partial\rho}$, and mode-mixity, $\frac{\partial B}{\partial\rho}$. On the other hand, the equations for Criterion
570 2 are found by introducing equations (B.6) and (B.7) in equations (B.5) and (B.8). Also the radial
571 slopes of the mixed-mode displacement jump, $\frac{\partial\lambda}{\partial\rho}$, and mode-mixity, $\frac{\partial B}{\partial\rho}$, are required. Finally, for the
572 evaluation of Criterion 3 only the slope of the mixed-mode displacement jump in the radial direction,
573 $\frac{\partial\lambda}{\partial\rho}$, is needed (see equations (B.9) and (B.10)).

574 Moreover, in this work, the criteria are applied to the CZM presented in [15, 17] to exemplify their
575 capabilities. In this particular case, the factors F_B and F_λ are reduced to equations (B.11) and (B.12),
576 for Criterion 1, and reduced to equations (B.13) and (B.14), for Criterion 2. Equations (B.11) and
577 (B.12) are obtained by introducing equations (B.15)-(B.24) into equations (B.2) and (B.3). Equations
578 (B.13) and (B.14) are obtained by introducing equations (B.15)-(B.19) and (B.25)-(B.29) into equations
579 (B.6) and (B.7). Also, the derivation of the radial slopes of the mixed-mode displacement jump and
580 mode-mixity, $\frac{\partial\lambda}{\partial\rho}$ and $\frac{\partial B}{\partial\rho}$, after the particular application to the CZM from [15, 17] is detailed in section
581 2.3.

| Criterion ID | Functions to solve | F_B | F_λ |
|--------------|---|---|--|
| 1 | $\frac{\partial \mathcal{D}^e}{\partial \varphi} \frac{\partial \rho}{\partial \rho} = \frac{\partial}{\partial \varphi} \left(F_B \frac{\partial B}{\partial \rho} + F_\lambda \frac{\partial \lambda}{\partial \rho} \right) = 0 \quad (\text{B.1})$ $\frac{\partial^2 \mathcal{D}^e}{\partial \varphi^2} \frac{\partial \rho}{\partial \rho} = \frac{\partial^2}{\partial \varphi^2} \left(F_B \frac{\partial B}{\partial \rho} + F_\lambda \frac{\partial \lambda}{\partial \rho} \right) > 0 \quad (\text{B.4})$ | $\frac{\partial \left(\frac{\omega_d}{\mathcal{G}_c} \right)}{\partial \omega_d} \left(\frac{\partial \omega_d}{\partial \lambda_o} \frac{\partial \lambda_o}{\partial \mu_o} + \frac{\partial \omega_d}{\partial \lambda_c} \frac{\partial \lambda_c}{\partial \mu_o} \right) \frac{\partial \mu_o}{\partial B} + \left(\frac{\partial \left(\frac{\omega_d}{\mathcal{G}_c} \right)}{\partial \omega_d} \frac{\partial \omega_d}{\partial \lambda_c} + \frac{\partial \left(\frac{\omega_d}{\mathcal{G}_c} \right)}{\partial \mathcal{G}_c} \right) \frac{\partial \mathcal{G}_c}{\partial B} \quad (\text{B.2})$ | $\frac{\partial \left(\frac{\omega_d}{\mathcal{G}_c} \right)}{\partial \omega_d} \frac{\partial \omega_d}{\partial \lambda} \quad (\text{B.3})$ |
| 2 | $\frac{\partial}{\partial \varphi} \frac{\partial \left(\frac{\omega_{tot}}{\mathcal{G}_c} \right)}{\partial \rho} = \frac{\partial}{\partial \varphi} \left(F_B \frac{\partial B}{\partial \rho} + F_\lambda \frac{\partial \lambda}{\partial \rho} \right) = 0 \quad (\text{B.5})$ $\frac{\partial^2}{\partial \varphi^2} \frac{\partial \left(\frac{\omega_{tot}}{\mathcal{G}_c} \right)}{\partial \rho} = \frac{\partial^2}{\partial \varphi^2} \left(F_B \frac{\partial B}{\partial \rho} + F_\lambda \frac{\partial \lambda}{\partial \rho} \right) > 0 \quad (\text{B.8})$ | $\frac{\partial \left(\frac{\omega_{tot}}{\mathcal{G}_c} \right)}{\partial \omega_{tot}} \left(\frac{\partial \omega_{tot}}{\partial \lambda_o} \frac{\partial \lambda_o}{\partial \mu_o} + \frac{\partial \omega_{tot}}{\partial \lambda_c} \frac{\partial \lambda_c}{\partial \mu_o} \right) \frac{\partial \mu_o}{\partial B} + \left(\frac{\partial \left(\frac{\omega_{tot}}{\mathcal{G}_c} \right)}{\partial \omega_{tot}} \frac{\partial \omega_{tot}}{\partial \lambda_c} + \frac{\partial \left(\frac{\omega_{tot}}{\mathcal{G}_c} \right)}{\partial \mathcal{G}_c} \right) \frac{\partial \mathcal{G}_c}{\partial B} \quad (\text{B.6})$ | $\frac{\partial \left(\frac{\omega_{tot}}{\mathcal{G}_c} \right)}{\partial \omega_{tot}} \frac{\partial \omega_{tot}}{\partial \lambda} \quad (\text{B.7})$ |
| 3 | $\frac{\partial}{\partial \varphi} \frac{\partial \lambda}{\partial \rho} = 0 \quad (\text{B.9})$ $\frac{\partial^2}{\partial \varphi^2} \frac{\partial \lambda}{\partial \rho} > 0 \quad (\text{B.10})$ | — | — |

Table B.5: Equations to solve for each criteria to determine the growth driving direction, φ .

| Criterion ID | F_B | | F_λ | |
|--------------|--|--------|--|--------|
| 1 | $\frac{\eta(\mathcal{G}_{IIc} - \mathcal{G}_{Ic}) B^{(\eta-1)} \lambda}{K \lambda_c \lambda_o (\lambda_o - \lambda_c)}$ | (B.11) | $\frac{1}{\lambda_c - \lambda_o}$ | (B.12) |
| 2 | $\frac{2\eta(\mathcal{G}_{IIc} - \mathcal{G}_{Ic}) B^{(\eta-1)} \lambda (\lambda_c - \lambda)}{K \lambda_c^2 \lambda_o (\lambda_o - \lambda_c)}$ | (B.13) | $\frac{2(\lambda_c - \lambda)}{\lambda_c (\lambda_c - \lambda_o)}$ | (B.14) |

Table B.6: Expressions for the factors F_B and F_λ after application of the CZM formulation presented in [15, 17].

| Dependencies | Partial derivatives | |
|---|---|--------|
| $\lambda_o(\mu_o)$ | $\frac{\partial \lambda_o}{\partial \mu_o} = \frac{1}{K}$ | (B.15) |
| $\lambda_c(\mu_o, \mathcal{G}_c)$ | $\frac{\partial \lambda_c}{\partial \mu_o} = -\frac{2\mathcal{G}_c}{\mu_o^2}$ | (B.16) |
| | $\frac{\partial \lambda_c}{\partial \mathcal{G}_c} = \frac{2}{\mu_o}$ | (B.17) |
| $\mu_o(B)$ | $\frac{\partial \mu_o}{\partial B} = \frac{\eta(\tau_{IIo}^2 - \tau_{Io}^2) B^{\eta-1}}{2\mu_o}$ | (B.18) |
| $\mathcal{G}_c(B)$ | $\frac{\partial \mathcal{G}_c}{\partial B} = \eta(\mathcal{G}_{IIc} - \mathcal{G}_{Ic}) B^{\eta-1}$ | (B.19) |
| $\omega_d(\lambda_o, \lambda_c, \lambda)$ | $\frac{\partial \omega_d}{\partial \lambda_o} = \frac{1}{2} K \lambda_c \frac{\lambda_o^2 - 2\lambda_c \lambda_o + \lambda_c \lambda}{(\lambda_o - \lambda_c)^2}$ | (B.20) |
| | $\frac{\partial \omega_d}{\partial \lambda_c} = \frac{1}{2} K \lambda_o^2 \frac{\lambda_o - \lambda}{(\lambda_o - \lambda_c)^2}$ | (B.21) |
| | $\frac{\partial \omega_d}{\partial \lambda} = \frac{1}{2} K \lambda_o \lambda_c \frac{1}{(\lambda_c - \lambda_o)}$ | (B.22) |
| $\mathcal{D}^e(\omega_d, \mathcal{G}_c)$ | $\frac{\partial \left(\frac{\omega_d}{\mathcal{G}_c}\right)}{\partial \omega_d} = \frac{1}{\mathcal{G}_c}$ | (B.23) |
| | $\frac{\partial \left(\frac{\omega_d}{\mathcal{G}_c}\right)}{\partial \mathcal{G}_c} = \frac{-\omega_d}{\mathcal{G}_c^2}$ | (B.24) |
| $\omega_{tot}(\lambda_o, \lambda_c, \lambda)$ | $\frac{\partial \omega_{tot}}{\partial \lambda_o} = \frac{1}{2} K \lambda_c (\lambda_o - \lambda) \frac{\lambda - 2\lambda_c + \lambda_o}{(\lambda_o - \lambda_c)^2}$ | (B.25) |
| | $\frac{\partial \omega_{tot}}{\partial \lambda_c} = \frac{1}{2} K \lambda_o \frac{(\lambda_o - \lambda)^2}{(\lambda_o - \lambda_c)^2}$ | (B.26) |
| | $\frac{\partial \omega_{tot}}{\partial \lambda} = K \lambda_o \frac{\lambda_c - \lambda}{\lambda_c - \lambda_o}$ | (B.27) |
| $\frac{\omega_{tot}}{\mathcal{G}_c}(\omega_{tot}, \mathcal{G}_c)$ | $\frac{\partial \left(\frac{\omega_{tot}}{\mathcal{G}_c}\right)}{\partial \omega_{tot}} = \frac{1}{\mathcal{G}_c}$ | (B.28) |
| | $\frac{\partial \left(\frac{\omega_{tot}}{\mathcal{G}_c}\right)}{\partial \mathcal{G}_c} = \frac{-\omega_{tot}}{\mathcal{G}_c^2}$ | (B.29) |

Table B.7: Dependencies and partial derivatives of the variables in the system using the CZM presented in [15, 17].

Highlights:

- The concept of growth driving direction for cohesive zone models is introduced.
- The growth driving direction is normal to the damage isolines.
- A point-wise criterion to predict the growth driving direction is formulated.
- Three different alternatives of the criterion are presented and discussed.
- The developed criteria can be applied to general 3D structures.