

# 1 **A novel cohesive zone modelling approach to represent mixed mode loading** 2 **and bond line thickness effects**

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6 Accurate representation of the traction-separation response for mixed mode loading in a  
7 cohesive zone model (CZM) is critical to predicting the response of adhesive joints in a  
8 number of applications, including transportation and vehicle crashworthiness. Traditionally,  
9 the Mode I and Mode II responses are treated independently, with mixed mode response  
10 determined by relationships between the degree of mode mixity and separation, potentially  
11 leading to overprediction of the plateau traction and underprediction of the plateau length in  
12 mixed mode loading. This poor fit is due to the indirect relationship between mixity and  
13 traction and having minimal fitting options for separation-to-plateau and softening. To  
14 address this limitation, a mixed mode CZM approach is proposed, based on measured mixed-  
15 mode traction-separation results for a toughened epoxy adhesive. The effects of bond line  
16 thickness were considered, to examine the ability of the proposed approach to include  
17 additional effects (beyond mode mixity) that are known to affect the traction-separation  
18 response. The CZM implementation was assessed using the original test data and was shown  
19 to capture the measured experimental traction-separation response across a range of mixed  
20 mode loading and bond line thickness more accurately compared to traditional CZM  
21 treatments.

22 Keywords: cohesive zone modeling, mixed mode loading, bond line thickness, adhesive  
23 joining, finite element modeling

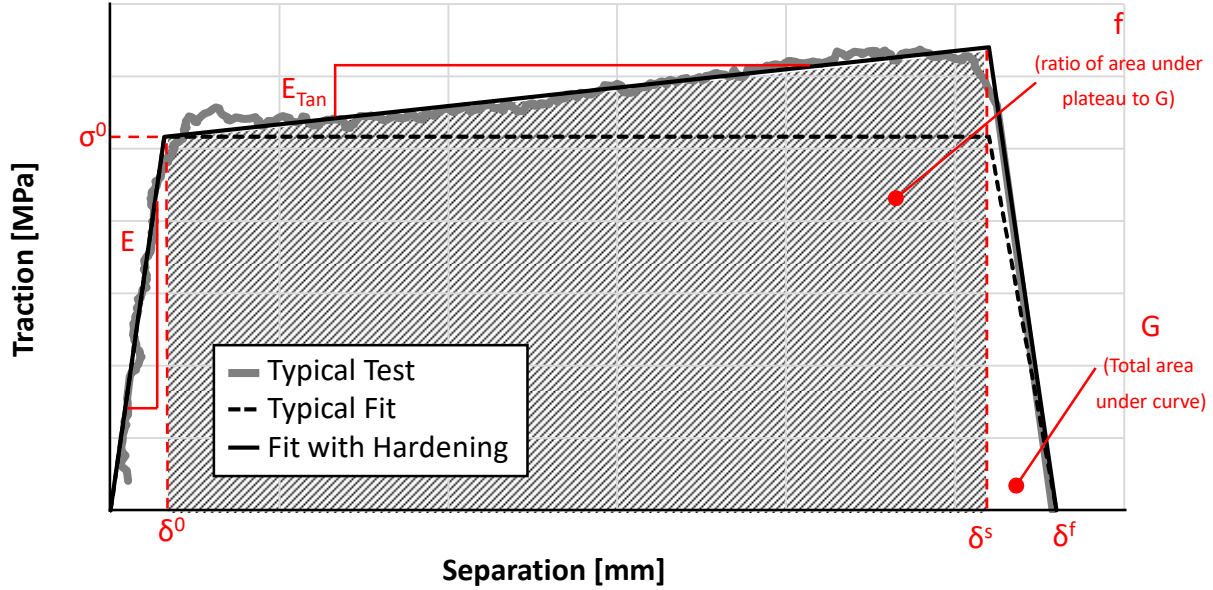
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## 25 **1 Introduction**

26 While a number of approaches can be used to model the failure of adhesive joints [1], one of the  
27 most attractive methods to simulate adhesive joints in large-scale explicit finite element models is

1 to represent the joint using a cohesive zone model (CZM) [2-4]. The CZM approach has been used  
2 in analysis for fields as varied as dental implants [5], flexible piping structures for the oil sector  
3 [6], and bonding of dissimilar metals for advanced body-in-white design applications [37]. An  
4 interface or thin layer where a crack may initiate and propagate can be modeled using CZM  
5 elements, without the need for a predefined defect in the bond line [8], defined using a traction-  
6 separation response [9]. A general limitation of this method is that the path of the crack must be  
7 known prior to defining the model geometry; however, the crack path for modern structural  
8 adhesives with thin bond lines (on the order of 0.2 mm to 1 mm) can be approximated using the  
9 CZM method. Implementations of CZMs usually involve defining the Mode I and Mode II  
10 traction-separation response independently, which are often simplified to bi-linear [10] or  
11 trapezoidal [11,12] shapes for ease of implementation in finite element codes, while still  
12 representing adhesive joint responses. For modeling toughened adhesive joints the trapezoidal  
13 shape is often used [13-15]. A trapezoidal traction-separation curve (Figure 1) can be divided into  
14 three phases: the initial phase during which the traction is proportional to the separation, the plateau  
15 phase where the traction response is constant, and the softening phase, in which the traction  
16 reduces from the plateau value to zero. These regions are differentiated by the separation-to-  
17 plateau ( $\delta^0$ ) and separation-to-softening ( $\delta^s$ ) before failure occurs at the separation-to-failure ( $\delta^f$ )  
18 value [4,16]. Fully defining a trapezoidal traction-separation response requires the initial slope of  
19 the traction-separation response ( $E$ ), plateau traction ( $\sigma_0$ ), critical energy release rate ( $G$ ), and the  
20 ratio of area under the plateau to the area under the entire traction-separation response (termed  
21 area ratio ( $f$ ), for brevity) to be defined. Trapezoidal CZM implementations commonly assume a  
22 constant plateau and do not allow for experimentally observed softening [17] or hardening [18].  
23 Although some CZM implementations which include softening [17] and hardening [19] have been

- 1 implemented in the literature, their adoption in popular finite element solvers has been limited. To
- 2 account for the slope of the plateau,  $E_{Tan}$  must also be defined.



3

4 **Figure 1: Trapezoidal traction-separation response highlighting parameter definition and**  
 5 **separation measurements used in fit**

6

7 The ratio of the Mode II separation ( $\delta_{II}$ ) to the Mode I separation ( $\delta_I$ ), mixity ( $\beta$ ), is used to define  
 8 the resultant mixed mode separation-to-plateau and separation-to-softening (Table 1). Separation-  
 9 to-failure ( $\delta^f$ ), which is the separation at which the element no longer supports load and is removed  
 10 from the simulation, is generally defined using relationships based on critical energy release rates  
 11 ( $G_{IC}$ ,  $G_{IIC}$ ), such as the failure criterion suggested by Benzeggagh and Kenane [20] or power law  
 12 relationships such as that proposed by Camanho & Dávila [16]. To define failure criteria based on  
 13 critical energy release rates, the initial stiffness in Mode I and Mode II loading ( $E_I$  and  $E_{II}$ ,  
 14 respectively) are also required.  $\delta^0$ ,  $\delta^s$ , and  $\delta^f$  are recalculated at each timestep in the finite element  
 15 simulation as the ratio between separation in the Mode I and Mode II directions evolves, although

1 the other parameters are typically fixed throughout the simulation based on the material parameters  
 2 defined in the model input. To account for potential non-linearities in the mixed mode failure  
 3 response, an experimentally measured mixity failure parameter ( $\eta$ ) has been proposed to control  
 4 the mixed mode separation to failure [4,16], although the ability to fit the model traction-separation  
 5 response to the experimental data can be somewhat limited.

6 **Table 1: Summary of trapezoidal cohesive zone model mixity treatments**

Separation Measure	Resultant separation expressed using mode mixity ( $\beta = \delta_{II} / \delta_I$ )
Separation-to-Plateau [16]	$\delta^0 = \delta_I^0 \cdot \delta_{II}^0 \sqrt{\frac{1 + \beta^2}{(\delta_{II}^0)^2 + (\beta \delta_I^0)^2}}$
Separation-to-Softening [16]	$\delta^s = \delta_I^s \cdot \delta_{II}^s \sqrt{\frac{1 + \beta^2}{(\delta_{II}^s)^2 + (\beta \cdot \delta_I^s)^2}}$
Separation-to-Failure (Power law [16])	$\delta^f = \frac{2(1 + \beta^2)}{\delta_0} \left[ \left( \frac{E_I}{G_{IC}} \right)^\eta + \left( \frac{\beta^2 \cdot E_{II}}{G_{IIC}} \right)^\eta \right]^{-1/\eta} + \delta_0 - \delta_s$
Separation-to-Failure (Benzeggagh-Kenane [20])	$\delta^f = \frac{2 \left[ G_{IC} + (G_{IIC} - G_{IC}) \left( \frac{\beta^2 \cdot E_{II}}{E_I + \beta^2 \cdot E_{II}} \right)^\eta \right]}{\delta_0 \left( \frac{E_I + \beta^2 \cdot E_{II}}{1 + \beta^2} \right)} + \delta_0 - \delta_s$

7

8 In general, the initial Mode I and Mode II stiffness values are not equal, so care must be taken  
 9 when assessing the mixed mode measurement because the resultant traction and resultant  
 10 separation vectors will not align [18]. Due to the Mode I and Mode II plateau tractions being  
 11 calculated based on the multiplication of the respective initial stiffness and separation-to-plateau  
 12 for each mode, there is also little flexibility in representing the value of the resultant plateau  
 13 traction.

14 Factors such as the thickness of the bond line [21-23], the rate of loading [17,24], previous cyclic  
 15 loading history [25], humidity [26], and temperature of the adhesive joint [27,28] can affect the  
 16 response of the adhesive. These effects are particularly well documented for the critical energy

1 release rate and plateau (or peak) traction [4]. For the bond line thicknesses considered in the study  
2 presented in the current work (0.18 mm to 0.6 mm), increasing bond line thickness tends to reduce  
3 the peak traction [29] and increase the critical energy release rate for toughened epoxy adhesives  
4 [30]. CZM implementations generally only consider a single bond line thickness, so different sets  
5 of material parameters are required for each bond line thickness used in a finite element model.

6 Watson *et al.* [18,31] developed test methodologies to measure the complete traction-separation  
7 response of structural adhesives. In that study, the authors used these new test methodologies to  
8 measure the complete traction-separation response for Mode I, Mode II and a pair of mixed modes  
9 of loading (45° and 75°) for three bond line thicknesses (0.18 mm, 0.3 mm and 0.64 mm). The  
10 Mode I response was measured using the Rigid Double Cantilever Beam (RDCB) test specimen  
11 in which the force-displacement response was converted into traction-separation by using  
12 adherends with a large second-moment of area in the bending direction. This design allows for the  
13 assumption that the adherend is effectively rigid, concentrating the deformation in the adhesive  
14 bond line [31]. A similar approach was taken to design specimens in which the bond line could be  
15 loaded at 45°, 75°, and 90° with large bending resistance in the direction of loading. By using  
16 optical methods to measure separation across the bond line and dividing the measured force by the  
17 original bond line area measured prior to testing, the Mode II and mixed mode traction-separation  
18 response could be extracted. The measured parameters ( $G_C$ ,  $E$ ,  $f$ , and  $\sigma_0$ , for Mode I and Mode II)  
19 were fit to a trilinear CZM using a power law separation-to-failure with  $\eta = 1$  (see line 3 in Table  
20 1) [32] implemented using CZM elements in a commercial finite element solver (LS-DYNA). The  
21 prediction of the traction-separation response of the CZM under mixed mode loading was found  
22 to be poor [18] with the CZM overpredicting the mixed mode plateau traction. Additionally, the  
23 separation-to-softening was generally underpredicted for the mixed mode cases, leading to a

1 shorter plateau and an extended softening region than was observed in the experiments.  
2 Additionally, three separate sets of material parameters were required to define each of the three  
3 bond line thicknesses investigated.

4 In the current study, an enhanced CZM was developed to address shortcomings of CZM  
5 implementations to accurately capture the traction-separation response across a range of mode  
6 mixity and bond line thickness combinations for toughened adhesives identified by Watson *et al.*  
7 [18]. The new approach utilized an evolving set of CZM parameters ( $E$ ,  $E_{Tan}$ ,  $\sigma_0$ ,  $G$  and  $f$ ) based  
8 on the mode mixity of each element throughout the simulation and the bond line thickness at the  
9 start of the simulation. The proposed model was then verified by modeling experimental  
10 characterization tests of Mode I, Mode II and mixed mode loading. The EMC was compared to a  
11 CZM implemented using an approach to mixity outlined in Table 1 (with a power law separation-  
12 to-failure definition using  $\eta = 1$ ) [32], termed the ‘Baseline’ model, in order to demonstrate the  
13 ability of the new model to better represent the measured material response.

## 14 **2 Model Methodology**

### 15 **2.1 Enhanced Mixed Mode Cohesive Zone Model Methodology**

16 A new CZM, termed the ‘Enhanced Mixed Mode Cohesive Zone’ (EMC) Model, was developed  
17 to predict the traction-separation response of adhesive joints, improving on aspects of the mixed-  
18 mode response identified by Watson *et al.* [31] and adding effects of bond line thickness into a  
19 new CZM implementation. While the CZM approach was developed for zero or near-zero  
20 thickness bond lines with thicker bond lines potentially being modeled using a series of solid and  
21 CZM elements, the ultimate goal for this work is to utilize the EMC in large-scale finite element  
22 models for automobile crashworthiness applications. Solid element formulations of the adhesive

1 were not investigated due to the small timestep sizes that would be associated with solid elements  
 2 having thicknesses on the order of the bond line thicknesses used in the present study. The  
 3 measured traction-separation responses presented by Watson *et al.* [31] were used to verify the  
 4 EMC and compare it to a baseline CZM. The philosophy guiding the EMC was to use the resultant  
 5 traction ( $\sigma$ )-resultant separation ( $\delta$ ) (*i.e.* the vector summation of Mode I and Mode II traction and  
 6 separation) along the direction of mixed separation, rather than treat the two responses  
 7 independently, as is typically the case, in order to predict the mixed-mode traction and failure of  
 8 adhesive joints under complex loading. Furthermore, the EMC approach alleviates the  
 9 misalignment of the traction and separation vectors under mixed mode loading due to unequal  
 10 Mode I and Mode II stiffnesses noted by Watson *et al.* [31].

11 In the EMC model, a series of functions of mixity,

$$\Theta = \frac{2}{\pi} \cdot \text{atan} \left( \frac{\delta_{II}}{\delta_I} \right), \quad (1)$$

12 and initial thickness of the element ( $t$ ) are used to define the parameters necessary to construct the  
 13 traction-separation response ( $E$ ,  $\sigma_0$ ,  $G$ ,  $f$ ,  $E_{Tan}$ , see Figure 1). The intention of this using this  
 14 definition of mixity rather than the more traditional definition ( $\beta = \delta_{II}/\delta_I$ ), was to define mixity  
 15 between zero in Mode I and 1.0 in Mode II, rather than zero to infinity. The finite bounds of the  
 16 new mixity definition were required for the parameter fitting described below. Furthermore, the  
 17 new definition avoids values that approach infinity when the Mode I separation is very small,  
 18 which could lead to round-off errors. Throughout the simulations, the mixity is calculated for each  
 19 timestep, while the thickness is kept constant (equal to the initial thickness of the element). The  
 20 separation-to-plateau ( $\delta^0$ ) of the resultant traction-resultant separation response for a given  
 21 combination of  $\Theta$  and  $t$  is defined in the typical manner found in the literature [16];

$$\delta^0 = \frac{\sigma_0}{E}. \quad (2)$$

1 The introduction of the hardening parameter  $E_{Tan}$  (see Figure 1), leads to definitions of the traction  
 2 at the end of the plateau ( $\sigma_s$ ) of

$$\sigma_s = \sigma_0 + E_{Tan} \cdot (\delta^s - \delta^0) \quad (3)$$

3 And the area under the plateau of

$$f \cdot G_C = \frac{1}{2} \cdot (\sigma_0 + \sigma_s) \cdot (\delta^s - \delta^0). \quad (4)$$

4 The total area under the traction-separation response ( $G_C$ ) can be defined as

$$G_C = \frac{1}{2} \cdot \sigma_0 \cdot \delta^0 + f \cdot G_C + \frac{1}{2} \cdot \sigma_s \cdot (\delta^f - \delta^s). \quad (5)$$

5 Equation (3), Equation (4) and Equation (5) represent three equations with three unknown values  
 6 ( $\delta^s$ ,  $\delta^f$ , and  $\sigma_s$ ). By rearranging and substituting these equations the separation-to-softening ( $\delta^s$ ) can  
 7 be shown to be as

$$\delta^s = \frac{\frac{2\sigma_0 E_{Tan}}{E} - 2\sigma_0 + \sqrt{\left(2\sigma_0 - \frac{2\sigma_0 E_{Tan}}{E}\right)^2 - \frac{2E_{Tan}^2 \sigma_0^2}{E^2} - \frac{8E_{Tan} \sigma_0^2}{E} - 8fGE_{Tan}}}{2E_{Tan}}, \quad (6)$$

8 and the separation-to-failure ( $\delta^f$ ) is defined as

$$\delta^f = \frac{2 \cdot G(1-f) - \frac{\sigma_0^2}{E}}{\sigma_0 + E_{Tan}(\delta^s - \delta^0)} + \delta^s. \quad (7)$$

9 For a complete definition of the EMC, as with all CZM implementations, damage must be  
 10 considered. For ease of calculation, two separate parameters are introduced. The first damage  
 11 parameter ( $D$ ) governs the traction response during unloading and reloading of the CZM element  
 12 [33];



$$D = \max \left( 1 - \frac{\delta^0}{\delta}, 1 - \frac{\delta^0}{\delta} \cdot \frac{\delta^f - \delta}{\delta^f - \delta^s}, D_{previous}, 0 \right). \quad (8)$$

1 The *previous* subscript denotes the damage from the previous time step. In this definition,  $D$  begins  
 2 to accumulate once the resultant separation exceeds the  $\delta^0$  value. This formulation ensures the  
 3 traction response returns to zero when the element is unloaded at any point during the loading  
 4 history, without a permanent plastic set. This behaviour follows the conclusions found by Biel &  
 5 Stigh [34], who measured the effect of damage on bonded DCB specimens and concluded that,  
 6 while some residual displacement may be present, the unloading response is best described by a  
 7 relationship that returns to zero separation when fully unloaded, with no permanent deformation.

8 A softening parameter ( $S$ ),

$$S = \max \left( 1 - \frac{\delta^f - \delta}{\delta^f - \delta^s}, S_{previous}, 0 \right), \quad (9)$$

9 is added to govern the traction response between  $\delta^S$  and  $\delta^f$ . Conceptually, this parameter can be  
 10 thought of as a damage parameter related to failure (rather than  $D$ , which is used to govern the  
 11 unloading response). Unlike  $D$ , the softening parameter ( $S$ ) only begins to increase after the  
 12 resultant displacement exceeds  $\delta^S$ . When  $S$  reaches unity, the element is unable to support further  
 13 load and is eroded (removed) from the model.

14 The manner in which traction is calculated is dependent on the level of separation in the previous  
 15 time step, namely,

$$\sigma = \begin{cases} (\delta - \delta_{t-1}) \cdot \left( (1 - D) \cdot (E - E_{Tan} \cdot (1 - S)) + E_{Tan} \cdot (1 - S) \right) + \sigma_{previous} & \text{if } \delta - \delta_{previous} < 0 \\ (\sigma_0 + E_{Tan} \cdot (\delta - \delta^0))(1 - S) & \text{otherwise} \end{cases} \quad \text{or } \sigma_{previous} < (\sigma_0 + E_{Tan} \cdot (\delta - \delta^0))(1 - S). \quad (10)$$

16 The first step in calculating traction from a set of separation values for a given timestep, is to  
 17 calculate the incremental displacement between the current resultant separation ( $\delta$ ) and the  
 18 resultant separation from the previous time step ( $\delta_{previous}$ ). If the change in displacement is less than

1 zero (unloading) or the resultant traction from the previous timestep ( $\sigma_{previous}$ ) is less than the  
 2 plateau traction (which can occur during initial loading, reloading after unloading and the portion  
 3 of the response between  $\delta^S$  and  $\delta^f$ ), an incremental portion of traction is added to  $\sigma_{previous}$  (as  
 4 described in the first condition of Equation (10)). This traction increment accounts for any damage  
 5 and softening, which may have occurred since the start of the simulation. Otherwise, the traction  
 6 is set to the plateau traction for a given resultant separation along the direction of mixity (as  
 7 described in the final condition of Equation (10)).

8 After calculating the resultant traction, the traction in Mode I and the two Mode II directions is  
 9 required by the finite element solver. The resultant traction can be apportioned in the Mode II  
 10 directions by

$$\sigma_{II,i} = \frac{\sigma \cdot \tan\left(\frac{\pi}{2}\theta\right)}{\sqrt{1 + \tan^2\left(\frac{\pi}{2}\theta\right)}} \cdot \frac{\delta_{II,i}}{\delta_{II}}, \quad i = x, y. \quad (11)$$

11 The Mode I traction is somewhat more complicated due to the elastic, undamaging compression  
 12 traction response typically assumed in CZM implementations. To account for this asymmetry, the  
 13 Mode I traction is calculated as

$$\sigma_I = \begin{cases} \frac{\sigma}{\sqrt{1 + \tan^2\left(\frac{\pi}{2}\theta\right)}} & \text{if } \delta_I \geq 0 \\ E_{0^\circ} \cdot \delta_I & \text{if } \delta_I < 0 \end{cases}, \quad (12)$$

14 where  $E_{0^\circ}$  is the initial Mode I ( $0^\circ$ ) stiffness calculated for the bond line thickness originally defined  
 15 for the given CZM element.

## 1 2.2 EMC Model Parameter Fitting from Characterization Data

2 To define the EMC model, the Mode II and mixed mode test presented in Watson *et al.* [18] were  
3 refit to include hardening, using a least squares approach for each test. Five test repeats of each  
4 mode of loading and bond line thickness combination were considered in the parameter fitting and  
5 model comparison. The Mode I test response did not exhibit appreciable hardening behaviour,  
6 although to avoid an infinite value for separation-to-softening (Equation (6)), an  $E_{Tan}$  value of  
7  $1 \times 10^{-9}$  GPa/mm was used in all Mode I cases. Other adhesives may exhibit more hardening (or  
8 softening) in Mode I loading, which would be admissible using the current modelling approach.  
9 The average value of the CZM parameters were calculated for each combination of bond line  
10 thickness and mode mixity by curve fitting the individual tests presented in Watson *et al.* [18] to  
11 Equation (2) through Equation (7) using a non-linear least squares fitting approach. The mean  
12 values for each condition were then calculated to develop ‘average’ traction-separation responses  
13 (Table 2). Using these average parameters, a trapezoidal traction-separation response could be  
14 defined for each loading mode and bond line thickness combination tested.

15

1 **Table 2: Summary of experimental test results for parameter fitting**

Loading Angle [°]	Mixity ( $\theta$ )	Average bond line Thickness ( $t$ ) [mm]	Initial Stiffness ( $E$ ) [GPa/m]	Plateau Traction ( $\sigma_0$ ) [MPa]	Critical Energy Release Rate ( $G$ ) [kJ/m]	Area Ratio ( $f$ )	Tangent Stiffness ( $E_{Tan}$ ) [GPa/mm]
0	0	$0.19 \pm 0.04$	2589	53.38	1.57	0.51	$1 \times 10^{-9}$
		$0.31 \pm 0.01$	1762	51.24	2.13	0.49	$1 \times 10^{-9}$
		$0.63 \pm 0.01$	1259	48.72	2.22	0.36	$1 \times 10^{-9}$
45	0.5	$0.23 \pm 0.05$	2417	30.60	2.05	0.87	0.04
		$0.33 \pm 0.05$	2099	31.47	2.43	0.87	7.78
		$0.60 \pm 0.04$	1242	28.42	3.60	0.79	0.03
75	0.833	$0.24 \pm 0.03$	2542	26.36	5.01	0.95	10.46
		$0.32 \pm 0.03$	1647	25.22	6.71	0.92	12.38
		$0.61 \pm 0.03$	777	23.95	10.56	0.91	3.90
90	1	$0.21 \pm 0.04$	2693	26.65	5.05	0.96	42.61
		$0.38 \pm 0.04$	1903	26.71	7.29	0.97	16.28
		$0.59 \pm 0.04$	772	23.65	13.76	0.95	8.33

2

3 For the baseline models, the CZM parameters presented in Watson *et al.* [18] were used directly  
4 to define the Mode I and Mode II behaviour using a trapezoidal traction-separation law. The mixed  
5 mode response was governed using a power law fit (see Table 1) with  $\eta = 1$ .

6 To identify functions of  $\theta$  and  $t$  for each parameter, surface fitting software (TableCurve 3D,  
7 Systat Software; San Jose, CA, USA) was used to determine the best fitting rational function. The  
8 rational function form that produced the highest  $r^2$  value for each parameter was used, disregarding  
9 the functions that produced singularities over the domain of interest. Furthermore, the surface  
10 generated from each fit was examined to ensure the relationship matched observed trends in the  
11 experiments by Watson *et al.* [18]. For example, in the experiments, the plateau traction  
12 monotonically increased with thickness and monotonically decreased with  $\theta$ . The  
13 phenomenological relationships used to describe each parameter should be considered valid only  
14 for the range of bond line thicknesses tested (0.18 mm to 0.64 mm). The functions used to generate  
15 each parameter were as follows:

$$E(\theta, t) = E_a + E_b\theta + E_ct + E_d\theta t + E_e\theta^2 + E_ft^2 + E_g\theta^2 t + E_h\theta t^2 \quad (13)$$

$$\sigma_0(\theta, t) = \sigma_{0,a} + \sigma_{0,b}\theta + \sigma_{0,c}t + \sigma_{0,d}\theta t + \sigma_{0,e}\theta^2 + \sigma_{0,f}t^2 + \sigma_{0,g}\theta^2 t + \sigma_{0,h}\theta t^2 \quad (14)$$

$$G(t, \theta) = \frac{G_a + G_b\theta + G_ct + G_dt^2}{1 + G_e\theta + G_f\theta^2 + G_g\theta^3 + G_ht} \quad (15)$$

$$f(\theta, t) = f_a + f_b\theta + f_ct + f_d\theta t + f_e\theta^2 + f_ft^2 + f_g\theta^2 t + f_h\theta t^2 \quad (16)$$

$$E_{Tan}(\theta, t) = E_{Tan,a} + E_{Tan,b}\theta + E_{Tan,c}t + E_{Tan,d}\theta t + E_{Tan,e}\theta^2 + E_{Tan,f}t^2 \\ + E_{Tan,g}\theta^2 t + E_{Tan,h}\theta t^2 \quad (17)$$

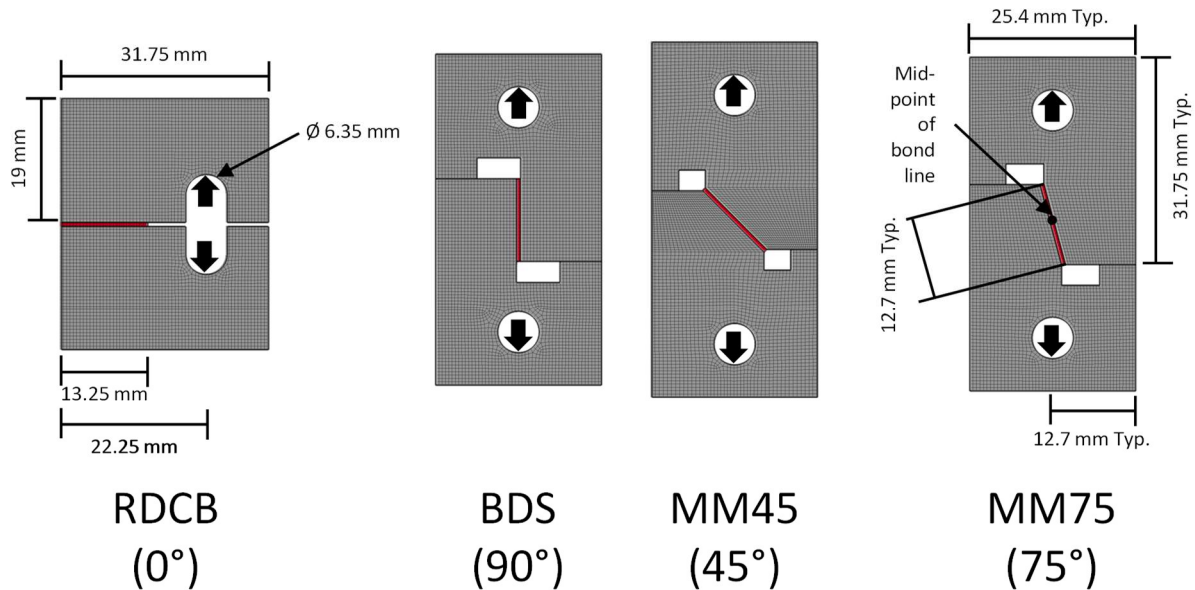
1 While Equation (13) to Equation (17) were selected due to their ability to phenomenologically  
 2 describe the test response well, further refinement to the function selection may simplify the input  
 3 necessary to the model. Furthermore, additional factors such as loading rate, temperature, or  
 4 environmental degradation due to surface contamination, or under or overcuring, could be included  
 5 in these functions to account for such effects in future work, provided that test data is available.

### 6 **2.3 Description of the Characterization Test Verification Models**

7 In order to verify the EMC, simulations of the characterization tests were performed. The EMC  
 8 model was implemented in a commercial explicit finite element solver (LS-DYNA Version 9.2.0  
 9 (build 119543), 64-bit, MPP, double precision) using a user-defined cohesive zone model  
 10 subroutine.

11 The models of each characterization test (Figure 2) used 0.5 mm fully integrated (LS-DYNA,  
 12 element type 2) hexahedral elements to model the adherends and loading pins in three dimensions  
 13 (*i.e.* not using plane strain or plane stress elements). The total thickness of each specimen was  
 14 modeled to match thickness from each test, 6.35 mm for the RDCB specimens and 3.18 mm for

1 the shear and mixed mode specimens. An elastic material property was applied to the adherends  
 2 ( $\rho = 7800 \text{ kg/m}^3$ ,  $E = 207 \text{ GPa}$  and  $\nu = 0.3$ ). The loading pins were defined as rigid with one pin  
 3 fixed in all directions and a prescribed velocity of  $1.0 \text{ mm/s}$  being applied to the other for 1 second  
 4 of simulation time. The force required to maintain the separation was output to track loading force.  
 5 For the RDCB models, displacement was measured by tracking the displacement of the loading  
 6 pin, while in the remaining characterization models the displacement was tracked by measuring  
 7 the relative displacement of the node on either side of the center of the bond line on the surface  
 8 element, as was reported in the experiments.



9

10 **Figure 2: Finite element mesh of specimen geometry [18] used to extract the traction**  
 11 **separation response under Mode I (RDCB), Mode II (BDS), and mixed mode (MM45 and**  
 12 **MM75) loading**  
 13

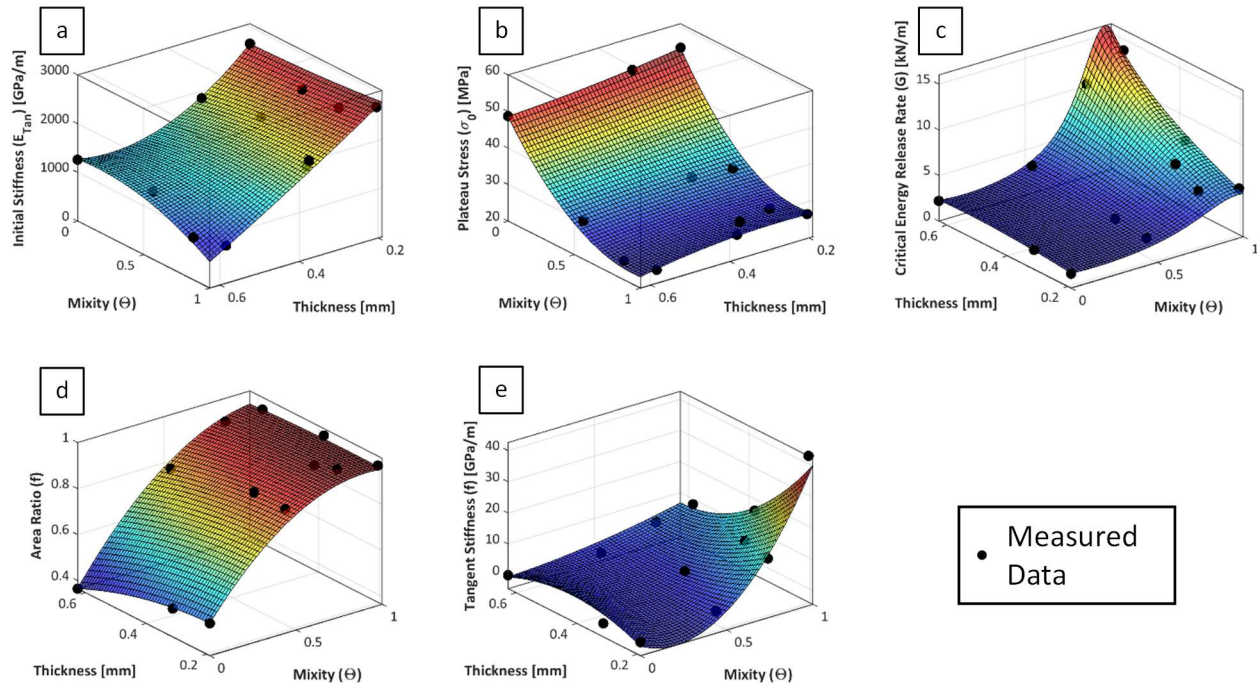
## 1 3 Results and Discussion

### 2 3.1 Fitting of the EMC Model to Experimental Characterization Test Data

3 When fitting the experimental data (Table 2) for each parameter (Table 3), the resulting surface  
 4 plots provided a good fit to the measured data (Figure 3), with an average  $r^2$  value of 0.97.  
 5 Parameter fitting was performed using average test responses for each loading mode/bond line  
 6 thickness combination. Using the individual test responses was found to only change the resulting  
 7 predicted traction-separation responses by a maximum of 2% for the separation responses of  
 8 interest ( $\delta^o$ ,  $\delta^S$ ,  $\delta^f$ ). The difference between the traction predicted using parameters fit from average  
 9 or individual tests was an order of magnitude lower (0.2%) than the separation responses, due to  
 10 lower variability in the force measurement in the characterization testing.

11 **Table 3: Summary of EMC parameter function fitting (see Equation (13) to Equation (17))**

Initial Stiffness ( $E$ ) Parameters		Plateau Traction ( $\sigma_0$ ) Parameters		Critical Energy Release Rate ( $G$ ) Parameters		Area Ratio ( $f$ ) Parameters		Tangent Stiffness ( $E_{Tan}$ ) Parameters	
$E_a$ [GPa m <sup>-1</sup> ]	4.46E+3	$\sigma_{0,a}$ [MPa]	5.68E+1	$G_a$ [kJN m <sup>-1</sup> ]	7.60E-1	$f_a$ [MPa]	4.90E-1	$E_{Tan,a}$ [GPa m <sup>-1</sup> ]	-1.40E+1
$E_b$ [GPa m <sup>-1</sup> ]	-1.29E+3	$\sigma_{0,b}$ [MPa]	-7.05E+1	$G_b$ [kJN m <sup>-1</sup> ]	1.30E-1	$f_b$ [MPa]	1.02E+0	$E_{Tan,b}$ [GPa m <sup>-1</sup> ]	-9.62E+0
$E_c$ [GPa m <sup>-2</sup> ]	-1.20E+1	$\sigma_{0,c}$ [MPa m <sup>-1</sup> ]	-2.13E-2	$G_c$ [kJN m <sup>-2</sup> ]	4.85E-3	$f_c$ [MPa m <sup>-1</sup> ]	2.10E-4	$E_{Tan,c}$ [GPa m <sup>-2</sup> ]	8.67E-2
$E_d$ [GPa m <sup>-2</sup> ]	8.94E+0	$\sigma_{0,d}$ [MPa m <sup>-1</sup> ]	5.24E-2	$G_d$ [kJN m <sup>-3</sup> ]	-5.74E-6	$f_d$ [MPa m <sup>-1</sup> ]	-2.30E-4	$E_{Tan,d}$ [GPa m <sup>-2</sup> ]	-1.59E-1
$E_e$ [GPa m <sup>-1</sup> ]	6.60E+2	$\sigma_{0,e}$ [MPa]	3.80E+1	$G_e$ [kJN m <sup>-1</sup> ]	1.11E+0	$f_e$ [MPa]	-5.70E-1	$E_{Tan,e}$ [GPa m <sup>-1</sup> ]	9.99E+1
$E_f$ [GPa m <sup>-3</sup> ]	1.10E-2	$\sigma_{0,f}$ [MPa m <sup>-2</sup> ]	1.31E-5	$G_f$ [kJN m <sup>-1</sup> ]	-4.13E+0	$f_f$ [MPa m <sup>-2</sup> ]	-6.50E-7	$E_{Tan,f}$ [GPa m <sup>-3</sup> ]	-1.04E-4
$E_g$ [GPa m <sup>-2</sup> ]	-2.74E+0	$\sigma_{0,g}$ [MPa m <sup>-1</sup> ]	-1.40E-2	$G_g$ [kJN m <sup>-1</sup> ]	2.46E+0	$f_g$ [MPa m <sup>-1</sup> ]	1.20E-4	$E_{Tan,g}$ [GPa m <sup>-2</sup> ]	-1.51E-1
$E_h$ [GPa m <sup>-3</sup> ]	-1.01E-2	$\sigma_{0,h}$ [MPa m <sup>-2</sup> ]	-4.35E-5	$G_h$ [kJN <sup>-1</sup> ]	-5.30E+2	$f_h$ [MPa m <sup>-2</sup> ]	5.10E-7	$E_{Tan,h}$ [GPa m <sup>-3</sup> ]	2.84E-4



1

2

**Figure 3: EMC parameter fitting as a function of mixity ( $\Theta$ ) and bond line thickness ( $t$ ) for initial stiffness (a,  $r^2 = 0.95$ ), plateau traction (b,  $r^2 = 0.99$ ), critical energy release rate (c,  $r^2 = 0.99$ ), area ratio (d,  $r^2 = 0.99$ ) and tangent stiffness (e,  $r^2 = 0.90$ ) (see Figure 1)**

4

5

6

7

### 3.2 Verification of the EMC Model Through Comparison to the Experimental Data

8

The verification models of the RDCB tests using the EMC approach provided a good fit to both

9

the output force-displacement response (Figure 4a, b, c) and calculated traction-separation

10

response (Figure 4d, e, f). The maximum force predicted by the EMC models was within 2.5% of

11

the experimental average. After converting the force-displacement response to traction-separation,

12

the average of the separation responses ( $\delta^0$ ,  $\delta^S$ ,  $\delta^f$ ) of the models was within 8% of the experimental

13

average, while the average plateau traction was within 2%. The baseline CZMs also demonstrated

14

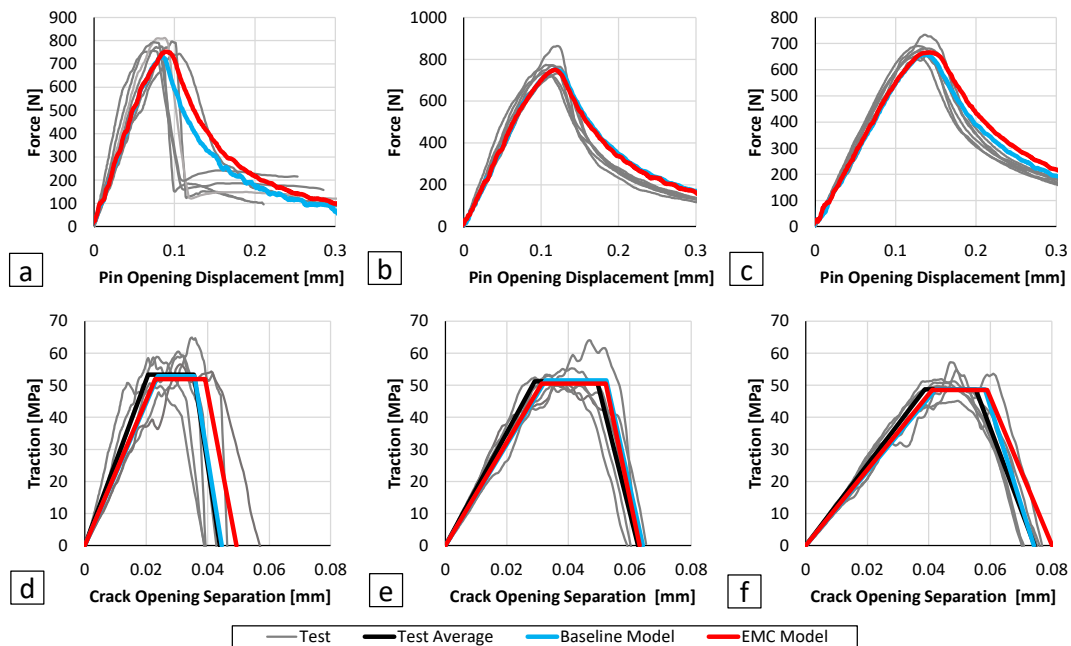
good agreement with the test response. Both the EMC and baseline models of the 0.18 mm nominal

15

bond line thickness did have some difficulty capturing the abrupt drop in the force-displacement



1 response that was observed during testing (Figure 4a). This lack of fit was partly due to the  
 2 underlying assumptions of the CZM approach, which assumes an area of damaged material is  
 3 present in front of the crack tip [35, 36], which was not the case in the brittle fracture present in  
 4 these tests. Despite the limitation of the CZM approach to capture brittle fracture, the traction-  
 5 separation response generated from the models of the RDCB test was able to capture the test  
 6 response reasonably well. Some discrepancy was apparent between the experimental (input)  
 7 average traction-separation responses and that generated by the models, due to the compliance of  
 8 the elastic adherends rather than the perfectly-rigid adherend assumption embedded in the analysis  
 9 technique [18, 31]. Additionally, the fixed 21 point running average used smooth the force-  
 10 displacement response to aid in the numerical differentiation required for conversion of the force-  
 11 displacement to traction-separation [31] may have introduced some differences between the model  
 12 and expected response due to the higher sampling rate of model compared to the tests.

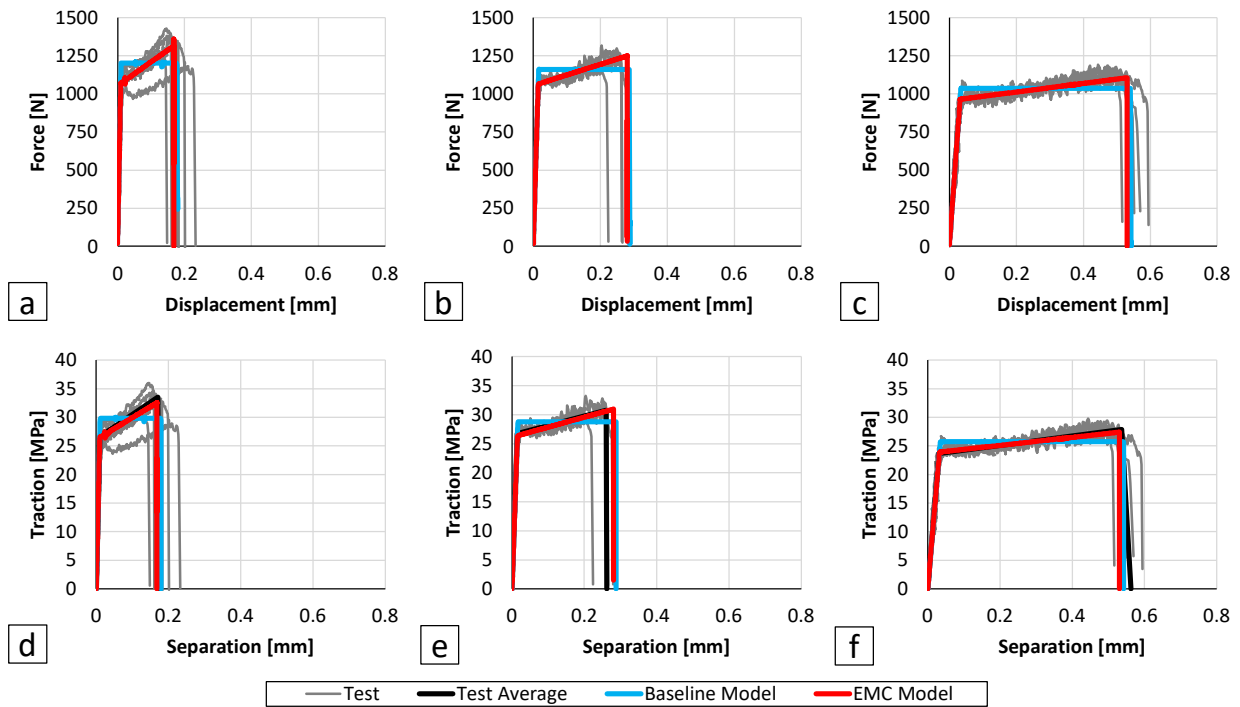


13

14 **Figure 4: Comparison of RDCB CZMs to experimental [18] force-displacement response**  
 15 **and corresponding output of traction-separation for nominal bond line thicknesses of 0.18**  
 16 **mm (a,d), 0.3 mm (b,e), and 0.64 mm (c,f)**

1

2 The models using the EMC approach were in good agreement with the measured response (Figure  
 3 5) with an average error of 5% and 1% for the separation values ( $\delta^0$ ,  $\delta^S$ ,  $\delta^f$ ) and average traction  
 4 values, respectively. The baseline model also provided the expected response, although without  
 5 capturing the hardening behaviour of the test data.

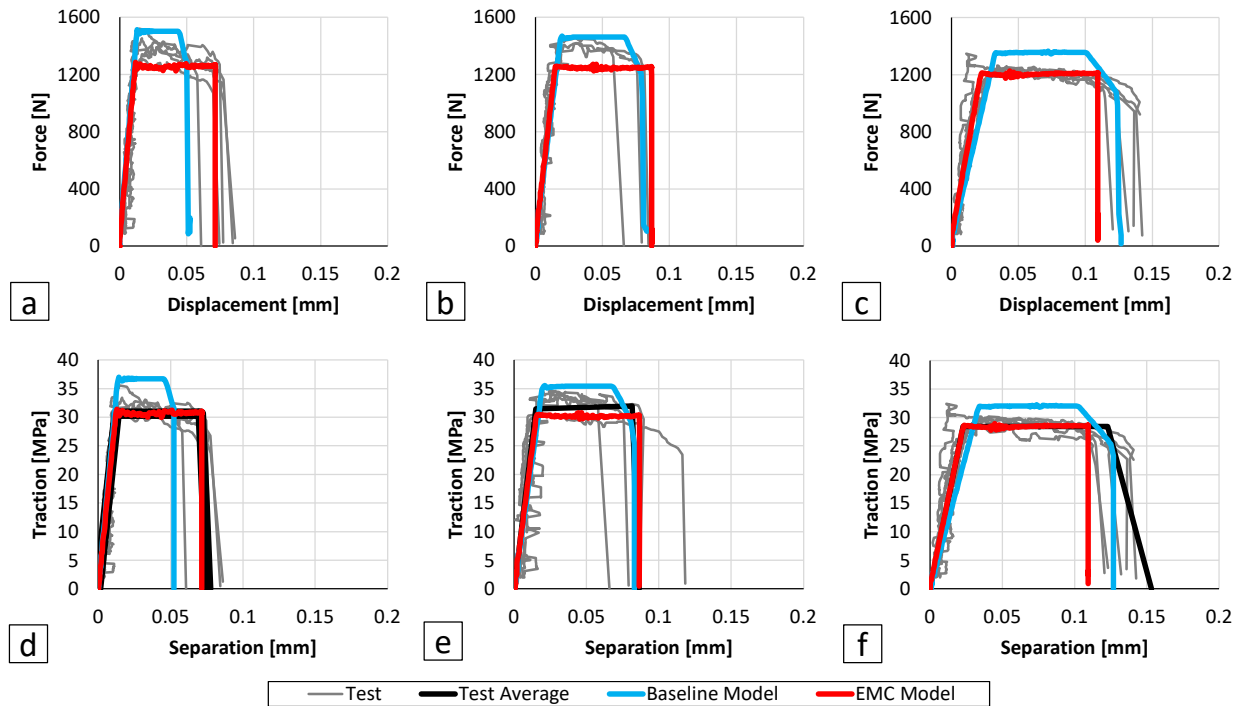


6

7 **Figure 5: Comparison of BDS CZMs to experimental [18] force-displacement response and**  
 8 **corresponding output of traction-separation for nominal bond line thicknesses of 0.18 mm**  
 9 **(a,d), 0.3 mm (b,e), and 0.64 mm (c,f)**

10 The 45° mixed mode EMC models generally reproduced the experimental response well, with the  
 11  $\delta^0$ ,  $\delta^S$ , and  $\delta^f$  values predicted within an average of 2% and average traction within 7%, compared  
 12 to 14% and 24%, respectively, for the baseline model (Figure 6). Despite the EMC models  
 13 reproducing the test response well, some deviation was apparent in the softening portion,  
 14 particularly for the thickest bond line (Figure 6c). For this bond line thickness, the mixity prior to  
 15 failure near the end of the bond line ranged from 0.48 to 0.53, compared to 0.5 in the ideal scenario.

1 This slight change in mixity led to differences in the traction-separation responses for individual  
 2 elements at the ends of the bond line. These deviations and the small difference between the  $\delta^S$  and  
 3  $\delta^f$  values, led to earlier softening of the elements at the end of the bond line compared to elements  
 4 away from the ends. A rebalancing of load across the bond line was then necessary, which led to  
 5 failure of the whole bond area earlier than would otherwise be expected. The minor variation in  
 6 mixity leading to abrupt failure occurred in the softening portion of the baseline model response  
 7 for all three bond line thicknesses, compared to the plateau portion of the response for the EMC  
 8 models. The baseline model also tended to exhibit a higher plateau traction, a lower separation  
 9 between the start and end of the plateau and a greater separation between softening onset and  
 10 failure.

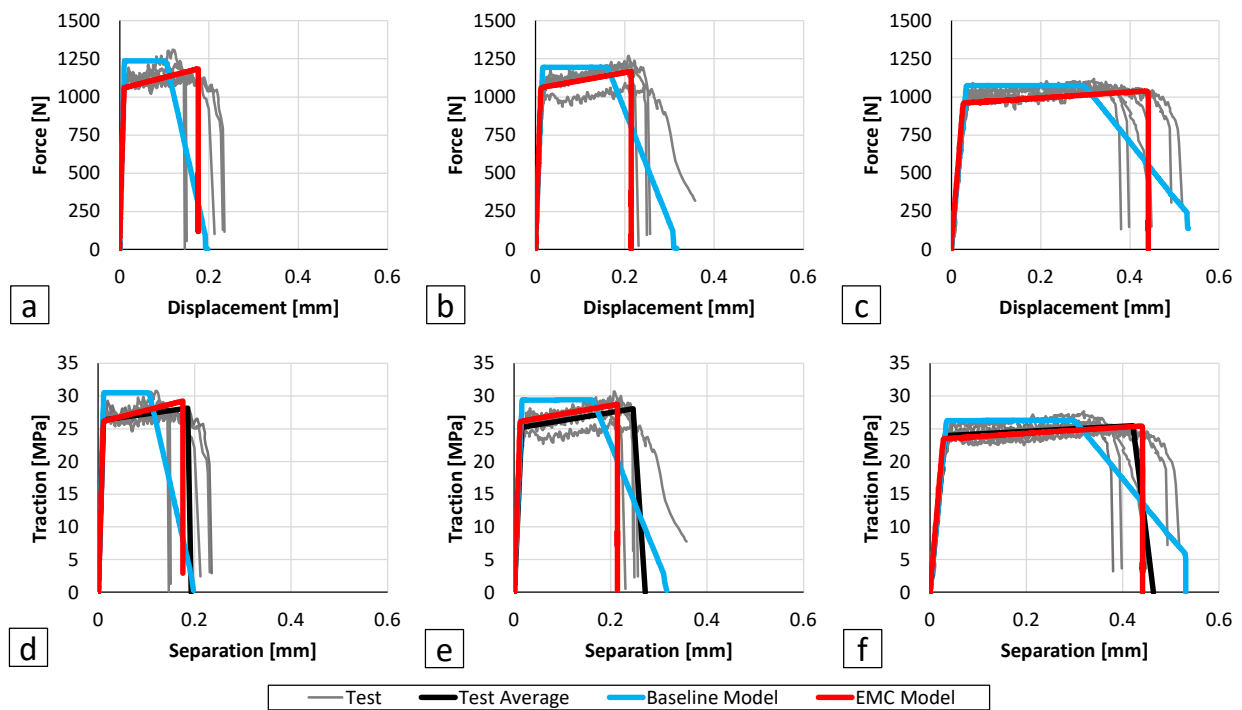


11

12 **Figure 6: Comparison of 45° MM CZMs to experimental [18] force-displacement response**  
 13 **and corresponding output of traction-separation for nominal bond line thicknesses of 0.18**  
 14 **mm (a,d), 0.3 mm (b,e), and 0.64 mm (c,e)**

15

1 As with the 45° mixed mode models, the 75° mixed mode ECM model was substantially better at  
 2 capturing the test response than the baseline models (Figure 7). Of particular note, the hardening  
 3 aspect of the test response was more pronounced in the 75° mixed mode compared to 45°, which  
 4 was captured by the rising plateau of the EMC models. Furthermore, the test and EMC models  
 5 exhibited very little softening, failing abruptly, unlike the baseline models that exhibited much  
 6 more pronounced softening behavior. Both the EMC and baseline models exhibited abrupt failure  
 7 of elements, with the EMC models failing with essentially no progressive softening, as in the  
 8 experiments. The baseline models, however, exhibited a large degree of softening prior to abrupt  
 9 failure from relatively low traction values (less than 10 MPa) in all the bond line thicknesses.



10

11 **Figure 7: Comparison of 75° MM CZMs to force-displacement response and corresponding**  
 12 **output of experimental [18] traction-separation for nominal bond line thicknesses of 0.18**  
 13 **mm (a, d), 0.3 mm (b, e), and 0.64 mm (c, f)**

14

1 The ability of the EMC model to accurately reproduce not only the pure Mode I and Mode II test  
2 response, but also the full traction-separation response for mixed modes of loading is an attractive  
3 feature of the EMC over traditional approaches, where control of the mixed mode response is  
4 somewhat limited. The average absolute difference between the model predictions and test average  
5 for  $\delta^0$ ,  $\delta^s$  and  $\delta^f$  were 11%, 8% and 12%, respectively, for the EMC models compared to 12%, 36%  
6 and 11% for the baseline CZM mixed mode models. Furthermore, the average absolute difference  
7 between the model and test traction at plateau and softening were 2% and 3%, respectively, for the  
8 EMC model, compared to 14% and 5% for the baseline CZM approach. Thus, it can be seen that  
9 the EMC approach addressed the over prediction of plateau traction and under prediction of plateau  
10 length under mixed mode loading identified by Watson *et al.* [18]. The reduction in error  
11 associated with the mixed modes of loading highlights the main advantage of the EMC approach  
12 over traditional treatment of mixed mode loading, despite providing similar levels of fit to the data  
13 for both approaches for pure Mode I and Mode II loading. The trade off for this improved fidelity  
14 in mixed mode response using the EMC approach is that testing is required to characterize the  
15 complete mixed mode traction-separation of a given adhesive [17, 18]. Furthermore, more data  
16 processing is required to derive a set of parameters to fully define the EMC model by first fitting  
17  $E$ ,  $E_{Tan}$ ,  $\sigma_0$ ,  $G$  and  $f$  to Mode I, Mode II and mixed mode test responses and then fitting these CZM  
18 parameters to Equation (13) through Equation (17) rather than only defining the Mode I and Mode  
19 II CZM parameters. However, a single set of parameters can be used to model a range of bond line  
20 thickness, potentially simplifying the input in large-scale models which use multiple bond line  
21 thicknesses.

22 The fit parameters used in the current study can only be used in a relatively narrow band of bond  
23 line thicknesses (between 0.15 mm and 0.7 mm) before the emergence of non-valid traction-

1 separation responses, caused by the combination of parameters leading to  $\delta^f$  values that are less  
2 than the corresponding  $\delta^S$ . Care must be taken to avoid these unphysical responses, although  
3 ideally one would ensure that the characterization tests were undertaken within the range of bond  
4 line thicknesses of interest for the models for which the EMC would ultimately be used.

5 The current study focused on the effects of bond line thickness on the traction-separation response  
6 under various modes of loading. However, the EMC approach could be adapted to investigate  
7 other effects such as temperature during loading, loading rate, the degree of under/overcuring of  
8 the adhesive or other environmental exposure effects. Obviously to investigate these effects,  
9 further experimentation would need to be carried out and Equation (13) through Equation (17)  
10 would need to be updated to include these effects for each parameter. A more refined definition of  
11 the model may also be required for effects that evolve during the simulation, such as the treatment  
12 of loading rate effects by May *et al.* [4]. Future work with the EMC model will involve validating  
13 the model by investigating the predictive capabilities using a series of cross tension tests with  
14 varying loading angles [37] to assess the model for a range of loading modes in scenarios beyond  
15 the verification carried out in the current study. Furthermore, an investigation which exercises the  
16 ability of the new CZM to assess the response of structures with bond lines of varying thicknesses  
17 (as opposed to a series of constant bond line thicknesses) will be carried out.

#### 18 **4 Conclusions**

19 The Enhanced Mixed Mode CZM (EMC) incorporates greater control over the mixed mode  
20 response compared to CZMs that are used in current FE solvers (such as the baseline model),  
21 incorporating a hardening response rather than a plateau and can be implemented with a single set  
22 of parameters for a range of bond line thicknesses. By accounting for hardening of the adhesive

1 joint under Mode II loading using the BDS specimen, the EMC approach eliminated the 13%  
2 average overprediction of traction at the start of the plateau and 10% underprediction of traction  
3 at the end of the plateau present in the baseline model. Furthermore, the EMC approach reduced  
4 the average difference between the model prediction and average test response for separation-to-  
5 plateau, softening and failure (8%) compared to a more traditional CZM approach (22%). The  
6 ECM approach can also readily be extended to account for factors altering the traction-separation  
7 response, such as temperatures, loading rate and environmental factors affecting curing.

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11 Advanced Manufacturing Consortium, Compute Canada and the Natural Sciences and  
12 Engineering Research Council of Canada (NSERC) for their support of this research.

## 13 **Data Availability**

14 The CZM developed in this study will be made available to the research community as a shared  
15 library that can be linked into the LS-DYNA finite element code. Please contact the corresponding  
16 author for information on accessing the CZM shared library.

## 17 **Disclosure Statement**

18 The authors report there are no competing interests to declare.

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