In-depth numerical analysis of the TDCB specimen for characterization of self-healing polymers

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Abstract. The Tapered Double Cantilever Beam (TDCB) is the common specimen to study self-healing thermosetting polymers. While this geometry allows characterizing the mode I fracture toughness without taking into account the crack length, the experiments show an important dispersion and unstable behaviour that must be taken into account to obtain accurate results. In this paper, finite element simulations have been used to understand the experimental behaviour. Static simulations with a
stationary crack give the local stresses and the stress intensity factors at the crack tip when the TDCB is under load. In addition, the eXtendend Finite Element Method (XFEM) has been used to make quasi-static crack propagation simulations. The results indicate that the crack tip has a curved profile during the propagation, advancing more at the edges than at the centre. The crack propagation begins when the applied load reaches a critical value. The unstable crack propagation noted in the experiments can be reproduced by introducing an unstable behaviour in the simulations. Finally, the sensitivity of the critical load has been studied as a function of the friction between pin and hole, tolerance of geometrical dimensions, and cracks out of the symmetric plane. The results can partially explain the dispersion of the experimental data.

1 Introduction

Self-healing polymers have the additional ability of recovering the structural properties with or without external aid (White et al., 2001). This ability is an advantage for structural polymers that are susceptible to suffer mechanical degradation due to damage in form of cracks. Self-healing polymers open a window to new structural materials such as self-healing composites. The study of self-healing polymers is the first step to approach such self-healing composites.

There are several self-healing concepts for polymers (Billiet et al., 2013; Y. C. Yuan et al., 2008). On the one hand, there are intrinsic self-healing polymers based on a matrix that can repair damage due to cracks by itself under a certain stimulation (Jud et al., 1981; Jud and Kausch, 1979; Meure et al., 2009; Raghavan and Wool, 1999), mostly heating. Currently,
most of these self-healing polymers cannot heal themselves without an external intervention. On the other hand, there are extrinsic self-healing polymers that have a healing agent embedded or encapsulated which is responsible for the repair (Toohey et al., 2007; White et al., 2001). The healing agent can be embedded into tubes making a vascular network or encapsulated in capsules. The size of these tubes or capsules can be of the order of microns. When the cracks break the tubes or capsules, the healing agent is released in the crack plane. In this case, the self-healing polymer usually does not need an external aid to repair the damage because there is a chemical trigger in the system. Consequently, the released healing agent in the crack plane is polymerized when coming into contact with the chemical trigger, and the structural integrity across the crack plane is re-established. They can be considered autonomous self-healing polymers.

This study deals with autonomous micro-encapsulated polymers. In these systems, the liquid healing agent is encapsulated in microcapsules which are dispersed in the polymer, and the chemical trigger can be found in solid state embedded inside the matrix (Blaiszik et al., 2008; Brown et al., 2005, 2002; White et al., 2001), or in liquid state encapsulated in a second sort of microcapsules (Yan Chao Yuan et al., 2008; Yuan et al., 2009). This second system with two types of microcapsules makes it possible to use a huge amount of click reactions in the design of self-healing polymers (Billiet et al., 2012; Hillewaere et al., 2014).

The studies about micro-encapsulated self-healing polymers evaluate self-repair by comparison of the final mechanical properties of the healed polymer and the initial properties of the virgin one (Wool, 1981). The most common value to quantify the self-healing performance is the ratio between the healed and virgin fracture toughness. Therefore, healing efficiency is defined as $\eta = \frac{K_{IC}^{healed}}{K_{IC}^{virgin}}$ (White et al., 2001). Several works employ a
Tapered Double Cantilever Beam (TDCB) fracture geometry to simplify the measurement of the healing efficiency (Brown et al., 2002, 2004, 2005; Rule et al., 2007; Brown, 2011). In the TDCB geometry, the fracture toughness is independent of the crack length $a$ and proportional to the critical load $P_C$ (Mostovoy et al., 1967), which triggers the crack growth. Then, the fracture toughness can be written as $K_{IC} = \alpha \cdot P_C$, where $\alpha$ is a constant obtained from the geometry and the material properties, and the healing efficiency is determined by the ratio of the critical loads, $\eta = \frac{P_{C_{\text{healed}}}}{P_{C_{\text{virgin}}}}$.

The TDCB geometry, adapted to simplify the study of self-healing polymers, is useful to obtain the healing efficiency, but several details must be taken into account to obtain accurate values. In addition, the limited fracture information extracted from the TDCB highlights the demand for other experimental geometries that may complete the characterization of the self-healing polymers. An accurate value of the fracture toughness and fracture energy can be obtained from the compact tension fracture test for plastic materials (ASTM Standard D 5045). In addition, tensile properties, such as Young’s modulus, Poisson’s ratio, yield strength and ultimate tensile strength, can be measured from the tensile test for plastic materials (ASTM Standard D 638).

The current paper focuses on the response of the TDCB specimen applied to study the healing performance of micro-encapsulated thermosetting polymers. We use the Finite Element Method (FEM) combined with recent techniques to follow the crack propagation based on eXtended Finite Element Method (XFEM). The commercial software ABAQUS has implemented this methodology. Simulations show in detail how the mechanical failure is produced in the TDCB experiments, giving information about the critical force, crack profile and the local stress intensity factor. First, we describe the TDCB specimen and the model in
detail. Then, the results from the simulations are explained and compared with experimental values. Finally, the effect of the geometry dimensions and boundary conditions has been studied.

2 TDCB specimen

2.1 Geometry

Although the TDCB geometry is described in several papers, we have taken the dimensions used by Brown et al. for samples with EPON 828 (Brown, 2011; Brown et al., 2004, 2002). Figure 1a shows the geometry and the dimensions. We have fixed the radius of the pin holes to 6 mm and the radius of the fillet edges to 2 mm. This geometry fits White’s protocol (White et al., 2001) to determine the healing efficiency.

The TDCB geometry is defined by the thickness $b$ and the height profile $h(a)$. The height profile of the geometry is designed so that the mode I fracture toughness $K_I$ is constant in the range of the crack length $a$ between 20 and 40 mm (Brown, 2011). Therefore, $K_I$ is linear with the load applied between the pins. This is possible because the change in compliance with respect to the crack length remains constant (Mostovoy et al., 1967). The differences between TDCB and other geometries have been fully discussed by Brown et al. (Brown, 2011). The crack propagation behaviour with constant compliance is shown in the experiments and it can be reproduced with the simulation as we show in the next section.
Figure 1. (a) TDCB geometry and dimensions, (b) detail of the horizontal plane, side grooves and symmetric planes ($xOz$ and $xOy$).

It is important to notice that two grooves along the horizontal plane $xOz$ were added to prevent the crack from changing its direction. The final thickness of the crack plane $b_n$ is lower than the thickness of the sample $b$ (see the detail of grooves in figure 1b). In order to define the geometry of the grooves, we have fixed an angle of $45^\circ$ for the side grooves and the two thicknesses, $b$ and $b_n$.

We have included an extra dimension in the geometry of the TDCB that has been neglected in previous works (Brown, 2011; Brown et al., 2004; White et al., 2001). This is a small height, $d_n$, in the horizontal plane (see figure 1b). One reason to introduce this dimension is that the real TDCB specimen always has a rounded end in the side of the grooves. Modelling these edges with a certain height $d_n$ is more realistic than a sharp geometry. In addition from the numerical point of view, the height $d_n$ is twofold: allows us to discretize the volume more easily and prevents numerical singularities.
It is needed to define a pre-crack in the geometry of the TDCB specimen to complete White’s protocol. The pre-crack is located in the horizontal plane $xOz$ with a length between 2 to 5 mm. In the experiments the pre-crack is performed by manually tapping with a razor. We have observed that the experimental results are strongly dependent on the performed pre-crack (Tsangouri et al., under submission). In section 5, we will discuss this issue and its sensitivity.

2.2 Material properties

In the present work we have used the epoxy EPON 828. This epoxy is well known in the aerospace industry and is fully characterized in the reference (Brown et al., 2004). It is noteworthy that EPON 828 has been used in several studies of self-healing polymers with micro-capsules (Brown et al., 2006, 2005, 2004, 2002; White et al., 2001). The EPON 828 resin and diethylenetri-amine (DETA) hardener are mixed in equimolar distribution (100/11 w/w ratio epoxy/hardener). The usual curing program is 24 h at room temperature and 24 h at 40 °C (Billiet et al., 2013). In this work we will consider EPON 828 as brittle material without plastic behaviour (see properties in Table 1). Because of the brittle behaviour of the polymer, we assume that the yield strength and the ultimate tensile strength are equal, $\sigma_Y = \sigma_{UT}$. 
Table 1. Properties of EPON 828. $E = $ Young’s modulus, $\nu = $ Poisson’s ratio, $\sigma_Y = $ yield strength, $\sigma_{UT} = $ ultimate tensile strength, $K_{IC} = $ fracture toughness, $G_{IC} = $ fracture energy, $\rho = $ density, $r_p = $ radius of plastic zone.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$ (MPa)</td>
<td>3400</td>
</tr>
<tr>
<td>$\nu$</td>
<td>0.38</td>
</tr>
<tr>
<td>$\sigma_Y = \sigma_{UT}$ (MPa)</td>
<td>39</td>
</tr>
<tr>
<td>$K_{IC}$ (MPa m$^{1/2}$)</td>
<td>0.55</td>
</tr>
<tr>
<td>$G_{IC}$ (N/m)</td>
<td>76</td>
</tr>
<tr>
<td>$\rho$ (Kg/m$^3$)</td>
<td>1160</td>
</tr>
<tr>
<td>$r_p$ ($\mu$m)</td>
<td>32</td>
</tr>
</tbody>
</table>

In addition to the epoxy properties, we have included the first order radius of the plastic zone around the crack tip, obtained from

$$r_p = \frac{1}{2\pi} \left( \frac{K_{IC}}{\sigma_Y} \right)^2$$  \hspace{1cm} (1)

where $K_{IC}$ is the mode I fracture toughness and $\sigma_Y$ the yield strength. The radius of the plastic zone $r_p$ has been used to find the correct size of the mesh elements along the crack plane and it is further discussed in the next section with the results of the model.

2.3 Experimental setup
The setup of the experiment with the TDCB specimen is described in references (Brown et al., 2004, 2002).

The specimen is supported by two pins inside each hole. Each pin allows free rotation along its rotational axis. During the experiment, a constant vertical displacement is applied in the upper pin while the lower pin is fixed. As a result, the crack propagates along the horizontal plane defined by the grooves. The reaction force and displacement in the upper pin is recorded during the experiment to obtain load-displacement curves. Then, the critical load $P_C$ can be obtained from the curves.

2.4 Model

The model has been built in ABAQUS® commercial software, version 6.13.1. Dimensions and displacements are in mm, stresses in MPa and force in N. We have assumed quasi-static hypothesis in our models.

The TDCB geometry has been divided in three parts (see figure 2). The upper and lower parts are located symmetrical with plane $xOz$ (see figure 1b). The central part will contain the crack. This latter part is connected with the upper and lower parts using tie constraints which allow continuity in displacements between the surfaces in contact.
Figure 2. TDCB sample geometry with parts in different colours. Beam constraints between the centres of each hole with the defined surface are used to model the pin contacts.

It is important to reproduce the real boundary conditions to obtain a good agreement with the experimental data. In the model, the pins are modelled with reference points located in the centre of each hole. Then, the contact between the pins and the internal surface of the holes has been modelled using beam constraints between the reference points and a certain area of the internal surface of the hole. In the upper hole, only the upper quarter of the surface is connected to the upper reference point, where the real pin will make contact (see figure 2). For the bottom hole, it is the bottom quarter of the surface which is connected to the reference point of this hole. We have not modelled the pins as rigid bodies to avoid the contact problem, which requires a finer mesh around the holes and increases the computational cost. The friction between pins and holes has been studied in section 5.

In this study we have used two different types of simulations: (i) static simulation with a stationary crack; and (ii) quasi-static crack propagation. Stress intensity factors have been studied with the static simulation, while load-displacement behaviour has been tackled with
quasi-static crack propagation. Although each simulation has a different objective, the geometry, mesh and boundary conditions have been built taking into account the compatibility between the results.

In the case of static simulations, the crack is defined in the geometry at the initial step. The crack plane is introduced as a partition in the central part, and it is defined as a seam crack. This means that the nodes at the crack plane are duplicated and two new surfaces are defined. The new surfaces are the lips of the crack, and they are joined at the tip. Around the crack tip an annular mesh with wedge elements is created using the sweep technique (see figure 3a). Therefore, degenerate elements are disposed around the crack tip to include the singular solution of linear elastic fracture mechanics. The stress intensity factors also require the direction of crack propagation along the positive X axis. The central part is built with linear hexahedral elements (C3D8 in ABAQUS designation), while quadratic hexahedral elements (C3D20) are used in the upper and lower parts.
Figure 3. Detail of the central part for each model: (a) static simulation crack tip with seam crack and wedge element shape around the tip; (b) quasi-static crack propagation mesh with pre-crack in XFEM model.

Several partitions have been made to locate smaller elements around the crack tip. We have defined the number of nodes in each edge of the geometry to describe completely the mesh in each part. In the static simulation, a mesh of 139720 elements and 197853 nodes has been
used. The mesh has two planes of symmetry corresponding with the planes $xOz$ and $xOy$ (see figure 1b).

In order to reproduce the experiment, the bottom reference point is fixed in displacement but is free to rotate around the $Z$ axis, while we applied a punctual force at the upper reference point in $Y$ positive direction (see $Pe$ in figure 2). Finally, to avoid movement around the $Y$ axis, the external points of the upper and lower parts have been fixed in $Z$ direction.

In the case of quasi-static crack propagation, the same geometry and parts have been used (see figure 2). In this case, the central part is enriched with XFEM elements and a pre-crack is located as an extra part (see figure 3b). There is no crack front singularity in the formulation of XFEM elements in ABAQUS. The crack propagation can be simulated using two different damage models, the cohesive damage or the Virtual Crack Closure Technique (VCCT). In the first model, XFEM-COHE, the cohesive damage with the criterion of maximum tensile stress has been applied to the XFEM elements. The results with this methodology depend strongly on the element size. In section 3, it is shown that the size of the elements must be small enough to obtain convergence in the solution. Due to this limitation, we have also used a second model where VCCT behaviour for crack propagation is applied to the XFEM elements. In this second model, XFEM-VCCT, the mesh dependency is lower than in the case of cohesive damage.

All the elements in the three parts are linear hexahedral elements (C3D8 in ABAQUS designation), which are compatible with XFEM enrichment. Several partitions have been made to locate smaller elements along the expected crack path. Four different refinements have been used in the central part to guarantee that the solution is independent of the mesh.
The coarse mesh in the central part is called mesh $rp4$ with 35360 elements. The smaller elements along the crack path have a size of 0.13 mm which is 4 times $r_p$. The mesh $rp3$ with 53960 elements has elements with 3 times $r_p$ size along the crack path. The mesh $rp2$ has 129600 elements and element size of 2 times $r_p$, 0.064 mm. And the finest mesh is mesh $rp1$ with 212400 elements and element size of $r_p = 0.032$ mm. The upper and lower parts have 11664 elements each.

In the case of quasi-static propagation, the bottom reference point is again fixed in displacement and free to rotate around the Z axis, while we applied a continuous displacement at the upper reference point in Y positive direction, see $U_y$ in figure 2. The rigid body movements are avoided fixing the external points of the upper and lower parts in Z direction.

### 3 Results of simulation

We have separated the results of static simulation and quasi-static crack propagation. The results of both simulations are complementary to one another and give a full description of the problem.

#### 3.1 Static simulations

In the static simulation, we apply a fixed load $P_c$ at the upper reference point, and the stress and displacement are calculated. The material behaviour is linear elastic without plastic effect or damage when the yield strength is reached. Stress intensity factors in mode I, $K_I$, are computed along the crack front.
We started with a simple crack which is located in the symmetric horizontal plane $xOz$ with a thickness $b_n = 2.5$ cm and a fixed crack length $a$ (see figure 3a). It is important to notice that the crack tip is straight and perpendicular to the direction of crack propagation $X$. $K_I$ has been calculated using the contour integrals around the front within the framework of LEFM. Figure 4 shows the $K_I$ along the crack tip for the EPON epoxy for three different crack lengths ($a = 24, 29, 33$ mm) and two loads ($P_c = 39, 49$ N) applied in the upper reference point. The value of the punctual force $P_c = 39$ N has been obtained from the quasi-static crack propagation simulation (see next section) and the value $P_c = 49$ N is from reference (Brown, 2011). The values of $K_I$ along the crack tip for $P_c = 39$ N are almost the same for the three different crack lengths (see figure 4). This result confirms that the geometry of TDCB is independent of the crack length for ranges between 20 and 40 mm. When the punctual force increases to $P_c = 49$ N, the stresses and $K_I$ increase along the crack tip. $K_I$ is higher than the fracture toughness of the material, $K_{IC} = 0.55$ MPa m$^{1/2}$, when $P_c = 49$ N. Therefore, crack propagation is expected at lower loads than the experimental values as discussed in the next section.

It is noteworthy that in all the cases the $K_I$ is higher at the edges of the crack tip due to the effects of the side grooves (Lemmens et al., 2014) (see figure 4). This indicates that the crack propagation will start at these edges. As a consequence, a curved profile of the crack tip is expected during the propagation along the symmetric plane $xOz$. The edges of the crack tip will be more advanced than the centre.
Figure 4. $K_I$ profile along the crack tip for static simulation with three crack lengths ($a = 24, 29, 33$ mm) and two applied loads ($P_c = 40, 49$ N).

The stress field around the straight crack tip gives more information about the crack propagation. Figure 5a shows the region where the Von Mises stress is higher than the yield strength, $\sigma_Y = \sigma_{UT} = 39$ MPa in brittle behaviour. The stresses into the plastic zone are fully treated as linear elastic material following LEFM. This region can be identified as the plastic zone around the crack tip under the hypothesis of LEFM. Due to the linear elastic behaviour of the material, the stresses into the plastic zone increase over the yield strength when the distance to the crack tip decreases. It is important to remark three aspects: (i) the usual shape of plane strain is observed along the crack tip except at the edges, therefore, the plane strain hypothesis is valid for the thickness geometry $b_n = 2.5$ mm; (ii) the plastic zone is larger at the edges because the stresses in $Y$ direction are concentrated due to the grooves (Yasufumi and Tomokazu, 1982); (iii) the stresses in $Z$ direction along the crack tip modify the plastic zone and introduce an out-of-plane constraint (Fernandez-Canteli et al., 2006; Giner et al., 2014).

The high value of $K_I$ reached at the edges and the large plastic zone indicates that this solution cannot be real. We need to take into account that, during the experiment, $P_c$
increases when the vertical displacement is applied continuously to the upper centre. For that reason, it is expected that $K_I$ at the edges reaches the fracture toughness when the punctual force is lower than $P_c$. At this point, the crack propagation starts at the edges and the profile of the crack tip becomes curved.

**Figure 5.** Crack tip plastic zone represented by Von Mises stress iso-surfaces with values higher than 39 MPa in static simulation, $P_c = 39$ N and $a = 23$ mm: (a) straight crack tip; (b) elliptic curved crack tip. Note: The crack propagation is from left to right in both figures.

Static simulations with elliptic curved profile of the crack tip have been made for the same applied load, $P_c = 39$ N. In these simulations, only a quarter of the geometry has been computed using the two symmetry planes, $xOz$ and $xOy$. Due to the curved profile of the crack tip, the mesh requires several partitions to obtain a regular mesh with quadratic hexahedral elements in all the geometry. **Figure 5 (b)** shows the plastic zone along the elliptic crack profile with minor axis $r_b = 1$ mm and eccentricity $e = 0.78$. In this case, the plastic zone at the edges is much smaller, and it is not connected with the highly stressed area located in the $45^\circ$ angle of the grooves. LEFM can be applied properly to calculate the stress intensity factors along the crack tip.
Four elliptic profiles have been studied, keeping the minor axis constant to $r_b = 1$ mm. When the eccentricity decreases, the curvature of the elliptic profile diminishes up to the straight crack tip at zero eccentricity. Figure 6 shows the $K_I$ values for the different elliptic profiles with eccentricity, $e = 0.78, 0.72, 0.63, 0.43$ and $0$. It is observed that $K_I$ at the edges decreases when the curvature increases (eccentricity increases). On the other hand, the $K_I$ value in the centre of the thickness increases when the curvature increases. The real curved profile cannot be represented with an elliptic one, but it must be close to the elliptic profile with $e = 0.63$ where $K_I$ is almost constant along the whole width of the crack tip.

![Figure 6. $K_I$ stress intensity factor for elliptic profiles at different eccentricities.](image)

In conclusion, the crack tip has a curved profile along the expected crack path. The elliptic profile is in good agreement with the marks of the crack in the experiments observed under the microscope (see Figure 7).
Figure 7 Microscope picture of the crack path with a curved crack arrest. The crack propagation is from left to right.

3.2 Quasi-static crack propagation simulation

Simulations of crack propagation are based on XFEM elements implemented in ABAQUS. There are two different methodologies to describe the advance of the crack with the XFEM method: the cohesive damage (XFEM-COHE) and Virtual Crack Closure Technique (XFEM-VCCT). The main difference is that cohesive damage assumes ductile fracture over a smeared crack while VCCT assumes brittle fracture using LEFM along the defined crack front. The material behaviour is linear elastic until the crack propagation is activated in each methodology. We have studied and compared both methodologies under the assumption of quasi-static crack propagation.

We have started with the simulation of crack propagation along the symmetric plane $xOz$, which is the ideal one. An initial pre-crack of 5 mm ($a = 24$ mm) with straight tip is defined in the central part using the level set of XFEM elements. Then, a vertical monotonous displacement of the upper centre is imposed like in the real experiments. The stress fields and deformations are calculated while the vertical displacement increases. The numerical time
steps are reduced to capture the crack propagation. The reaction force at the upper reference point is recorded as a function of the vertical displacement.

In the case of cohesive behaviour XFEM-COH, the crack propagation is modelled with a linear traction-separation law. The damage evolution describes the degradation of the material stiffness with a linear behaviour after a certain damage initiation. The crack initiates into an element when the cohesive tensile stress exceeds the critical value, $\sigma_{UT}$, and releases the critical strain energy, $G_{IC}$, when the element is fully cracked. The profile of the crack tip is curved during all the propagation (see figure 8a). The crack advances first at the edges until it reaches the curved profile, then, the entire curved crack tip advances along the crack plane. The reaction force at the upper reference point increases linearly with the displacement until it reaches the critical load when the crack propagation starts. Then, the reaction force remains constant during the crack propagation (see XFEM-COH curves in figure 8b).

Figure 8. (a) Curved crack profile during quasi-static crack propagation using XFEM. The crack propagation is from left to right. (b) Load-displacement curves of the upper reference point for quasi-static crack propagation, using XFEM-COH (solid lines) and XFEM-VCCT methods (dashed lines).
Figure 8b shows the reaction force in the upper centre versus the vertical displacement for the different meshes. In XFEM-COHE, the critical load $P_c$ decreases when the mesh is more refined along the crack tip. The solution has convergence when the size of the elements along the path crack matches the size of the plastic radius $r_p$. It is important to reproduce the stress field around the crack tip to obtain an accurate solution using XFEM-COHE due to the damage model. The problem is that the fine mesh $rp1$ has a huge computational cost. The curve XFEM-COHE rp1 corresponds to one week simulation with 8 Intel Xeon cpus, model E5-2667 at 2.90GHz. Other modelling is needed to afford the crack propagation simulation.

We have also performed simulation of crack propagation based on XFEM using the VCCT, XFEM-VCCT. In this case, the crack propagates when the strain energy release rate exceeds the fracture energy $G_{IC}$. LEFM is used to propagate the existing crack front. In VCCT a pre-crack must be defined and the damage properties are specified via an interaction property between the lips of the crack. The reaction force versus displacement of the upper reference point is represented in figure 8b for EPON epoxy. The behaviour is the same as before, the reaction force increases linearly until $P_c$ is reached, and then the load remains constant (see XFEM-VCCT curves in figure 8b). In XFEM-VCCT, the critical load obtained from the 3 different meshes is constant around 39 N. The small fluctuation around this value is due to numerical instabilities. This method seems to be more convenient because there is much less effect of the mesh element size. As a consequence, the computational cost can be dramatically reduced (< one day) using rp4 mesh.

Finally, the fracture energy has been calculated using

$$G_{IC} = \frac{4P_c^2}{E\beta^2}m$$

(2)
with

\[ m = \frac{Eb}{8} \frac{dC}{da} \]  

(3)

where \( P_C \) is the critical load, \( E \) the Young’s modulus, \( b \) is the thickness of the specimen, \( dC/da \) is the variation of compliance, and \( \beta \) is the effective thickness. These equations are described in detail in ref. (Brown, 2011; Lemmens et al., 2014) where three different effective thicknesses are studied to take into account the effect of the grooves:

Mostovoy (Mostovoy et al., 1967)  
\[ \beta^{\text{Mostovoy}} = \sqrt{bb_n} \]  

(4)

ASTM Standard E1820  
\[ \beta^{\text{ASTM}} = b - (b - b_n)^2 / b \]  

(5)

Freed and Kraft (Freed and Krafft, 1966)  
\[ \beta^{\text{F&K}} = b^{(1-N)b_n^N} \]  

(6)

We have obtained from the crack propagation \( P_C = 39 \) N and \( dC/da = 2.55 \times 10^{-4} \) N\(^{-1}\). The material properties of EPON and the geometry complete the values in the equations 2 and 3. The fracture energy for Mostovoy and ASTM effective thickness are \( G_{IC}^{\text{Mostovoy}} = 77.68 \) N/m and \( G_{IC}^{\text{ASTM}} = 75.86 \) N/m, respectively. These values are close to the one set in the simulation, 76.12 N/m (see table 1). In equation 6, there is a parameter \( N \) that depends on the groove shape. Using the theory values between 0.5 and 1.0 (Freed and Krafft, 1966), the fracture energy goes from \( G_{IC}^{\text{F&K}} = G_{IC}^{\text{Mostovoy}} = 77.68 \) N/m, when \( N = 0.5 \), to \( G_{IC}^{\text{F&K}} = 194.19 \) N/m, when \( N = 1 \). In our case, the best fit is \( N = 0.5 \), which is also in good agreement with the value \( N = 0.51 \) reported by Lemmens et al. (Lemmens et al., 2014) for the stress intensity factors obtained at the mid-point of the crack (\( z = 0 \)). We want to remark that a variation of 1
N in $P_c$ leads to a change of 4 N/m in the fracture energy obtained, which makes that the values are still in good agreement.

As a conclusion, the static simulation and crack propagation give a full description of the experimental setup of TDCB. The critical load of 39 N is in agreement with the fracture energy of the material, and the $K_I$ profiles along the crack tip with this critical load have also values close to the fracture toughness $K_{IC} = 0.55$ MPa m$^{1/2}$.

4 Discussion between experimental data and simulations

The crack propagation along the TDCB specimen can be followed experimentally with the load-displacement curve of the upper centre (see experimental curve XHER55 in figure 9). The load increases proportionally when the imposed displacement $U_y$ increases. When the load reaches the critical value $P_{ci}$ (crack initiation load), the crack propagates in an unstable manner and the load drops suddenly to a lower value $P_{ca}$ (crack arrest load). After that, the load starts to increase again until it reaches the value $P_{ci}$ once more, giving the stick-slip behaviour while the crack propagates through the specimen. The stick-slip crack propagation is in agreement with other references (Meure et al., 2009; Y. C. Yuan et al., 2008). The unstable behaviour gives two load limits, while only one is expected from the theory and simulations. In addition, the values of the loads, $P_{ci}$ and $P_{ca}$, are larger than the critical load from the simulations (see simulation curve XFEM-VCCT in figure 9). In this section we discuss the difference between the experimental data and simulations.
Figure 9. Load-displacement curves of EPON, one representative from the experimental data and other from the simulations. Experimental mean values of $P_{ci}$ and $P_{ca}$ are represented with dashed lines.

Although the experimental and simulation curves have almost the same slope before the crack growth, it is important to mention that the experimental displacement is not a good reference due to the possible accumulated clearances in the setup. Therefore, only experimental load values are considered in this work.

The stick-slip behaviour has been studied in detail in ref. (Macon et al., 2001). The unstable crack propagation can be due to inertia forces, rate dependent material behaviour and reflected stress waves. The authors conclude that, under stick-slip propagation between $P_{ci}$ and $P_{ca}$, a portion of the fracture energy release is due to kinetic energy. Therefore, the crack arrest load $P_{ca}$ is associated with the material properties and not with the load setup. The authors also noted that the magnitude of the kinetic energy depends on the shape of the crack. Sharper cracks lead to unstable behaviour, but the kinetic energy is lower than for the blunt cracks.
We have studied the unstable behaviour including this effect in the simulations. In Abaqus version 6.13.1, an unstable growth tolerance can be specified in the VCCT fracture criterion (Abaqus 6.13, 2013). The results using XFEM-VCCT show small differences between stable and unstable crack propagation. Therefore, we have performed VCCT-debond simulations without XFEM elements to study the unstable behaviour. With this model, VCCT-debond, the crack plane must be defined in advance. We have included a new surface in the central part through the horizontal symmetric plane $xOz$. We have reused the same meshes as in the XFEM simulations, taking into account that the new surface introduces new nodes when it divides the elements along the plane $xOz$. Again, linear hexahedral elements with full integration (C3D8) are used in the central part. The upper and lower parts have the same mesh and elements than in previous simulations. The fracture energy of the material is introduced in the behaviour of the new surface $xOz$, while the rest of properties are applied in all the elements.

Figure 10 shows the results of the VCCT-debond simulations using the mesh $rp3$. When the unstable behaviour is not applied, the load displacement curve follows the same behaviour as the XFEM simulations (see stable curve in figure 10). After the critical load $Pc$ is reached, the load remains constant during the crack propagation. It can be noted that $Pc$ the critical load is 37 N instead of 39 N from the XFEM simulations. This difference cannot be explained, so we have assumed that it is an internal issue of the software between regular FEM and XFEM. In addition, the value of the critical load does not disturb our study. When the unstable behaviour is included in VCCT-debond simulations, the stick-slip crack propagation can be reproduced (see the unstable curve in figure 10). Figure 10 shows that the crack arrest load of the unstable simulation, $Pca*$-Pca, corresponds with the critical load $Pc$ of the stable simulation. Therefore, the $Pc$ obtained in the XFEM simulations (see section
3.1) represents the simulated crack arrest load $P_{ca*}$ because they are stable simulations under as expected from the theory in quasi-static hypothesis.

![Graph showing load-displacement curves using VCCT debond simulation for stable and unstable, unstable and enhanced behaviour.]

**Figure 10.** Load-displacement curves using VCCT debond simulation for stable and unstable, unstable and enhanced behaviour.

Omitting the unstable behaviour, figure 9 shows that the experimental value of $P_{ca}$ is values of $P_{ca}$ are usually larger than the critical load of the simulations $P_c$, which is $P_{ca*}$ (see figure 9). This mismatch can be due to different conditions or effects between the theoretical model and the experimental setup. There can be differences in the material properties, TDCB geometry or applied boundary conditions. For example, if we change our material properties increasing the fracture energy to 94 N/m, value taken from (Brown, 2011), $P_c$ increase 4 N, adding one fracture energy for crack initiation, 90 N/m, and a second one for crack propagation, 76 N/m, the load limits ($P_{ci}$ and $P_{ca}$) increase (see enhanced curve in figure 10). The study of the material behaviour is out of the scope of this paper. In this study, EPON is a well-known material, so we have only used the material properties noted in table 1. Other
issues related with the geometry and boundary conditions, which can modify the critical load $P_c$, will be studied in the next section.

It is important to note that the mean load limits $P_{ci}$ and $P_{ca}$ have been obtained from almost 300 experiments. The values represented in figure 9 are the mean ones, $P_{ci} = 60.7$ N and $P_{ca} = 51.5$ N, with a standard deviation of 7 N each. The mean crack arrest load $Pca$ is close to the value of 49 N reported by Brown et al. (Brown, 2011) with the same polymer, virgin EPON 828. The high dispersion in the experimental data is something usual, but in the case of TDCB is more significant. That is the second argument to make a parametric study of the TDCB setup.

5 Parametric study with static simulation

Although the references show the reproducibility of the experiments, it is important to mention that some parameters of the experiment must be very well controlled to obtain accurate results. In this section, several parameters have been studied in order to quantify the possible errors.

5.1 Friction

The friction between pins and holes of the specimen affects the experimental results. We have studied this effect in the framework of static simulation, adding to the model a constant coefficient of friction between the pin-hole contact surfaces. The friction introduces a moment in the centre of each hole that modifies the stress around the crack tip as in SENT specimens (Pook, 1968). Therefore, the critical load is also modified by the friction. Figure
11 shows that the critical load for crack propagation increases with the friction coefficient, reaching a value of 47 N in the worst case. This increment of the critical load can explain, along with other factors such as unstable crack propagation, why the numerical results are below the experimental ones. In addition, the friction can introduce a great dispersion in the experimental data if the contact surfaces are not properly lubricated. From the simulation, one can estimate a 5% error in the measurements due to the friction when the friction coefficient is 0.2.

It is noteworthy to mention that with the maximum coefficient of friction, the pin-hole surfaces are still not blocked because the load applied induces a limited moment. If the setup blocks the free rotation completely, the critical load reaches its highest value of 70 N.

![Graph showing critical load as a function of friction coefficient](image)

**Figure 11.** Critical load as a function of the friction coefficient between pins and holes.

The moment introduced by the friction modifies the fracture energy, $G_{ic}$, and the variation of the compliance $dC/da$. Therefore, the TDCB geometry fails to meet the constant value of fracture toughness over the crack length. It is important to keep the friction as low as possible.
5.2 Geometry: thickness, angle of grooves, round fillet radius, pin radius

Variations in the geometrical dimensions of the TDCB modify the critical load $Pc$. Although the specimens are built with a precise mould, there are always some tolerances in these dimensions. We have studied the influence of the tolerance of several dimensions and we have expressed it as an error of the critical load. Table 2 summarizes the range, tolerance, error in percentage and error direction for the following dimensions: $b_n =$ thickness of the crack path, $b =$ thickness of the specimen, $d_n =$ height in the horizontal plane $xOz$, $\varphi =$ angle of the grooves, $r^{fillet} =$ radius of the round fillet; and $r^{pin} =$ radius of the pin.

When the thickness along the crack path, $b_n$, increases, the $K_I$ along the crack tip decreases. Therefore, a larger critical load $Pc$ is needed to start the crack propagation. For an increment of 0.1 mm in $b_n$, the critical load increases 1 N. That means that the $b_n$ tolerance of 0.1 mm introduces an error of 2.5% from the nominal critical load $Pc$ (see table 2). This result is valid in the range of 2 to 3 mm of $b_n$. In addition, we have noted as positive error direction the fact that when $b_n$ increases, $Pc$ also increases. The same procedure has been applied with the thickness of the specimen $b$. In this case, the tolerance of 0.1 mm introduces an error of 1% in the critical load, and $Pc$ increases when the thickness increases (see table 2).

We have also estimated the influence of $d_n$ and $\varphi$, related with the V-shape of the groove. When $d_n$ increases 0.03 mm, $Pc$ decreases with 1% error from the nominal $Pc$. Therefore, the error direction is noted as negative. And when the angle $\varphi$ increases 10 degrees, $Pc$ also decreases 1%. Finally the dimensions $r^{fillet}$ and $r^{pin}$ have less influence in the estimation of $Pc$ (see table 2). Huge variations of these radius, 1 mm, only lead to errors lower than 0.1%. 
It is difficult to correlate directly the error of the healing efficiency, $\Delta \eta$, with the error of the critical load, $\Delta P_C$. Using the error propagation theory, we can obtain from $\eta = \frac{P_C^{\text{healed}}}{P_C^{\text{virgin}}}$ that $\frac{\Delta \eta}{\eta} = \frac{\Delta P_C^{\text{healed}}}{P_C^{\text{healed}}} + \frac{\Delta P_C^{\text{virgin}}}{P_C^{\text{virgin}}}$. Therefore, if the error of the critical load is 5%, the error of the healing efficiency will be 10%. But the expected error must be lower because the geometry and the boundary conditions of the setup are almost the same in the load and re-load after healing. Due to the possible errors in the experimental data, it is important to make several experiments with the same material in order to reduce the error of the healing efficiency.

Table 2. Geometrical parameter and its influence in the critical load.

<table>
<thead>
<tr>
<th>Dimension</th>
<th>Range</th>
<th>Tolerance</th>
<th>Error (%)</th>
<th>Error direction</th>
</tr>
</thead>
<tbody>
<tr>
<td>$b_n$</td>
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<td>0.1 mm</td>
<td>2.5</td>
<td>+</td>
</tr>
<tr>
<td>$b$</td>
<td>5.25-7.25 mm</td>
<td>0.1 mm</td>
<td>1</td>
<td>+</td>
</tr>
<tr>
<td>$d_n$</td>
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<td>0.03 mm</td>
<td>1</td>
<td>-</td>
</tr>
<tr>
<td>$\varphi$</td>
<td>35-65 degrees</td>
<td>10 degrees</td>
<td>1</td>
<td>-</td>
</tr>
<tr>
<td>$r^{\text{fillet}}$</td>
<td>1-3 mm</td>
<td>1 mm</td>
<td>0.1</td>
<td>-</td>
</tr>
<tr>
<td>$r^{\text{pin}}$</td>
<td>5-7 mm</td>
<td>1 mm</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

5.3 Non-symmetrical problem.

The geometry studied until now has a symmetry plane along the crack propagation plane xOz. In this section we introduce the non-symmetric problem, when the crack deviates from its path. Non-symmetric problems can be caused by a non-symmetric geometry, a bad position
of the sample in the pins, a different friction in both pins or a deviated pre-crack. Finally, the result is a crack out of the symmetric plane $xOz$.

Simulations of crack propagation out of the symmetric plane are very difficult, because they imply finer meshes and restricted numerical parameters of the XFEM method to reach a solution of convergence. Therefore, static simulations with stationary crack have been used to study the non-symmetric problem.

We have studied horizontal cracks with straight front located above the symmetric crack plane $xOz$, positive $Y$ axis. The stationary cracks are located in the grooves with an offset $y^*$ ranging from $d_n/2$ to $y_b$. The upper limit $y_b$ is the $Y$ coordinate where the grooves finish and the thickness is $b$. Therefore, $y_b$ can be calculated from the geometry dimensions as

$$y_b = b - b_n \cdot \tan(\phi/2) + \frac{d_n}{2}. \quad (7)$$

The thickness of the horizontal crack $t^*$ goes from $b_n$ to $b$ in the range of $y^*$. The relation between the offset $y^*$ and thickness of the crack $t^*$ is

$$t^* = \frac{2 \cdot y^*}{\tan(\phi/2)} + b_n. \quad (8)$$
Figure 12. (a) Detail of the central part of the model with a seam stationary crack at $y^* = 2.45$. (b) Stress intensity factors in mode I, II and III ($K_I$, $K_{II}$ and $K_{III}$) along the crack tip for a non-symmetrical crack. Crack propagation direction, $\theta$, along the crack tip.

Figure 12 (a) shows the stationary crack located in the grooves with an offset $y^* = 0.47$ mm. The crack thickness is $t^* = 4.53$ mm and the crack length is 25 mm. The fracture toughness in mode I, II and III have been calculated along the straight tip when a load of 39 N is applied in the upper reference point (see figure 12b). The first difference is that the $K_I$ is higher in the centre than in the edges, contrary to what happened in the cracks located in the symmetric plane $xOz$. It is important to notice that $K_I$ is null at the edges. In addition, $K_{II}$ and $K_{III}$ become relevant at the edges of the crack tip (see figure 12b).

The crack propagation direction, $\theta$, has been computed along the crack tip taking the maximum tangential stress criterion (Abaqus 6.13, 2013). Figure 12b shows the crack propagation direction $\theta$ which is zero at the centre of the crack tip and negative at the edges. This means that the edges will propagate with an inclination to lead the crack to the symmetric plane (see figure 12a). Although $K_I$ is close to the fracture toughness, $K_{IC} = 0.55$ MPa m$^{1/2}$, at the centre of the tip, the stress intensity factors at the edges are low. A higher
critical load is required to propagate the crack at the edges. In addition, more fracture energy will be demanded to change the direction of the crack starting from the edges.

The increment of initial critical load due to the non-symmetrical crack has been studied experimentally in detail from the TDCB experimental data (Tsangouri et al., under submission). Non-symmetric cracks propagate at values higher than the mean initial critical load $Pci$, but when the crack has returned to the symmetric plane $xOz$, the initial critical load decreases to the mean value $Pci$ of the symmetric experiment.

We have compared and validated the static simulation of non-symmetrical cracks with the experimental data extracted from Digital Image Correlation (DIC). This technique cannot see what happens into the grooves due to geometrical limitations, but the strain fields at the beam surfaces give information about the crack propagation. Figure 13a shows the strain field in vertical direction $Y$ obtained from DIC. Although the resolution of the DIC is limited, we can observe the non-symmetric pattern that the simulation predicts. From the simulations, one can extract the strain fields at the surfaces of the TDCB specimen (see figure 13b). These strain fields are in good agreement with DIC experiments.
Figure 13. (a) Strain field in vertical direction $Y$ extracted from Digital Image Correlation (DIC) of a non-symmetrical crack. (b) Strain field in vertical direction $Y$ extracted from the static simulation of a non-symmetrical crack.

6 Conclusions

A full numerical study of the TDCB geometry has been performed, using static simulations with stationary crack and crack propagation simulations under the hypothesis of quasi-static behaviour.

The static simulations give information about the stresses located around the crack front. A curved profile of the crack tip is expected from the computed stress intensity factor. The quasi-static crack propagation simulations along the symmetry plane $xOz$ show that the propagation starts in the edges of the crack front until it reaches a curved profile. Then, the curved crack tip propagates along the plane $xOz$ while the load in the upper pin remains constant. The critical load $P_c$ can be extracted from the simulations.

A stick-slip behaviour during the crack propagation is observed in the experiments. Two limits of critical load are noted $P_{ci}$ and $P_{ca}$ with a standard deviation of 7 N. The stick-slip behaviour can be simulated adding the unstable behaviour to the model. The crack arrest load from the unstable simulation $P_{ca^*}$ is related to the critical load $P_c$ obtained from the quasi-static theoretical simulations, which remains constant during the stable crack propagation.

Omitting the unstable behaviour, a large difference is noted between the experimental critical load and the simulated one. The material properties and the experimental setup should be carefully analysed. This paper focus on the latter. can modify unstable behaviour increases this
value (not consider in paper) but there are other issues to take into account. In that direction we have studied the pin-hole friction, some geometric dimensions and the crack out of the symmetric plane—non-symmetrical problem. The highest error can be introduced by the friction between pin and hole and the non-symmetrical crack out of the symmetric plane. These factors must be controlled in order to obtain accurate results.

As a general conclusion, the TDCB geometry specimen is a good specimen to study self-healing thermosetting polymers, however experimentalists must should be aware of about the limitations of this geometry.

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References


