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Potential-based and non-potential-based cohesive zone formulations under mixed-mode separation and over-closure. Part I: Theoretical Analysis

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Abstract
This paper presents a thorough analysis of potential-based and non-potential-based cohesive zone models (CZMs) under conditions of mixed-mode separation and mixed-mode over-closure. Problems are identified with the well established potential-based Xu-Needleman (XN) model and a number of new potential-based and non-potential-based models are proposed. It is demonstrated that derivation of traction-separation relationships from a potential function can result in non-physical repulsive normal tractions and instantaneous negative incremental energy dissipation under displacement controlled monotonic mixed-mode separation when the work of tangential separation exceeds the work of normal separation. A modified potential-based (MP) model is proposed so that the zone in which repulsive normal tractions occur can be controlled. The MP model also provides an additional benefit of correct penalisation of mixed-mode over-closure, in contrast to the XN model. In order to fully eliminate the problem of repulsive normal tractions a non-potential-based CZM (NP1) is also proposed. This model is shown to provide physically realistic behaviour under conditions of displacement controlled mixed-mode separation and over-closure. Noting that the form of the traction-separation equations differ for mode I and mode II separation for the XN, MP and NP1 models, an additional non-potential-based model (NP2) is proposed so that near mode-independent behaviour can be achieved in displacement controlled separation, while correctly penalising over-closure. Following from the NP2 model, a non-potential-based model in which coupling is based on the separation magnitude is considered (SMC model). In the final part of the paper the performance of each model under traction controlled mixed-mode separation is investigated by numerically inverting the traction-separation equations. Separation paths for the XN model reveal a strong bias toward mode I separation while the NP1 model exhibits a bias towards mode II separation. Interestingly, the NP2 model exhibits a high degree of mode sensitivity under traction controlled conditions, in contrast to its near mode independence under displacement controlled conditions. It is demonstrated that incorrect weighting of the coupling terms in non-potential models can lead to the existence of a singularity under traction controlled conditions. Finally, it is demonstrated that the potential-based models fail to capture a gradual change from mode II to mode I work of separation, as reported experimentally for traction controlled interface separation. In a follow-on Part II companion paper a number of case studies are simulated, demonstrating that the theoretical findings of the present paper have significant implications for the finite element prediction of interface debonding.
1 Introduction

Cohesive zone models (CZMs) have been extensively used to describe the delamination process which occurs at the interface between two surfaces (Abdul-Baqi and Van der Giessen, 2001; Barenblatt, 1959; Camacho and Ortiz, 1996; Dugdale, 1960; Ural et al., 2009; Yan and Shang, 2009). CZMs have been used to model crack propagation in porous materials (Nakamura and Wang, 2001), ductile materials (Li and Chandra, 2003) and model coating failure in diamond-coated tools (Hu et al., 2008). CZMs can be coupled or uncoupled. In an uncoupled CZM, the normal traction is independent of the tangential opening separation and vice versa (Tijssens et al., 2000). Uncoupled CZMs are of limited use unless interface separation is constrained to occur in a single predefined direction (e.g. either mode I or mode II separation). Typically, however, CZMs are applied to engineering problems where the mode of interface separation is not predefined, requiring the use of mixed-mode formulations. Such mixed-mode applications require the use of a coupled CZM, whereby all components of the traction vector depend on both the normal and tangential interface separations, in order to provide a physically realistic response. For example if an interface undergoes a complete separation in the tangential direction, the resistance to a subsequent normal separation should be significantly reduced or eliminated. In the present study a detailed analysis of the performance of coupled CZMs under mixed-mode conditions is presented. Problems with existing models are identified and several new models are proposed to overcome such problems.

In addition to mixed-mode separation, mixed-mode over-closure must also be considered. The term over-closure refers to the phenomena whereby contacting surfaces penetrate into one another under a compressive contact stress. Clearly this is non-physical and should be correctly penalised by a CZM formulation. Most CZMs correctly penalise over-closure in pure mode I deformation, where no interface shear (tangential) displacement occurs. However, when the over-closure is mixed-mode, with both negative normal displacements and non-zero shear displacements, it is demonstrated that physically realistic over-closure behaviour is not trivially achieved by all CZM formulations.

The most commonly implemented coupled CZM is that developed by Xu and Needleman (XN) in which traction-separation relationships are obtained from the first derivatives of an interface potential function (Xu and Needleman, 1993). In this model, normal and tangential behaviour is coupled via exponentially decaying functions of normal and tangential separation. The ratio of the work of tangential separation to the work of normal separation, commonly denoted using the symbol “q”, determines the relative strength of the interface under mode I and mode II separation. A similar potential-based model was also proposed by Beltz and Rice, in which a sinusoidal tangential traction-separation relationship is coupled with a Xu-Needleman type normal traction-separation relationship (Beltz and Rice, 1992). Again, the ratio of work of tangential separation to the work of normal separation provides a critical coupling parameter in this model. Several experimental studies have been reported in which the work of normal and tangential separation are different (Dollhofer et al., 2000; Warrior et al., 2003; Yang et al., 2001). However, the ratio of tangential to normal work, q, is arbitrarily set to unity for mixed-mode implementations of the XN CZM (Rahulkumar et al., 2000; Yuan and Chen, 2003; Zavattieri et al., 2008). It should also be noted that a number of previous studies adopt a value of q ≈ 0.43 so that both the normal and tangential maximum tractions have the same value when the normal and tangential interface characteristic distances are assumed to be equal (Abdul-Baqi and Van der Giessen, 2002; Hattiangadi and Siegmund, 2005). A range of values of q ranging from 0.025 to 10.0 were considered in the
original application of the XN model to debonding of spherical inclusions in a metal matrix composite (Xu and Needleman, 1993). In the study of thin film delamination, values of \( q \) ranging from 0.086 to 0.7 were considered by Abdul-Baqi and Van der Giessen (2001) while most recently a value of \( q = 0.5 \) was used by Yan and Shang (2009). A second coupling parameter used in the XN model is the traction-free normal separation following complete shear separation (commonly denoted using the symbol “\( r \)” in the XN potential function). It was noted by Abdul-Baqi and Van der Giessen (2001) that physically realistic penalisation of normal over-closure was computed only if \( r \geq q \). However, the majority of studies that use the XN model set \( r = 0 \) (Rahulkumar et al., 2000; Xu and Needleman, 1993; Zavattieri et al., 2008). Further, a study by van den Bosch et al. (2006) suggests that physically realistic coupling is implemented by the XN model only when \( q = 1 \). An alternative non-potential-based cohesive zone formulation was proposed using the XN traction-separation equations when \( q = 1 \), with independent scaling factors then being applied to normal and tangential equations to account for differences in mode I and mode II interface strength.

To date, no comprehensive analysis of potential and non-potential-based CZMs has been published in which the complete range of diverse interface behaviour under mixed-mode separation and mixed-mode over-closure has been characterised. Furthermore, previous analyses of existing CZMs and proposed CZMs have relied on displacement controlled boundary conditions for model assessment (Abdul-Baqi and Van der Giessen, 2001; Mosler and Scheider, 2011; Park et al., 2009; van den Bosch et al., 2006), without considering traction controlled mode mixity. In Section 2.1 of the present paper an extensive analysis of the XN CZM under displacement controlled interface behaviour is presented, significantly expanding on the initial analyses of Abdul-Baqi and Van der Giessen (2001) and van den Bosch et al. (2006). It is demonstrated that no combination of model parameters provide physically realistic behaviour under both mixed-mode separation and mixed-mode over-closure for this potential-based model. A modified potential-based (MP) model is proposed in Section 2.2, which partially addresses a number of limitations uncovered for the XN model. In Section 3, non-potential-based CZMs are considered, starting with the model of van den Bosch, Schreurs and Geers (BSG model) (van den Bosch et al., 2006). Two alternative non-potential-based models (NP1,NP2) are then proposed, both of which provide physically reasonable coupling under displacement controlled mixed-mode separation and over-closure. A formulation that relies on separation magnitude for coupling of normal and tangential behaviour (SMC) is then considered. Finally, in Section 4 analysis of the aforementioned CZMs under traction controlled mode mixity is presented. Separation paths and work of separation are computed as a function of mode mixity, illustrating anomalous behaviour for both potential and non-potential-based models. Computed work of separation as a function of mode mixity for each model is compared to the theoretical relationship of Hutchinson and Suo (1992). Such traction controlled mode mixity analyses provide new insight into the behaviour of potential and non-potential-based CZMs. In addition to the total work of separation, instantaneous incremental energy dissipation (Cazes et al., 2009) is considered for all separation paths presented in the paper. The findings of the present study provide motivation for the development of mixed-mode finite element case studies in Part II of this two part study, in which the practical importance of the theoretical analysis presented in Part I is illustrated and the advantages of the CZMs proposed in the present study over the established XN and BSG models are demonstrated.
2 Potential-Based CZMs

2.1 Xu-Needleman (XN) Formulation

The XN cohesive zone law has frequently been used to model numerous fracture mechanics problems. This law is based on the definition of an interface potential, $\phi$, representing the work done when two opposing surfaces at an interface undergo a relative separation $\Delta$ (Xu and Needleman, 1993). The resulting tractions are given by:

$$ T(\Delta) = \partial \phi(\Delta)/\partial \Delta $$

(1)

The interface potential is given by:

$$ \phi(\Delta_n, \Delta_t) = \phi_n + \phi_n \exp \left(-\frac{\Delta_n}{\delta_n} \right) \left[ \left(1 - r + \frac{\Delta_n}{\delta_n} \right) \left(\frac{1 - q}{r - 1} \right) - \left\{ q + \left( \frac{r - q}{r - 1} \right) \frac{\Delta_n}{\delta_n} \right\} \exp \left(-\frac{\Delta_t^2}{\delta_t^2} \right) \right] $$

(2)

Coupling in this model is controlled through the parameters $q$ and $r$;

$$ q = \frac{\phi_t}{\phi_n} \quad r = \Delta_n^* / \delta_n $$

$\phi_n$ and $\phi_t$ are the work of normal and tangential separation respectively. The normal and tangential components of the interface separation vector, $\Delta$, are $\Delta_n$ and $\Delta_t$ respectively. The normal and tangential interface characteristic lengths are $\delta_n$ and $\delta_t$ respectively and $\Delta_n^*$ is the value of $\Delta_n$ after complete tangential separation takes place under the condition of normal tension being zero ($T_n = 0$).

Using equations (1) and (2), the interfacial tractions are obtained as follows;

$$ T_n(\Delta_n, \Delta_t) = \frac{\partial \phi}{\partial \Delta_n} = \left( \frac{\phi_n}{\delta_n} \right) \exp \left(-\frac{\Delta_n}{\delta_n} \right) \left[ \left(1 - r + \frac{\Delta_n}{\delta_n} \right) \left(\frac{1 - q}{r - 1} \right) - \left\{ q + \left( \frac{r - q}{r - 1} \right) \frac{\Delta_n}{\delta_n} \right\} \exp \left(-\frac{\Delta_t^2}{\delta_t^2} \right) \right] $$

(3)

$$ T_t(\Delta_n, \Delta_t) = \frac{\partial \phi}{\partial \Delta_t} = 2 \left( \frac{\phi_n}{\delta_t} \right) \left( \frac{\Delta_n}{\delta_n} \right) \left(\frac{r - q}{r - 1} \right) \exp \left(-\frac{\Delta_n}{\delta_n} \right) \exp \left(-\frac{\Delta_t^2}{\delta_t^2} \right) $$

(4)

The characteristic lengths $\delta_n$ and $\delta_t$ are given by;

$$ \delta_n = \phi_n / \left( \sigma_{max} \exp(1) \right) $$

(5)

$$ \delta_t = \phi_t / \left( \tau_{max} \left( 0.5 \exp(1) \right)^{0.5} \right) $$

(6)

Where $\sigma_{max}$ is the maximum normal traction without tangential separation and $\tau_{max}$ is the maximum tangential traction without normal separation.
Figure 1: Work of separation ($\phi/\phi_n$) as a function of normal ($\Delta_n/\delta_n$) and tangential ($\Delta_t/\delta_t$) components of the interface separation vector for the XN model: (a) $q = 2$, $r = 0$; (b) $q = 0.43$, $r = 0$. (c) Maximum normal traction ($T_n,max/\sigma_{max}$) as a function of tangential separation. (d) Normal traction ($T_n/\sigma_{max}$) as a function of normal separation ($\Delta_n/\delta_n$).

Figure 1 (a) shows the work of separation as a function of both normal and tangential separations for $q > 1$. Two paths are compared to obtain the same final mixed-mode interface separation configuration. Undergoing interface separation along the path indicated by the green arrows from the unseparated configuration ($\Delta_n/\delta_n = \Delta_t/\delta_t = 0$) to the final fully separated mixed-mode configuration ($\Delta_n/\delta_n = \Delta_t/\delta_t = 5$), it is clear that the work done during initial normal separation is $\phi_n$ (in accordance with equation (2)). As is also clear from equation (2), the work done for full mixed-mode separation must also be $\phi_n$. Therefore, no subsequent work is done for tangential separation following initial normal separation. In contrast to the path indicated by the green arrows, the red arrows outline a path in which tangential separation is followed by normal separation. For $q > 1$, clearly the work done during the initial tangential separation is greater than $\phi_n$. However, the work of full mixed-mode separation must be $\phi_n$, in accordance with equation (2). Therefore, following initial tangential separation, negative work (red arrow) must be performed to achieve full mixed-mode separation. This negative work gradient results in negative (repulsive) normal tractions for mixed-mode separation conditions.

Figure 1 (b) shows the work of separation as a function of both normal and tangential separations for $q < 1$. Considering the path outlined by the green arrows, the work done
during initial normal separation is again \( \phi_n \) and no subsequent work is done for tangential separation following normal separation. However, considering the path outlined by the red arrows, when \( q < 1 \), the work done during the initial tangential separation is less than \( \phi_n \). Therefore, in the case where \( q < 1 \), following initial tangential separation, normal work is still required to reach full interface separation configuration as the value of work at full mixed-mode separation must be \( \phi_n \). Therefore, positive normal tractions are computed following full tangential separation when \( q < 1 \).

A more physical coupling of normal and tangential behaviour should ensure that, following complete tangential separation at the interface, zero work (and consequently zero traction) should be required for normal separation and vice versa. Tensions which exist following complete interface separation in either the tangential or normal component directions are hereafter referred to as residual tensions. Figure 1 (c) shows the maximum normal tension \( T_{n,\text{max}} \) as a function of tangential separation \( (T_{n,\text{max}} \text{ refers to the maximum normal traction encountered during normal separation for a given tangential separation } \Delta_t \). For example, if \( \Delta_t=0 \), \( T_{n,\text{max}}=\sigma_{\text{max}} \). \( T_{t,\text{max}} \) is defined in a similar fashion). Residual normal tensions for mixed-mode interface separation are evident. The maximum normal traction, \( T_{n,\text{max}} \) after complete tangential separation can be expressed as;

\[
T_{n,\text{max}} = -\sigma_{\text{max}} \exp(-r) \left( \frac{1-q}{r-1} \right)
\]  

(7)

A coupling parameter set which has been widely chosen in literature is \( q = 0.43 \) and \( r = 0 \) (e.g. Abdul-Baqi and Van der Giessen, 2002; Hattiangadi and Siegmund, 2005) as this results in \( \tau_{\text{max}} = \sigma_{\text{max}} \) for \( \delta_n = \delta_t \). However, Figure 1 (c) shows that positive residual normal tensions are computed as \( \Delta_t/\delta_t \to \infty \) for \( q = 0.43 \) and \( r = 0 \). This phenomena occurs for all \( q < 1 \), as illustrated in Figure 1 (b). When \( q = 2 \) and \( r = 0 \), negative residual normal tensions (also referred to as repulsive normal tensions) occur for all values of \( \Delta_n \) following an initial tangential separation \( \Delta_t/\delta_t = 5 \), as shown in Figure 1(d). These unphysical residual tensions, computed when \( q \neq 1 \) are an artefact of the path-independent work of separation \( \phi(\Delta) \), as illustrated in Figure 1((a),(b)). Residual normal tensions can be avoided only if \( q = 1 \) (in which case the parameter \( r \) is redundant (see equations (3),(4))).

A positive value of \( T_{n,\text{max}} \) is computed when \( r = q \ (q \neq 1) \), as shown in Figure 1 (c) for \( r=q=2 \), in contrast to a negative or repulsive value of \( T_{n,\text{max}} \) for \( r=0 \) and \( q=2 \). Figure 1(c) suggests that when \( q > 1 \) the coupling is improved by choosing \( r = q \). However, this is not the case, as illustrated by the full normal traction-separation curves following an initial tangential separation \( (\Delta_t/\delta_t = 5) \) shown in Figure 1(d). If \( q > 1 \) and \( r > 1 \) significant repulsive traction occurs during initial normal separation, followed by residual normal traction. The normal separation at which the local maximum or minimum of normal traction occurs is given as;
\[
(Ar + A + 1)\exp\left(-\frac{\Delta \zeta}{\delta t}\right) - Ar - A
\]
\[
(A + 1)\exp\left(-\frac{\Delta \zeta}{\delta t}\right) - A
\]

where \( A = (1 - q)/(r - 1) \). Therefore if \( \Delta_t/\delta_t = 0 \), then \((\Delta_n/\delta_n)^{\text{max,min}}\) occurs at 1. However, if \( \Delta_t/\delta_t \to \infty \) then \((\Delta_n/\delta_n)^{\text{max,min}}\) occurs at \( r + 1 \). This can clearly be seen in Figure 1 (d). When \( r = q \) \((q \neq 1)\), negative normal tractions are computed for \( \Delta_n/\delta_n < r \) due to the shifting of the normal traction-separation response. The occurrence of residual positive normal tractions was considered by van den Bosch et al. (2006). However, the traction at \( \Delta_n/\delta_n = 1 \) was incorrectly reported as the peak traction for all values of \( \Delta_t/\delta_t \). Non-zero values of \( r \) have previously been used in finite element implementations of the XN model (e.g. Abdul-Baqi and Van der Giessen, 2001). Figure 1(c, d) demonstrate that this coupling parameter can have a pronounced affect on computed normal tractions.

![Figure 2](image_url)

**Figure 2:** (a) Maximum tangential traction \((T_{t,\text{max}}/\tau_{\text{max}})\) as a function of normal separation \((\Delta_n/\delta_n)\) for a range of \( r \) and \( q \) coupling parameters. (b) Work of separation \((\phi/\phi_n)\) as a function of normal \((\Delta_n/\delta_n)\) and tangential \((\Delta_t/\delta_t)\) components of the interface separation vector for \( q = 1 \).

The normal separation at which local maxima/minima tangential tractions occur is given as:

\[
(\Delta_n/\delta_n)_{T_{t,\text{max}}/\tau_{\text{max}}}^{\text{max,min}} = r(1 - q)/(r - q)
\]

Figure 2(a) shows that the maximum tangential traction response can be greatly affected, according to the specific parameter set chosen. Several previous studies have assumed \( q = 1 \) when implementing the XN model (Rahulkumar et al., 2000; Yuan and Chen, 2003; Zavattieri et al., 2008). For this specific case clearly the parameter \( r \) is redundant. However, for \( q = 1 \), unphysical tangential behaviour will be computed in cases of mixed-mode over-closure. Specifically, as illustrated in Figure 2 (a), maximum tangential tractions reduce as the magnitude of normal over-closure increases for \( q = 1 \). In fact for large magnitudes of normal over-closure\((\Delta_n/\delta_n < -1)\), negative maximum tangential tractions are computed. In addition to the specific case where \( q = 1 \), this problem also occurs for all values of \( q \) when \( r = 0 \). As previously mentioned, several studies have assumed that \( q = 0.43 \) and \( r = 0 \).
However, inaccuracies computed due to over-closure have not previously been investigated. A previous study by van den Bosch et al. (2006) suggests that penalisation of mode I normal over-closure will prevent the computation of reduced tangential traction in over-closure. In Part II of this study, simulation results are presented that illustrate that this is not the case.

Also shown in Figure 2 (a), repulsive tangential tractions develop during mixed-mode over-closure when \( r < q \) as highlighted by van den Bosch et al. (2006). It is only when \( r = q \) \( (q \neq 1) \) that a realistic physical response is obtained for mixed-mode over-closure, and maximum tangential tractions decreasing gradually with increasing normal separation. However, as demonstrated in Figure 1(d) negative normal tractions are computed for mixed-mode separation when \( r = q \) \( (q \neq 1) \) and residual normal tractions as \( \Delta_t / \delta_t \to \infty \).

The evolution of repulsive tractions during mixed-mode over-closure for \( q = 1 \) is further illustrated by considering the interface potential \( \phi \) (Figure 2(b)). For zero normal separation, \( \partial \phi / \partial \Delta_n > 0 \). This results in the expected form of pure mode II separation. However, normal over-closure leads to a decrease in \( \partial \phi / \partial \Delta_n \). At \( \Delta_n / \delta_n = -1 \), \( \partial \phi / \partial \Delta_t = 0 \). This results in the unphysical behaviour whereby there is no resistance to tangential separation, despite compression of the interface. Further over-closure leads to \( \partial \phi / \partial \Delta_n < 0 \), resulting in repulsive tangential traction. While this may be appropriate at an atomic length scale, it is unphysical at the length scales of most engineering applications.

![Figure 3](image-url)

**Figure 3:** (a) Normal traction \( (T_n / \sigma_{max}) \) as a function of normal separation \( (\Delta_n / \delta_n) \) for increasing tangential separations (b) Tangential traction \( (T_t / T_{max}) \) as a function of tangential separation \( (\Delta_t / \delta_t) \) for increasing normal separations (c) Work of separation \( (\phi / \phi_n) \) as a function of normal \( (\Delta_n / \delta_n) \) and tangential \( (\Delta_t / \delta_t) \) separations. In all cases \( q=0.3, r=0.5 \).

In a study by Abdul-Baqi and Van der Giessen (2001) thin film delamination during indentation was simulated using the XN CZM. A number of parameter sets were considered in this study whereby \( r \neq 0 \) and \( q \neq 1 \); here one such combination, namely \( r = 0.5 \) and
\( q = 0.3 \), is considered in order to further illustrate the unphysical behaviour that can be computed by the XN model. Again, two separation paths are considered (Figure 3(c)): Partial normal separation followed by shear separation (green arrows); partial tangential separation followed by normal separation (red arrows). We have shown in Figure 1(a),(b) that only the latter (red) path leads to unphysical behaviour if \( r = 0 \). However, when \( r \neq 0 \), unphysical behaviour is computed for both paths.

Considering the green path, following initial normal separation, negative tangential work is computed during subsequent tangential separation \((\partial \phi / \partial \Delta_t < 0)\). Resultant repulsive tangential tractions are illustrated in Figure 3(b) following initial normal separations of \( \Delta_n/\delta_n = 2 \) and \( \Delta_n/\delta_n = 3 \). The tangential response for pure mode II separation \((\Delta_n/\delta_n = 0)\) is also shown in Figure 3(b) for comparison. The unphysical repulsive forces computed under mixed-mode conditions are characterised by a change in sign of the computed tractions. As \( \Delta_n/\delta_n \to \infty \) the magnitude of negative tangential traction reduces.

Next, considering the red path: following initial tangential separation, negative normal work is computed during subsequent normal separation \((\partial \phi / \partial \Delta_n < 0)\). This response is shown in terms of normal traction in Figure 3 (a) \((\Delta_t/\delta_t = 2)\). The normal traction-separation response is shifted and the maximum normal traction occurs at \( r + 1 \) as discussed above. The traction-separation curve for pure mode I separation \((\Delta_t/\delta_t = 0)\) is also shown in Figure 3(a) for comparison.

### 2.2 Modified Potential (MP) Formulation

In an effort to overcome the problems uncovered above for the XN model we propose a modified form of the XN potential function:

\[
\phi(\Delta_n,\Delta_t) = \phi_n \left[ 1 + \exp \left( \frac{-f(\Delta_t)\Delta_n}{\delta_n} \right) \left( 1 - r + \frac{f(\Delta_t)\Delta_n}{\delta_n} \right) \left( \frac{1 - q}{r - 1} \right) - \exp \left( -\frac{\Delta_t^2}{\delta_t^2} \right) \left( q + \frac{f(\Delta_t)\Delta_n}{\delta_n} \left( \frac{r - q}{r - 1} \right) \right) \right] \tag{10}
\]

where

\[
f(\Delta_t) = 1 + m - m \exp \left( -\frac{\Delta_t^2}{\delta_t^2} \right) \tag{11}
\]

The new interface parameter, \( m \), provides additional coupling between normal and tangential tractions. All other variables and parameters have the same meaning as defined for the XN model.

Once again, interface traction-separation relationships are obtained from \( T(\Delta) = \partial \phi(\Delta) / \partial \Delta \), giving the following expressions:

\[
T_n(\Delta_n,\Delta_t) = \frac{\partial \phi}{\partial \Delta_n} = f(\Delta_t) \left( \frac{\phi_n}{\delta_n} \right) \exp \left( \frac{-f(\Delta_t)\Delta_n}{\delta_n} \right) \left( \frac{f(\Delta_t)\Delta_n}{\delta_n} \exp \left( -\frac{\Delta_t^2}{\delta_t^2} \right) + \frac{1 - q}{r - 1} \left[ 1 - \exp \left( -\frac{\Delta_t^2}{\delta_t^2} \right) \right] \left( r - \frac{f(\Delta_t)\Delta_n}{\delta_n} \right) \right) \tag{12}
\]
and

$$T_t(\Delta_n, \Delta_t) = \frac{\partial \phi}{\partial \Delta_t} = 2 \left( \frac{\phi_n}{\delta_t} \right) \frac{\Delta_t}{\delta_t} \exp \left( - \frac{\Delta_t^2}{\delta_t^2} \right) \exp \left( - \frac{f(\Delta_t) \Delta_n}{\delta_n} \right) \left[ \left( q + \left( \frac{r}{r-1} \right) f(\Delta_t) \Delta_n \right) + \left( m \Phi_0 \Delta_n \right) \right]$$

$$+ \left( \frac{m \Delta_n}{\delta_n} \right) \left( \frac{1-q}{1-r} \right) \left( 1 - \exp \left( - \frac{\Delta_t^2}{\delta_t^2} \right) \right) \left( r - \frac{f(\Delta_t) \Delta_n}{\delta_n} \right)$$

(13)

**Figure 4**: Work of separation ($\phi/\phi_n$) as a function of normal ($\Delta_n/\delta_n$) and tangential ($\Delta_t/\delta_t$) components of the interface separation vector for the MP model with $q=2$ and $r=0$: (a) $m=0$ (XN model); (b) $m=1$; (c) $m=5$. Dotted line indicates a path comprising of mixed-mode separation followed by normal separation.

As with the XN model, the parameter, $q$, represents the ratio of work of pure mode II separation to the work of pure mode I separation. The parameter $m$ controls the zone of influence of mode II behaviour for mixed-mode conditions. If $m=0$, the potential function collapses to the XN model. An increasing value of $m$ leads to a decreasing region in which mode II behaviour dominates. To illustrate this point, Figure 4 considers the case where $\phi_t > \phi_n$ (a case where $\phi_t < \phi_n$ is presented in Appendix A). Three cases are considered, $m=0$ (the XN model), $m=1$, and $m=5$. All three potential functions are identical for pure mode I separation and also for pure mode II separation. Clearly, when $m=5$ the transition from mode II behaviour to mode I behaviour is confined to a narrow region near the mode II axis. In contrast, when $m=0$ (XN model) the transition from mode II to mode I behaviour is very gradual. The implications of reducing the transition zone become clear when one considers a separation path that follows a line at a shallow angle to the mode II axis followed by normal
separation, as shown in Figure 4. For the case of \( m = 0 \) (XN model), following the initial phase of the interface deformation, in which the separation is predominantly in the tangential direction, negative work of separation occurs during the second phase of the deformation in the normal direction. This results in repulsive normal tractions, as outlined in Section 2.1. However, as the parameter \( m \) is increased, the region in which repulsive normal tractions occur is reduced. Considering the case of \( m = 1 \) (Figure 4(b)), following the initial mixed-mode separation the negative gradient of \( \phi \) encountered during the subsequent normal separation is significantly reduced from that computed for the XN model \((m = 0)\) shown in Figure 4(a). Hence, the magnitude of repulsive normal tractions is reduced when \( m > 0 \). For \( m = 5 \), as shown in Figure 4(c), no significant repulsive normal tractions are computed for the same path. In this case the transition zone from mode II to mode I separation is sufficiently small such that the illustrated path does not encounter any negative gradients of \( \phi \) during the second normal phase of the separation. It is important to note, however, that the possibility of computing repulsive normal tractions cannot be fully eliminated for any potential-based model where the mode II work of separation exceeds the mode I work of separation \((q > 1)\). This is very clearly illustrated in Figure 4(c) \((m = 5)\): despite the significantly reduced zone in which repulsive normal tractions are computed, a pure mode II separation will necessarily lead to the computation of repulsive normal tractions. In fact for a given value of \( q \), the magnitude of repulsive normal tractions computed following a pure mode II separation will be highest for potential surfaces with smaller transition zones between mode II and mode I separation.

![Figure 5](image)

**Figure 5:** (a) Tangential traction \((T_{t}/\tau_{\text{max}})\) as a function of tangential displacement \((\Delta_{t}/\delta_{t})\) for \( q=2 \) and \( r=0 \) during a mixed-mode separation where \( Tan^{-1}(\Delta_{n}/\Delta_{t}) = 20^\circ \). (b) Normal traction \((T_{n}/\sigma_{\text{max}})\) as a function of normal displacement \((\Delta_{n}/\delta_{n})\) representing a normal separation subsequent to the mixed-mode separation shown in (a). Curves are shown for the XN model and the MP model \((m=1, 2 \text{ and } 5)\). Instantaneous incremental energy dissipation \((d\phi_{i}/\phi_{n})\) during loading paths considered in (a) and (b) are plotted in (c) and (d) respectively.
Figure 5(a) shows the tangential traction-separation curves for a mixed-mode separation at 20° to the mode II axis for the XN model and for the MP model with $m = 1, 2$ and 5. The initial slope is identical for all models. Additionally, the peak traction is not strongly affected by the value of $m$ in the MP model. It can be noted, however, that larger values of $m$ lead to a more rapid decrease in tangential traction for increasing separation post peak. When this mixed-mode separation is followed by an increase in normal separation (with tangential separation held constant at $\Delta_t / \delta_t = 5$), a repulsive normal traction of $T_n / \sigma_{\text{max}} = -0.8$ is computed at $\Delta_n / \delta_n \approx 2$ for the XN model, as shown in Figure 5(b). Repulsive normal tractions reduce as normal separation increases, but in the case of the XN model, repulsive normal tractions are still evident at a normal separation of $\Delta_n / \delta_n = 8$. For the MP model with $m = 1$, the magnitude of repulsive normal tractions are significantly reduced from the XN case. Additionally, repulsive normal tractions are negligible when $\Delta_n / \delta_n \geq 4$. A further reduction is evident when $m = 2$, with no significant repulsive normal tractions being computed when $\Delta_n / \delta_n \geq 3$. Finally, it is demonstrated in Figure 5(b) that no repulsive normal tractions are computed during the normal separation phase when $m = 5$. Again, this corresponds to the potential plot of Figure 4(c), in which the reduced zone in which repulsive normal tractions are computed does not coincide with the separation path.

Energy dissipation at the interface is analysed by considering a weak criterion and a strong criterion for positive dissipation:

- **Weak criterion** – the CZM produces a "globally" dissipative loading i.e. net positive work over a separation path.
- **Strong criterion** – the CZM produces instantaneous positive incremental dissipation over the entirety of a loading path.

An expression for the instantaneous incremental dissipation (Cazes et al., 2009) is given as:

$$d \phi_i = 0.5(T d \Delta - \Delta d T)$$  \hspace{1cm} (14)

Clearly a potential-based model will satisfy the weak criterion for any loading path that starts at the reference undeformed configuration. In the case of a closed deformation loop a potential-based model will yield zero net dissipation. However, in the absence of damage the aforementioned strong criterion will not be satisfied by a potential-based model during a closed deformation loop; instantaneous positive dissipation will occur during part of the cycle (loading) while negative dissipation will also occur during part of the cycle (unloading). However, negative instantaneous dissipation in potential-based CZMs is not limited to closed deformation loops under cyclic loading. The loading path in Figure 4, in which the interface displacement magnitude increases monotonically, gives rise to negative dissipation, particularly during the second part of the loading path when repulsive normal tractions are computed, as shown in Figure 5(b). Figure 5(d) confirms the MP model reduces negative dissipation during this part of the loading path. Interestingly, as shown in Figure 5(c), during the first part of the loading path, in which near mode II loading occurs ($\tan^{-1}(\Delta_n / \Delta_t) = 20°$), negative dissipation is also observed, again due to the computation of negative normal tractions for both the XN and MP models.
Figure 6: Instantaneous incremental energy dissipation \( (d\phi_i/\phi_n) \) during constant separation mode \( (\theta = Tan^{-1}(\Delta_n/\Delta_t)) \) loading paths with \( q=4, r=0 \). (a) XN model and (b) MP model \( (m=5) \).

Figure 6 presents an examination of instantaneous incremental dissipation during monotonic loading to failure for a range of separation mode angles, \( \theta \), again where \( \theta = Tan^{-1}(\Delta_n/\Delta_t) \) for the XN model (Figure 6(a)) and the MP model with \( m=5 \) (Figure 6(b)). In both cases the work of mode II separation exceeds the work of mode I separation \( (q=4) \). As expected, identical pure mode I and pure mode II separation is computed for both models with \( d\phi_i > 0 \) throughout separation. However, for mixed-mode separation paths, negative dissipation is computed \( (d\phi_i < 0) \). In the case of the XN model, prolonged negative dissipation occurs. When the separation magnitude reaches a value of \( \Delta_e/\delta_n = 8 \) significant negative dissipation still occurs. In fact for a separation mode angle of \( \theta = 3\pi/8 \) the instantaneous dissipation remains negative until \( \Delta_e/\delta_n \approx 25 \). In contrast, for the MP model negative instantaneous dissipation is computed over a short range of separation magnitude, with all mixed-mode separation paths exhibiting zero dissipation for \( \Delta_e/\delta_n > 4 \). It should be noted however, that the \( d\phi_i \) exhibits a stronger negative peak than is the case for the XN model.

In summary, the aforementioned weak criterion for dissipation is satisfied for both the XN and MP model. However, when \( \phi_i > \phi_n \), even in the case of monotonic loading, neither model satisfies the strong condition \( d\phi_i > 0 \). The MP model reduces the zone of repulsive normal traction and consequent negative dissipation, but at the price of increasing the magnitude of repulsive tractions within this zone, as can be observed by comparing Figure 7 (MP model) to Figure 1 (XN model).

Figure 7: MP model with \( q = 2 \) and \( r = 0 \): (a) Maximum normal traction \( (T_{n,max}/\sigma_{max}) \) as a function of tangential separation; (b) Normal traction \( (T_n/\sigma_{max}) \) as a function of normal separation \( (\Delta_n/\delta_n) \).
Figure 8: (a) Work of separation \(\phi/\phi_n\) as a function of normal \((\Delta_n/\delta_n)\) and tangential \((\Delta_t/\delta_t)\) components of the interface separation vector for the MP model with \(m=1, q=1\) and \(r=0\). Green arrow highlights the positive gradient of \(\phi\) w.r.t. \(\Delta_n\). Red arrow highlights the positive gradient of \(\phi\) w.r.t. \(\Delta_t\) indicating correct penalisation of mixed-mode overclosure, with resistance to tangential separation increasing with increasing normal overclosure. (b) Maximum tangential traction \(T_{t,max}/\tau_{max}\) as a function of normal separation \((\Delta_n/\delta_n)\) for the MP model. Curves are shown in both separation and overclosure for \(m=0\) (XN model), \(m=1\), \(m=2\) and \(m=5\).

Figure 8(a) shows the potential surface for the MP model \((m = 1)\) for the case of \(q = 1\). It should be recalled that the XN model fails to correctly penalise mixed-mode over-closure for \(q = 1\) (see Figure 2(b)), with a negative gradient of \(\phi\) in the tangential direction leading to repulsive tangential tractions. In contrast to the XN model, increasing over-closure in the MP model is accompanied by increasing gradients of \(\phi\) in the tangential direction. This leads to an increasing penalisation of tangential separation with increasing normal over-closure, resulting in a physically realistic penalisation of mixed-mode over-closure. It should be noted however, that for \(\Delta_t/\delta_t > 1\) the gradient of \(\phi\) in the tangential direction becomes negative, leading to reduced penalisation of tangential separation, and repulsive tangential tractions at high values of \(\Delta_t/\delta_t\). Despite this limitation, the MP model represents an improvement on the XN model where resistance to tangential separation is reduced for the entire over-closure regime. The relationship between tangential traction and normal separation for the MP model for \(q = 1\) is further examined in Figure 8(b). The XN model \((m = 0)\) is included for comparison, again highlighting the unphysical reduction in maximum tangential traction, \(T_{t,max}\), with increasing normal over-closure \((\Delta_n < 0)\). In contrast to the XN model, the MP model correctly penalises mixed-mode over-closure, with maximum tangential traction increasing with increasing normal over-closure for all cases considered. An increase in the coupling parameter, \(m\), results in an increased penalisation of mixed-mode over-closure. In separation \((\Delta_n > 0)\), the MP relationship between \(T_{t,max}\) and \(\Delta_n\) is very similar to the XN model. However, for \(m = 5\) a slight increase in \(T_{t,max}/\tau_{max}\) to a value of 1.11 can be observed for \(0 < \Delta_n/\delta_n < 0.35\). This affect is less pronounced for \(m = 2\) and is not significant for \(m = 1\).
3 Non-Potential-Based CZMs

3.1 BSG Formulation

A modification of the XN model has been proposed by van den Bosch et al. (2006) (BSG model) to provide improved coupling under mixed-mode conditions. Essentially this model uses the traction-separation equations for the XN CZM for \( q = 1 \) and then applies independent scaling factors in the normal and tangential directions to prescribe the peak tractions. The resultant traction-separation relationships are given as:

\[
T_n(\Delta_n, \Delta_t) = \left( \frac{\phi_n}{\delta_n^2} \right) \frac{\Delta_n}{\delta_n} \exp\left(-\frac{\Delta_n}{\delta_n}\right) \exp\left(-\frac{\Delta_t^2}{\delta_t^2}\right)
\]

(15)

\[
T_t(\Delta_n, \Delta_t) = 2 \left( \frac{\phi_t}{\delta_t} \right) \frac{\Delta_t}{\delta_t} \left[1 + \frac{\Delta_n}{\delta_n} \right] \exp\left(-\frac{\Delta_n}{\delta_n}\right) \exp\left(-\frac{\Delta_t^2}{\delta_t^2}\right)
\]

(16)

\( \phi_n \) and \( \phi_t \) (the work of mode I and mode II separation, respectively) are independent model parameters. If \( \phi_n \neq \phi_t \) the traction-separation relationships cannot be derived from a potential function (i.e. \( \partial T_n/\partial \Delta_t \neq \partial T_t/\partial \Delta_n \)), so the work done during mixed-mode separation is path-dependent. Such a non-potential-based CZM eliminates several problems associated with mixed-mode separation (as described in the previous section). However, given that this model is based on XN traction-separation relationships for \( q = 1 \), unphysical behaviour is similarly computed in mixed-mode over-closure. This is illustrated in Figure 9, which shows the work done when a normal displacement of \( \Delta_{n,\text{max}} \) is followed by a complete tangential separation, whereby \( \Delta_t \) increases from 0 to \( \infty \). In addition to total work, the work of normal separation and the work of tangential separation are plotted and both normal separation and over-closure are considered. Model parameters are chosen such that \( \phi_t = 0.34\phi_n \) so that \( \tau_{\text{max}} = 0.8\sigma_{\text{max}} \). Firstly, as shown in Figure 9(a), this model provides a monotonic increase in total work with increasing \( \Delta_{n,\text{max}} \) as reported previously by van den Bosch et al. (2006). However, focusing on the over-closure regime, the work of tangential separation reduces with increasing normal over-closure. In fact, for large values of normal over-closure (\( \Delta_n/\delta_n < -1 \)) negative tangential work is computed, resulting in repulsive tangential forces. A case study is presented in Part II of this study to demonstrate that this unphysical behaviour in mixed-mode over-closure can lead to inaccurate simulation of coating buckling from a stent surface.
Figure 9: Work performed where an interface first undergoes pure normal separation until $\Delta_n = \Delta_{n,max}$ followed by a complete tangential separation for (a) BSG model (b) NP1 model (c) NP2 model and (d) SMC model. In all cases $\tau_{\max} = 0.8 \sigma_{\max}, \delta_n = \delta_t = 1$.

### 3.2 Non-Potential-Based Formulation 1 (NP1)

In order to correct the unphysical behaviour of the BSG CZM in mixed-mode over-closure we propose a modified form of the tangential traction-separation relationship. The term $(1 + \Delta_n / \delta_n)$ in equation (16) is removed, thus eliminating reductions in peak tangential traction during mixed-mode over-closure. The resultant traction-separation relationships are expressed as

\[ T_n(\Delta_n, \Delta_t) = \sigma_{\max} \exp(1) \left( \frac{\Delta_n}{\delta_n} \right) \exp \left( -\frac{\Delta_n}{\delta_n} \right) \exp \left( -\frac{\Delta_n^2}{\delta_n^2} \right) \tag{17} \]

\[ T_t(\Delta_n, \Delta_t) = \tau_{\max} \sqrt{2} \exp(1) \left( \frac{\Delta_t}{\delta_t} \right) \exp \left( -\frac{\Delta_n}{\delta_n} \right) \exp \left( -\frac{\Delta_n^2}{\delta_n^2} \right) \tag{18} \]

where $\sigma_{\max}$ and $\tau_{\max}$ are the peak tractions computed during pure mode I and pure mode II separation, respectively. Equations 17 and 18 cannot be derived from a potential function.

Figure 9(b) shows the work done when a normal displacement of $\Delta_{n,max}$ is followed by a complete tangential separation again with $\tau_{\max} = 0.8 \sigma_{\max}$. The tangential work, $W_t$, increases with increasing normal over-closure, providing a physically realistic representation of mixed-mode over-closure, in contrast to the BSG model. However, it should be noted that a slight reduction in $W_{\text{total}}$ is computed as $\Delta_{n,max}$ initially increases from 0. This is due to a
rapid decrease in tangential work as $\Delta_{n,max}$ increases from 0. This is in contrast to the monotonic increase in $W_{total}$ computed by the BSG model (Figure 9(a)).

### 3.3 Non-Potential-Based Formulation 2 (NP2)

It should be noted that the three CZMs presented thus far (XN, BSG and NP1) have different forms for mode I and mode II separation. In all three cases normal tractions for mode I separation are of the form $\sigma_{max} \exp\left(-\frac{\Delta_n}{\delta_n}\right)$ while tangential tractions for mode II separation are of the form $\tau_{max} \exp\left(-\frac{\Delta_t}{\delta_t}\right)$. Therefore, no model parameters can be chosen so that identical mode I and mode II traction-separation relationships are obtained for these three models. In order to overcome this limitation a non-potential-based formulation (NP2) is proposed:

$$T_n(\Delta_n, \Delta_t) = \sigma_{max} \exp(1) \left(\frac{\Delta_n}{\delta_n}\right) \exp\left(-\frac{\Delta_n}{\delta_n}\right) \exp\left(-\alpha \frac{\Delta_t^2}{\delta_t^2}\right)$$  \hspace{1cm} (19)

$$T_t(\Delta_n, \Delta_t) = \tau_{max} \exp(1) \left(\frac{\Delta_t}{\delta_t}\right) \exp\left(-\frac{\Delta_t}{\delta_t}\right) \exp\left(-\beta \frac{\Delta_n}{\delta_n}\right)$$  \hspace{1cm} (20)

This model provides identical behaviour in mode I and mode II separation when $\sigma_{max} = \tau_{max}$ and $\delta_n = \delta_t$. The parameters $\alpha$ and $\beta$ can be used to specify the weighting of the mixed-mode coupling terms. For the case of $\alpha = \beta = (\sqrt{2} - 1)$ it can easily be demonstrated that identical normal and tangential components of the traction vector are obtained for $45^\circ$ mixed-mode separation ($\Delta_n = \Delta_t$) with the effective traction ($\sqrt{T_n^2 + T_t^2}$) versus effective separation ($\sqrt{\Delta_n^2/\delta_n^2 + \Delta_t^2/\delta_t^2}$) curve being identical to that of mode I or mode II separation. For the remainder of the present study it is assumed that $\alpha = \beta = (\sqrt{2} - 1)$ for the NP2 model unless otherwise stated. Equations 19 and 20 cannot be derived from a potential function.

In order to assess the mixed-mode behaviour of NP2 when $\tau_{max} \neq \sigma_{max}$, Figure 9(c) shows the work done when a normal displacement of $\Delta_{n,max}$ is followed by a complete tangential separation when $\tau_{max} = 0.8 \sigma_{max}$. Firstly, in contrast to the BSG model (Figure 9(a)) and to NP1 (Figure 9(b)), it should be noted that the ratio the of work of mode I separation to the work of mode II separation is identical to the ratio of $\sigma_{max}$ to $\tau_{max}$, as expected given the identical forms of mode I and mode II traction-separation. A drawback of NP2 is that a monotonic increase in $W_{total}$ is not obtained for increasing $\Delta_{n,max}$ with a maximum value of $W_{total}$ being computed at $\Delta_{n,max}/\delta_n \approx 4.4$. Next considering NP2 in over-closure, tangential work increases with increasing normal over-closure, providing physically realistic mixed-mode over-closure similar to that of NP1.
3.4 Separation Magnitude Coupling Formulation (SMC)

Finally, a third non-potential-based model is considered (SMC) in which the effective separation \( \Delta n^2 \delta n^2 + \Delta t^2 \delta t^2 \) is used to couple the normal and tangential interface tractions, as shown in equations (21) and (22):

\[
T_n(\Delta n, \Delta t) = \sigma_{max} \exp(1) \left( \frac{\Delta n}{\delta n} \right) \exp \left( - \frac{\Delta n^2}{\delta n^2} \frac{\Delta t^2}{\delta t^2} \right)
\]

\[
T_t(\Delta n, \Delta t) = \tau_{max} \exp(1) \left( \frac{\Delta t}{\delta t} \right) \exp \left( - \frac{\Delta n^2}{\delta n^2} \frac{\Delta t^2}{\delta t^2} \right)
\]

This model provides identical behaviour in mode I and mode II separation when \( \sigma_{max} = \tau_{max} \) and \( \delta n = \delta t \). Additionally, it is clear that the traction magnitude \( \sqrt{T_n^2 + T_t^2} \) is independent of the mode mixity, depending only on the effective separation. Additionally, it can easily be demonstrated that \( \partial T_n / \partial \Delta t = \partial T_t / \partial \Delta n \), i.e. the traction separation equations can be derived from a potential function

\[
\phi(\Delta n, \Delta t) = \phi_0 + \sigma_{max} \exp(1) \left( 1 + \frac{\Delta n^2}{\delta n^2} + \frac{\Delta t^2}{\delta t^2} \right) \exp \left( - \frac{\Delta n^2}{\delta n^2} \frac{\Delta t^2}{\delta t^2} \right)
\]

only when \( \sigma_{max} = \tau_{max} \) and \( \delta n = \delta t \). A similar observation has been reported for bi-linear “truss-like” CZMs by Goutianos and Sørensen (2012).

The SMC model is non-potential-based and path-dependent if \( \tau_{max} \neq \sigma_{max} \) or if \( \delta n \neq \delta n \) (i.e. \( \partial T_n / \partial \Delta t \neq \partial T_t / \partial \Delta n \)). Considering the mixed-mode behaviour of SMC when \( \tau_{max} \neq \sigma_{max} \), Figure 9(d) shows the work done when a normal displacement of \( \Delta n_{max} \) is followed by a complete tangential separation when \( \tau_{max} = 0.8 \sigma_{max} \). In contrast to the NP2 formulation, SMC provides a monotonic increase in \( W_{total} \) for increasing \( \Delta n_{max} \). However, it is clear from equations (21, 22) and from Figure 9(d) that the SMC formulation provides identical traction-separation behaviour in over-closure and in separation. Therefore, as over-closure is not penalised in a physically realistic fashion it is suggested that the SMC model should be used for separation (\( \Delta n \geq 0 \)) only. In cases where both separation and over-closure may be encountered the SMC model could be used in separation with the NP2 formulation being used in over-closure. Such a scheme is computationally attractive as the NP2 and SMC CZMs have an identical mode II traction-separation relationship.

In summary, three non-potential-based cohesive zone formulations have been proposed in order to achieve physically realistic coupling between normal and tangential tractions in mixed-mode separation and mixed-mode over-closure. Figure 10 (a) demonstrates that maximum normal traction, \( T_{n, max} \) reduces with increasing tangential separation for all models (NP1, NP2, SMC). The details of the coupling differ between models with the steeper coupling terms \( \exp - (\Delta n^2 / \delta n^2) \) of NP1 leading to the disappearance of normal tractions at a low tangential separation \( \Delta t / \delta t \approx 3 \) in contrast to NP2 and SMC. Figure 10 (b)
demonstrates that maximum tangential traction, $T_{t,\text{max}}$, reduces with increasing normal separation ($\Delta_n/\delta_n > 0$) for all models (NP1,NP2, SMC). However, as previously stated, only NP1 and NP2 provide a physically realistic penalisation of mixed-mode over-closure.

Figure 10: (a) Maximum normal traction ($T_{n,\text{max}}/\sigma_{\text{max}}$) as a function of tangential separation ($\Delta_t/\delta_t$). (b) Maximum tangential traction ($T_{t,\text{max}}/\tau_{\text{max}}$) as a function of normal separation ($\Delta_n/\delta_n$). NP1: $\delta_n = 1; \delta_t = \sqrt{2}\delta_n$, NP2: $\delta_n = \delta_t = 1$, SMC: $\delta_n = \delta_t = 1$.

The ability of each model to provide mode-independent interface behaviour is next considered. Again, model parameters are chosen such that $\sigma_{\text{max}} = \tau_{\text{max}}$ with separations at peak traction being identical for mode I and mode II separation. In Figure 11(a) the maximum traction magnitude ($|T|_{\text{max}} = \max (\sqrt{T_n^2 + T_t^2})$) is plotted as a function of separation mode angle, $\theta$, where $\theta = \tan^{-1}(\Delta_n/\Delta_t)$. A plot of the separation magnitude at which $|T|_{\text{max}}$ occurs ($|\Delta|_{\text{max}}$) is shown in Figure 11(b). The potential-based XN and MP models are also included for comparison. As specified in equations (21-22), the SMC formulation provides a mode-independent response. For NP2, identical behaviour is obtained for mode I, mode II and pure mixed-mode ($\theta = \pi/4$) separation. For NP1, the BSG and XN models, the peak traction is highly mode-dependent, as is the separation magnitude at which it occurs. It should again be noted that while in Figure 11 model parameters are chosen so that $|T|_{\theta=0} = |T|_{\theta=\pi/2}$ and $|\Delta|_{\theta=0} = |\Delta|_{\theta=\pi/2}$, the form of the traction-separation curve is different for mode I and mode II separation for NP1, BSG and XN models.

Figure 11(c) shows the work of separation as a function of separation mode angle $\theta$, again with $\sigma_{\text{max}} = \tau_{\text{max}}$ for all models. In the case of the XN model the work of separation is approximately constant ($\approx \phi_n$) for $\theta \leq \pi/3$. The work of separation gradually decreases to the mode II value for $\theta \gtrsim 0.3\pi$. A similar trend is computed for the MP model, with the work of separation being constant ($\approx \phi_n$) over a larger range of $\theta$ than for the XN model before gradually decreasing to the mode II value. As can be seen in Figure 11(c), $W(\theta) \approx \phi_n$ for $\theta \gtrsim 0.45\pi$ for the MP model with $m = 2$. In contrast to the potential-based models, the work of separation for the BSG model monotonically decreases from the mode I value to the mode II value. Similarly for NP1, the work is dependent on the separation mode angle for all theta and decrease from mode I to mode II is not monotonic, with a minimum work of separation being computed for NP1 at $\theta \approx 0.37\pi$. In contrast to the aforementioned models, for $\sigma_{\text{max}} = \tau_{\text{max}}$, NP2 yields an identical work of separation for mode I and mode II separation,
and for $\theta = 0.25\pi$. However, slight reductions in work of separation are computed for intermediate mode angles. The SMC model provides a constant work of separation for all theta and is not shown in Figure 11(c) for clarity. It is worth noting that constant work of separation is computed by the XN, MP and BSG model if $\phi_n = \phi_t$, but this clearly prohibits the setting of $\sigma_{max} = \tau_{max}$.

Figure 11: (a) Maximum effective traction ($|T|_{max}/\sigma_{max}$) as a function of separation controlled mode angle $\theta$ for all CZMs. (b) Separation magnitudes at which maximum effective traction occurs ($|\Delta|_{max}/\delta_n$) as a function of separation controlled mode angle $\theta$ for all CZMs. (c) Work of separation ($W(\theta)/\phi_n$) as a function of separation controlled mode angle $\theta$ for all CZMs except SMC. For all models $\sigma_{max} = \tau_{max}$. For XN, BSG and NP1 models $\delta_t = \sqrt{2}\delta_n$. For NP2 and SMC models $\delta_n = \delta_t$.

From equation 14 (Cazes et al., 2009), it is straightforward to show that a monotonic increase in $\Delta_n$ and $\Delta_t$ will result in positive energy dissipation if (i) repulsive tractions do not occur, and (ii) the CZM coupling terms enforce that an increase in $\Delta_n$ results in a decrease in $T_t$ and an increase in $T_n$ results in a decrease in $T_n$. Clearly, in the separation regime, these conditions are satisfied by all non-potential CZMs considered in this study, where the coupling terms essentially provide an exponential decay in traction. Hence, as the load-paths considered in Figures 9, 10 and 11 entail monotonic increase in separation, the strong condition for positive instantaneous dissipation is satisfied throughout. Figure 12 demonstrates that, in contrast to the XN and MP potential-based models, each non-potential CZM provides positive instantaneous dissipation during interface separation at a constant separation mode angle when $\phi_t > \phi_n$. 
Figure 12: Normalised instantaneous incremental energy dissipation ($d\phi_i/\phi_n$) during constant separation mode $\theta = Tan^{-1}(\Delta_n/\Delta_t)$ loading paths where $\phi_t = 4\phi_n$: (a) BSG; (b) NP1; (c) NP2; (d) SMC.

4 Traction Controlled Mode Mixity

The mixed-mode behaviour of CZMs under imposed separation paths can provide insight on the effect of coupling, as demonstrated in Figure 11. However, mode mixity is more generally expressed in terms of traction mode angle $\psi$, where $\psi = Tan^{-1}(T_n/T_t)$. For a constant value of $\psi$ both the separation path and the work of separation are strongly influenced by the coupling terms of the CZM, as illustrated in Figure 13 and 14. By numerically inverting the cohesive zone equations and imposing a constant traction ratio, a separation path can be determined for a given value of $\psi$ (such a numerical inversion is necessary only for the path-independent non-potential-based models, as the tractions and hence traction ratios are directly specified by the potential function for potential-based models). Figure 13 shows the paths followed during a mixed-mode separation for constant values of $\psi$. Separation paths are shown for $\psi$ ranging from $\psi = 0.005\pi$ (near mode I) to $\psi = 0.495\pi$ (near mode II) in increments of 0.035$\pi$. Figure 14 shows the corresponding total, normal and tangential work of separation as a function of $\psi$. Firstly, the separation paths for the XN model with $\sigma_{max} = \tau_{max}$ are plotted in Figure 13(a). Interestingly, for $\psi \geq 0.21\pi$ the normal component $\Delta_n$ increases during the initial stages of separation and then decreases, so that the final separation vector is close to mode II. In contrast, for $\psi \leq 0.21\pi$ the separation path is dominated by the normal component. The corresponding work of
separation is shown in Figure 14(a), illustrating a step change in total work from $\phi_n$ to $\phi_t$ at $\psi = 0.21\pi$. Step changes are also observed in the work of normal and tangential separation. Setting $q = 1$ (i.e. $\phi_n = \phi_t$) for the XN model it is shown in Figure 13(b) that the separation paths for constant $\psi$ tend strongly towards normal separation. This occurs due to the fact that $\tau_{max} = \sigma_{max}\sqrt{\epsilon}$, leading to asymmetry between normal and tangential work of separation despite a constant total work of separation, as illustrated in Figure 14(b). Again, it should be noted that the BSG and XN models are identical for $q = 1$. Considering next the BSG model with $\sigma_{max} = \tau_{max}$ in Figure 13(c): Here the paths of constant $\psi$ tend strongly towards normal separation with a monotonic reduction in total work of separation from $\phi_n$ to $\phi_t$ as $\psi$ moves from mode I to mode II (Figure 14(c)). This behaviour is very different to that computed for the XN model with $\sigma_{max} = \tau_{max}$ (Figures 13(a), 14(a)). Next, the NP1 model with $\sigma_{max} = \tau_{max}$ is considered in Figure 13(d). Proportional separation is computed, i.e. $\Delta_n/\Delta_t$ is constant for constant $\psi$ leading to linear separation paths. However it should be noted that separation paths are clustered towards the mode II axis, signifying a slight bias towards tangential separation. It can be seen in Figure 14(d) that the total work of separation does not reduce monotonically from $\phi_n$ to $\phi_t$ as $\psi$ moves from mode I to mode II, but reaches a local minimum at $\psi = 0.3\pi$. The NP1 model with $\phi_t = \phi_n$ ($\tau_{max} = \sigma_{max}\sqrt{\epsilon}$) is considered in Figure 13(e). Evenly distributed proportional loading paths are computed. However, as shown in Figure 14(e), the mixed-mode work of separation is lower than the mode I and mode II work of separation for $0 \leq \psi \leq 0.5\pi$, again with a local minimum being observed.

NP2 is next considered in Figure 13(f) with $\sigma_{max} = \tau_{max}$ and $\alpha = \beta = (\sqrt{2} - 1)$, recalling that these parameters provide identical effective traction-separation curves for mode I, mode II and $45^\circ$ separation. However, for mixed-mode separation at a constant $\psi$ it is shown in Figure 13(f) that for $\psi > 0.25\pi$, normal separation initially increases and then decreases, leading to separation paths that tend toward mode II. The opposite is the case for $\psi < 0.25\pi$ with separation paths tending towards mode I. Proportional separation is computed only for $\psi = 0.25\pi$, but examination of the total work of separation (Figure 14(f)) reveals a singularity at this point. The existence of this singularity can be explained as follows: Considering a horizontal line on Figure 13(f) representing a constant normal separation (e.g. $\Delta_n/\Delta_t = 2$): As $\Delta_n/\Delta_t$ increases along this line, $\psi$ should increase monotonically. Hence, the existence of a local max/min $\psi$ along this line signifies the existence of a region on the plot which does not contain a constant $\psi$ separation path. It is trivial to show that such a region occurs if $\alpha, \beta < 1$. Hence, while the imposition of displacement controlled conditions suggests that the NP2 model provides a reasonable approximation of mode-independent behaviour, as shown in Figure 11, it is demonstrated in Figure 13(f) that the NP2 model results in strongly mode-dependent behaviour under traction controlled conditions. As shown in Figure 13(g), setting $\alpha = \beta = 1$ for the NP2 model removes the existence of a singularity and results in proportional loading paths. However, the total work of separation under mixed-mode conditions is lower than that prescribed for mode I and mode II, with a minimum occurring at $\psi = 0.25\pi$ as shown in Figure 14(g). Finally, as expected, it is shown in Figures 13(h) and 14(h) that the SMC model provides perfectly proportional separation paths and mode-independent total work of separation.
Figure 13: Paths followed during constant traction controlled mode mixity $\psi$, i.e. $\psi$ is constant along each line/path shown in $\Delta_n - \Delta_t$ space. Separation paths are shown for $\psi$ ranging from $\psi = 0.005\pi$ (near mode I on vertical axis) to $\psi = 0.495\pi$ (near mode II on horizontal axis) in evenly spaced intervals of $0.035\pi$. For XN, BSG and NP1 models $\delta_t = \sqrt{2}\delta_n$. For NP2 and SMC models $\delta_n = \delta_t$. (a) XN model, $\sigma_{max} = \tau_{max}$; (b) XN/BSG model, $\phi_t = \phi_n (\tau_{max} = \sigma_{max}\sqrt{\epsilon})$; (c) BSG model, $\sigma_{max} = \tau_{max}$; (d) NP1 model, $\sigma_{max} = \tau_{max}$; (e) NP1 model, $\phi_t = \phi_n (\tau_{max} = \sigma_{max}\sqrt{\epsilon})$; (f) NP2 model $\phi_t = \phi_n (\sigma_{max} = \tau_{max})$ and $\alpha = \beta = (\sqrt{2} - 1)$; (g) NP2 model $\phi_t = \phi_n (\sigma_{max} = \tau_{max})$ and $\alpha = \beta = 1$; (h) SMC model $\phi_t = \phi_n (\sigma_{max} = \tau_{max})$.
Figure 14: Work of separation $W(\psi)$ as a function of traction controlled mode mixity $\psi$. Normal ($W_n$) and tangential ($W_t$) contributions to total work of separation are also shown. For XN, BSG and NP1 models $\delta_x = \sqrt{2} \delta_n$. For NP2 and SMC models $\delta_n = \delta_t$. (a) XN model, $\sigma_{max} = \tau_{max}$; (b) XN/BSG model, $\phi_t = \phi_n$ ($\tau_{max} = \sigma_{max}\sqrt{\epsilon}$); (c) BSG model, $\sigma_{max} = \tau_{max}$; (d) NP1 model, $\sigma_{max} = \tau_{max}$; (e) NP1 model, $\phi_t = \phi_n$ ($\tau_{max} = \sigma_{max}\sqrt{\epsilon}$); (f) NP2 model $\phi_t = \phi_n$ ($\sigma_{max} = \tau_{max}$) and $\alpha = \beta = (\sqrt{2} - 1)$; (g) NP2 model $\phi_t = \phi_n$ ($\sigma_{max} = \tau_{max}$) and $\alpha = \beta = 1$; (h) SMC model $\phi_t = \phi_n$ ($\sigma_{max} = \tau_{max}$).
It can be noted in Figure 13 that $\Delta_n$ and $\Delta_t$ do not increase monotonically during constant traction mode separation in the case of the XN model (Figure 13(a)) and the NP2 model (Figure 13(f)). Figure 15 illustrates the instantaneous incremental dissipation along each path. In the case of the XN model, as $\psi \to 0.21\pi$ negative dissipation is computed. It should be noted that the negative dissipation occurs due to the decrease in the normal component of separation, and not due to the computation of repulsive forces (as $q < 1$ in Figure 15(a)). In the case of the NP model the rate of reduction of $\Delta_n$ and $\Delta_t$ is quite low and negative dissipation is not computed (Figure 15(b)). For all other models in Figure 13 instantaneous positive dissipation occurs throughout.

**Figure 15**: Normalised instantaneous incremental energy dissipation ($d\phi_t/\phi_n$) during constant traction controlled mode mixity $\psi$: (a) XN model, $\sigma_{max} = \tau_{max}$, corresponding to Figure 13(a) (insert); (b) NP2 model $\phi_t = \phi_n (\sigma_{max} = \tau_{max})$, corresponding to Figure 13(f) (insert).

Mixed-mode behaviour is next considered when $\phi_t > \phi_n$. Specifically, for the case of $\phi_t = 4\phi_n$. Figure 16 shows the paths followed during a mixed-mode separation for constant values of $\psi$. Figure 17 shows the corresponding total, normal and tangential work of separation as a function of $\psi$. Firstly, considering the XN model, Figure 16(a) demonstrates that all separation paths ultimately follow a normal trajectory (with the sole exception of pure mode II separation). Even for cases that are very close to mode II, $\psi \to 0.5\pi|^{-}$, $\Delta_t/\delta_t$ does not exceed a value of 0.74, ultimately resulting in a pure normal trajectory to complete separation. Such behaviour can be related to the existence of regions of repulsive normal traction for potential-based models when $\phi_t > \phi_n$, as $\psi < 0$ in such regions. The corresponding total work of separation (Figure 17(a)) is equal to $\phi_n$ for all values of $\psi < 0.5\pi$. Only for pure mode II separation ($\psi = 0.5\pi$) is the work of separation greater than $\phi_n$. It is worth noting that the MP model provides an identical relationship between total work of separation and $\psi$ to that computed for the XN model, with only the distribution of normal and tangential work of separation being affected by the parameter $m$. The separation paths for the MP model are also very similar to those of the XN model: As an example, when $m = 2$, $\Delta_t/\delta_t$ does not exceed a value of 0.73, again resulting in pure normal trajectory to complete separation for $\psi < 0.5\pi$. As demonstrated previously, the MP model provides an improvement on the XN model under displacement controlled conditions in terms of limiting the size of regions of repulsive normal tractions, as shown in Figure 5. Under traction controlled conditions, however, separation paths are bounded by the lower limits of the
regions of repulsive normal traction, hence a reduction of size of this region has little effect on the separation behaviour. Given the similarity of the XN and MP models under traction controlled separation, results are not presented here for the MP model. The separation paths computed for the BSG model (Figure 16(b)) also contain a heavy bias towards normal separation. However, unlike the potential-based models, the BSG model is not hindered by an “exclusion zone” as this non-potential-based formulation does not predict regions of repulsive normal traction. However, as shown in the total work of separation plot (Figure 17(b)), following a plateau near $\psi = 0.5\pi$, the work of separation reduces rapidly with decreasing $\psi$ so that $W(0.5\pi) \approx 1.04\phi_n$. In contrast to the BSG model, NP1 (Figure 16(c)) provides proportional loading with a constant ratio of normal to tangential separation being computed for all $\psi$. Additionally, the transition from mode I to mode II is more gradual for the NP1 model than for the BSG model. This is also evident from the work of separation (Figure 17(c)), where $W(0.5\pi) \approx 1.07\phi_n$. It should also be noted that no plateau is computed for the work of separation near $\psi = 0.5\pi$. Next considering NP2 with $\alpha = \beta = (\sqrt{2} - 1)$ in Figure 16(d): As previously discussed, if $\alpha, \beta < 1$ a local max/min exists for $\psi$, leading to “exclusion zones” in which $\psi$ does not decrease monotonically from mode II to mode I. In the case of $\phi_t = 4\phi_n$ the NP2 model predicts near mode II separation for all $\psi \geq 0.418\pi$ and near mode I separation for all $\psi \leq 0.418\pi$. In terms of the work of separation, this results in a discontinuity at $\psi = 0.418\pi$ as shown in Figure 17(d). In fact the total work is separation is slightly lower than $\phi_n$ for $0 < \psi \leq 0.35\pi$. By setting $\alpha = \beta = 1$ for NP2 proportional separation is achieved (Figure 16(e)) without the existence of an “exclusion zone”. Additionally, work of separation is continuous over the range of $\psi$ as shown in Figure 17(e). However, the reduction in work from the pure mode I value, $\phi_n$, with increasing $\psi$ is more pronounced than is the case in Figure 17(d) for $\alpha = \beta = (\sqrt{2} - 1)$. Plots are presented for the SMC model in Figures 16(f) and 17(f). Proportional separation paths are computed and a gradual monotonic decrease from mode II to mode I work of separation is computed, with a plateau being computed at $\psi = 0.5\pi$. Finally, it should be noted that positive instantaneous dissipation is computed for all paths shown in Figure 16 (see Appendix B).
Figure 16: Paths followed during constant traction controlled mode mixity $\psi$ when $\phi_t = 4\phi_n$. [Similar to Figure 12 above, $\psi$ is constant along each line/path shown in $\Delta_n - \Delta_t$ space. Separation paths are shown for $\psi$ ranging from $\psi = 0.005\pi$ (near mode I on vertical axis) to $\psi = 0.495\pi$ (near mode II on horizontal axis) in evenly spaced intervals of $0.035\pi$. For XN, BSG and NP1 models $\delta_t = \sqrt{2}\delta_n$. For NP2 and SMC models $\delta_n = \delta_t$. (a) XN model; (b) BSG model; (c) NP1 model; (d) NP2 model, $\alpha = \beta = (\sqrt{2} - 1)$; (e) NP2 model, $\alpha = \beta = 1$; (f) SMC model.]
The classical work of Hutchinson and Suo (1992) proposed the following relationship between work of separation and $\psi$:

$$W(\psi) = \phi_n \{1 + Tan^2[(1 - \lambda)\psi]\}$$  \hspace{1cm} (24)

where the model parameter $\lambda$ determines the ratio of $\phi_n$ to $\phi_t$.

Equation (24) is found to provide an accurate representation of experimentally measured mixed-mode fracture of a plexiglass-epoxy interface (Wang and Suo, 1990) for $\lambda = 1.665$ (approximating to $\phi_t = 4\phi_n$), as shown in Figure 18. Plots of $W(\psi)$ computed for the CZMs in Figure 17 are also reproduced in Figure 18 for comparison with the Hutchinson and Suo.
theoretical curve. Clearly the XN model does not provide a reasonable approximation of the theoretical curve, with the work of separation being equal to the mode I value for all $\psi < 0.5\pi$. Once again, it is important to note that an identical work of separation versus $\psi$ relationship will be reproduced for all potential-based CZMs (including the MP model), as the existence of zones of repulsive normal traction when $\phi_t > \phi_n$ will ultimately lead to normal separation for all mixed-mode paths of constant $\psi$. The BSG model represents a significant improvement on the potential-based XN model, but exhibits a very rapid transition from mode II to mode I work of separation. The BSG model also exhibits a plateau region near mode II, unlike the theoretical curve. The NP1 model provides a closer correlation to the theoretical curve than the BSG model with more gradual transition from mode II to mode I being predicted. Additionally, the NP1 model does not predict a plateau region near $\psi = 0.5\pi$, similar to the theoretical curve of Hutchinson and Suo (1992). It is important to note that the NP1 and BSG curves cannot be forced to exactly reproduce the theoretical curve by altering the coupling terms. As an example, if the coupling term $\exp(-\Delta_t^2/\delta_t^2)$ in equations (16) and (18) is replaced with $\exp(-\kappa\Delta_t^2/\delta_t^2)$ it can easily be shown that a singularity occurs for both models for $\kappa < 1$, leading to a step change in work of separation, similar to the case of NP2. On the other hand, if $\kappa > 1$ it can easily be shown that the transition from mode II to mode I is accelerated for the BSG and NP1 models, providing a more inaccurate representation of the Hutchinson and Suo curve. Finally, it can be seen that the SMC model provides the best approximation of the Hutchinson and Suo curve, with the exception of a plateau region near mode II separation.

![Figure 18: Comparison of work of separation $W(\psi)$ as a function of traction controlled mode mixity $\psi$ when $\phi_t = 4\phi_n$ for XN, BSG, NP1 and SMC models with theoretical mode mixity relationship of Hutchinson and Suo (1992).](image)
5 Discussion

In this paper an analysis of potential-based and non-potential-based CZMs in mixed-mode separation and over-closure is performed. It is demonstrated that derivation of traction-separation relationships from a potential function results in non-physical behaviour under mixed-mode conditions. In the case of the XN potential-based model repulsive normal tractions and negative instantaneous incremental energy dissipation (Cazes et al., 2009) can be computed during mixed-mode separation if \( \phi_t > \phi_n \). Similarly, positive/adhesive residual normal tractions can be computed following mode II or mixed-mode separation if \( \phi_t < \phi_n \).

In the present paper a modified potential-based (MP) CZM is proposed in which the zone in which repulsive \((\phi_t > \phi_n)\) or residual \((\phi_t < \phi_n)\) normal tractions occur is reduced. However, the reduction of the zones of repulsive/residual tractions is achieved at the price of increasing the magnitude of repulsive/residual tractions within this zone. When traction-separation relationships are derived from a potential function, with \( \phi_t \neq \phi_n \), repulsive/residual tractions will be computed for certain mixed-mode separations. In essence, if a potential function must capture mode I interface fracture, such that \( \partial \phi / \partial \Delta_n \rightarrow 0 \) as \( \Delta_n \rightarrow \infty \), while also capturing mode II interface fracture, such that \( \partial \phi / \partial \Delta_t \rightarrow 0 \) as \( \Delta_t \rightarrow \infty \), then when \( \phi_t \neq \phi_n \), either repulsive or residual tractions are inevitable under mixed-mode conditions. Both the XN and MP models are formulated such that as \( \Delta_n \rightarrow \infty \) then \( \phi = \phi_n \) for all values of \( \Delta_t \), hence repulsive normal tractions and associated negative dissipation emerge in the mixed-mode transition region if \( \phi_t > \phi_n \). If a potential function is formulated such that \( \phi = \phi_t \) as \( \Delta_t \rightarrow \infty \) for all values of \( \Delta_n \), then the unphysical phenomenon of residual tangential tractions and further positive dissipation following full mode I fracture will emerge when \( \phi_t > \phi_n \). Additionally, for such a potential function if \( \phi_t > \phi_n \) then repulsive tangential tractions will be computed under mixed-mode conditions. A potential function proposed by Sørensen et al. (2008) based on a micromechanical analysis of fibre-bridging during cracking of fibre reinforced composites exhibits a near constant value of \( \partial \phi / \partial \Delta_t (= T_t) \) occurs for all values of \( \Delta_n \) and \( \Delta_t \). The existence of a constant tangential traction during mode II separation that is independent of the magnitude of \( \Delta_t \) may be specific to fibre reinforced composites. Indeed a subsequent experimental study (Sørensen and Jacobsen, 2009) has demonstrated a constant value of \( T_t \) under mode II separation for fibre reinforced composites. However such behaviour is not typical for mode II interface fracture; generally mode II fracture is characterised by a reduction in tangential traction as complete interface separation occurs, i.e. \( T_t \rightarrow 0 \) (or \( \partial \phi / \partial \Delta_t \rightarrow 0 \) for a potential-based model) as \( \Delta_t \rightarrow \infty \). Considering that several experimental studies report that \( \phi_t > \phi_n \) (Dollhofer et al., 2000; Yang et al., 2001; Warrior et al., 2003), it is critically important that the conditions leading to emergence of repulsive-residual tractions from a potential function are identified.

In the potential-based model of Park et al. (2009) normal tractions are arbitrarily set to zero if repulsive normal tractions emerge from the potential function when \( \phi_t > \phi_n \), with only tangential tractions being derived from the potential function subsequently. However, it can be shown that this approach results in path dependent behaviour, with the work of separation for a given deformed interface configuration being dependent on the path history, even when the interface separation increases monotonically. As an example, in the model of Parks et al., if \( \phi_t = 4 \phi_n \) and normal and tangential characteristic interface lengths are equal, potential derived normal tractions are set to zero resulting in path-dependent behaviour once \( \Delta_t \geq 0.196 L_t \), where \( L_t \) is the length at which complete tangential separation occurs \( (T_t \rightarrow 0 \text{ as } \Delta_t \rightarrow L_t) \). Hence this approach results in a non-potential-based path-dependent coupled CZM for the majority of the domain in which the CZM is applied. However such behaviour is not typical for mode II interface fracture whereby \( T_t \rightarrow 0 \) (or \( \partial \phi / \partial \Delta_t \rightarrow 0 \) for a potential-based
model) as $\Delta_t \to \infty$. Path-independence should be established through extensive experimental testing in order to justify the use of a potential-based CZM, as this feature may not be appropriate for all interfaces. Rigorous mixed-mode experimental testing (e.g. Sørensen and Jacobsen, 2009; Sørensen and Kirkegaard, 2006) should be performed in order to establish the existence of path-independence and to determine if residual/repulsive normal tractions occur during tangential separation. Potential functions that provide a sinusoidal shear traction-separation relationship (Beltz and Rice, 1991) may be appropriate for the simulation of periodic repulsive normal tractions due to the interaction of asperities under mode II loading.

A convenience of potential-based CZMs is that the work of separation depends only on the current interface separation, hence for a specified deformed interface configuration the fracture resistance is uniquely defined. A further advantage of potential-based CZM is that a weak dissipation criterion is fulfilled. Starting from an undeformed configuration, a potential-based model will assure that the overall or total dissipation is not negative following the completion of a separation path, even though instantaneous negative dissipation may occur during parts of the separation path. As an example, during a closed deformation loop zero net dissipation occurs during the debonding-rebonding process with positive dissipation occurring during debonding and negative dissipation occurring during rebonding. Such instantaneous negative dissipation may be appropriate for certain applications, such as molecular bonding of silicon wafers (Kubair et al., 2009), where Van de Waals forces are responsible for surface interactions. However, for the majority of applications interface rebonding will not occur during cyclic loading, requiring the introduction of internal CZM variables to account for damage or plasticity (Cazes et al., 2009; Roe and Siegmund, 2003). For CZMs that incorporate damage, typically a linear unloading to the undeformed configuration is implemented upon load reversal. However, in the current study we demonstrate that potential-based CZMs can result in negative instantaneous dissipation under monotonic mixed-mode loading conditions. Hence, for potential-based CZMs even the incorporation of damage upon load reversal is not sufficient to satisfy the strong dissipation criterion, i.e. instantaneous positive dissipation, which may occur prior to load reversal.

While non-potential CZMs give rise to path history dependent tractions and work of separation, coupling terms can be chosen such that repulsive normal tractions and negative dissipation during monotonic loading will not be computed, as demonstrated for the three non-potential CZMs proposed in the current study. Such formulations are not suitable for cyclic loading applications as the weak dissipation will not necessarily be satisfied, with the possibility of net negative dissipation for a closed deformation loop. However, as these formulations satisfy both the strong and weak dissipation criteria for monotonic loading conditions, suitable damage criteria or plasticity should be incorporated into these formulations for cyclic loading applications where rebonding does not occur. It should be noted that the computation of repulsive normal tractions and negative instantaneous dissipation is not necessarily eliminated due to the fact that a CZM is non-potential-based and hence path-dependent. In an effort to eliminate the repulsive normal tractions computed by the XN model when $\phi_t > \phi_n$, He and Xin (2011) multiply the XN normal tractions by the term $e^{-\Delta_t^2/\delta_t^2}$. However, it can easily be demonstrated that this modification: (i) is no longer path-independent ($\partial T_t/\partial \Delta_n \neq \partial T_n/\partial \Delta_t$); (ii) does not eliminate the possible computation of repulsive normal tractions and associated negative dissipation.

The XN model provides physically realistic coupling under mixed-mode separation only if the work of mode I separation and work of mode II separation are equal ($q = 1$). Based on
this observation van den Bosch et al. (2006) proposed a coupled non-potential-based CZM (the BSG model) that provides physically realistic coupling during mixed-mode separation. Using the XN traction-separations for \( q = 1 \), independent scaling factors were applied to the expressions for normal and tangential tractions in order to simulate cases where \( \phi_t \neq \phi_n \). However, similar to the XN model for \( q = 1 \), the BSG model does not provide correct penalisation of mixed-mode over-closure, with peak tangential tractions decreasing with increasing over-closure, becoming repulsive when the normal over-closure exceeds the characteristic distance. We propose an alternative model (NP1) that is identical to the XN and BSG models in pure mode I and pure mode II separation, again with physically realistic coupling in mixed-mode separation. However, in contrast to the BSG model, NP1 provides a physically realistic coupling in mixed-mode over-closure, i.e. the peak tangential traction increases with normal over-closure and repulsive tangential tractions are never computed. In a follow on case study, in Part II of the present study, we demonstrate that excessive mixed-mode over-closure is computed at a stent-coating interface by the BSG model, leading to an erroneous prediction of coating stress and buckling. In principle, different forms of the normal traction-displacement law could be enforced in the overclosure and in separation. However, the associated coupling and consequent tangential behaviour is not obvious for such an approach. It is not clear that a resultant discontinuity in the form of the tangential-separation would be appropriate, i.e. should a compression at an interface alter the form of the tangential traction-separation equations? Clearly rigorous experimental investigation of “mode II” delamination in the presence of an interface compression should be performed to determine the appropriate normal-tangential coupling in the overclosure regime.

A potential limitation of the XN, MP, BSG and NP1 formulations is that identical traction-separation relationships cannot be specified for mode I and model II separation. Even if peak mode I and mode II tractions are equal (\( \sigma_{max} = \tau_{max} \)) and occur at the same effective separation (\( \sqrt{2} \delta_n = \delta_t \)) the work of tangential separation will be lower than the work of normal separation (\( q \approx 0.607 \)). We propose a formulation (NP2) that provides identical “effective traction”-“effective separation” relationships for 90° (mode I), 0° (mode II) and 45° (pure mixed-mode) separation in addition to providing physically realistic behaviour in mixed-mode over-closure. We also consider a formulation (SMC model) in which the effective separation is used for mixed-mode coupling, following from the work of Tvergaard and Hutchinson (1993), providing mode-independent behaviour in separation but no penalisation of over-closure. We demonstrate that under displacement controlled mode mixity NP2 provides a closer approximation to the mode-independent separation behaviour of the SMC model than the XN, BSG or NP1 formulations. Given that NP2 is identical to the SMC model for 0°, 45° and 90° separation, a framework can be readily implemented in which NP2 is applied if \( \Delta_n < 0 \) and SMC is applied if \( \Delta_n \geq 0 \). It should be noted that in addition to providing identical mode I and mode II traction separation behaviour, the SMC model is path-independent if \( \sigma_{max} = \tau_{max} \) and \( \delta_n = \delta_t \). The potential-based model of Park et al. (2009) is also capable of providing identical mode I and mode II behaviour.

Cohesive zone formulations have generally been investigated using displacement controlled boundary conditions (van den Bosch et al., 2006; Park et al., 2009). However, experimental investigation of mixed-mode fracture generally provides the work of mixed-mode interface separation \( \psi = Tan^{-1}(K_{II}/K_I) \) (or \( \psi = Tan^{-1}(T_T/T_n) \)), leading to theoretical expressions for mixed-mode work of separation as a function of \( \psi \) in the classical paper of Hutchinson and Suo (1992). In the present paper the performance of potential-based and non-potential-based CZMs under traction controlled mode mixity is investigated. When \( \sigma_{max} = \tau_{max} \) the
following is demonstrated: (i) The XN model exhibits non-proportional separation paths, with all values of $\psi$ resulting in an effective mode I or mode II separation, with an associated discontinuity in the work of separation when plotted as a function of $\psi$; (ii) The BSG model exhibits non-proportional loading with a bias towards mode I separation; (iii) NP1 provides proportional loading but a local minimum mixed-mode work of separation is computed; (iv) The NP2 model \( (\alpha = \beta = (\sqrt{2} - 1)) \) exhibits proportional loading only if \( T_n = T_t \) \( (\psi = 0.25\pi) \) with a singularity being computed for the work of separation at this point. All other values of $\psi$ lead to non-proportional separation paths that ultimately tend towards either mode I or mode II separation; (v) The SMC model provides proportional loading, a constant work of separation for all $\psi$, and symmetry between normal and tangential work of separation. These findings highlight the fact that even though similar mode I and mode II behaviour may be specified for a cohesive zone formulation, the coupling between normal and tangential behaviour under mixed-mode conditions can lead to severe bias towards normal or tangential separation. The analyses represented in the present paper for NP2 demonstrate that coupling terms in cohesive zone equations must be weighted such that a continuous and monotonic increase in $\psi$ must be obtained for increasing tangential separation (and a corresponding continuous monotonic decrease in $\psi$ for increasing normal separation). Incorrect weighting of coupling terms can result in the creation of “exclusion zones” through which no separation paths of constant $\psi$ can be obtained, leading to a discontinuous work of separation as a function of $\psi$. This highlights the importance of considering traction controlled mode mixity in the development of non-potential-based cohesive zones. While the NP2 model provides physically realistic near-mode-independent behaviour under displacement controlled conditions, significant problems occur under traction controlled conditions, leading to physically unrealistic behaviour. The recent study of Mosler and Scheider (2011) presents a novel thermodynamically consistent formulation based on a stored Helmholtz energy, incorporating boundary potential terms on each side of the interface. An assessment of the contribution of such terms under traction controlled mixed-mode conditions would be of interest. As a practical example of a traction controlled mixed-mode case study, an analytical solution for the interface stress state at a bi-layered arch recently published by two of the authors (Parry and McGarry, 2012) reveals that the effective interface stress is independent of position along the interface, with perfect symmetry being observed between shear and normal stress. In Part II of this study we demonstrate that the choice of cohesive zone at the arch interface significantly influences the pattern of delamination leading to finite element predictions that contradict the analytical solution.

As previously mentioned, several experimental studies have reported interface fracture in which $\phi_t > \phi_n$ (Wang and Suo, 1990; Dollhofer et al., 2000; Warrior et al., 2003; Yang et al., 2001). Based on the experimental work of Wang and Suo (1990), Hutchinson and Suo (1992) proposed a classical theoretical relationship between work of separation (or interface toughness) and mode mixity $\psi$ whereby the work of separation gradually and monotonically reduces from the mode II value, $\phi_t$, to the mode I value, $\phi_n$ (Hutchinson and Suo, 1992). In the present study we demonstrate that potential-based CZMs cannot reproduce such a relationship: when $\phi_t > \phi_n$, regions of repulsive normal traction occur in significant regions of the $\Delta_n - \Delta_t$ space. Separation paths of constant $\psi$ cannot travel through such regions, with the result that an effective normal separation is obtained for all $\psi$ with the exception of pure mode II separation. This behaviour has been demonstrated for the XN and MP models in the present study. However, an identical form of work of separation versus $\psi$ is obtained for all potential-based CZMs where $\Delta_n \to \infty$ then $\phi = \phi_n$ for all values of $\Delta_t$. For example, similar to the behaviour reported here for the XN model, when $\phi_t > \phi_n$ it can readily be
demonstrated that the model of Park et al. (2009) predicts a work of separation equal to $\varnothing_n$ for all $\psi < 0.5\pi$, with $\Delta_t$ being less than the critical (conjugate) value for all mixed-mode separation paths of constant $\psi$. Such behaviour is not in agreement with the reported experimental results and the theoretical relationship of Hutchinson and Suo (1992). In contrast to potential-based models, the non-potential-based BSG, NP1 and SMC models provide a reasonable approximation of the theoretical curve of Hutchinson and Suo, with the latter two models proving slightly more accurate. Once again, the analysis of the NP2 model illustrates the importance of correctly weighting the coupling equations in a non-potential-based model. For $\alpha = \beta = (\sqrt{2} - 1)$ a separation path “exclusion zone” is again computed, resulting in a step change in work of separation as a function of $\psi$. On the other hand, while setting $\alpha, \beta \geq 1$ removes the “exclusion zone” leading to proportional separation, a local minimum in work of separation is computed at $\psi < 0.25\pi$. While the formulation of non-potential-based coupled cohesive zone formulations may at first seem relatively straightforward, the present study illustrates that non-potential-based formulations should be numerically inverted in order to investigate the mixed-mode behaviour under traction controlled conditions. The importance of such analyses is highlighted by NP2, which provides physically realistic behaviour under displacement controlled mixed-mode separation, but exhibits physically unrealistic behaviour under traction controlled mixed-mode separation.

6 Conclusions

In conclusion, the analyses presented in this study provide valuable guidance for future implementation of potential and non-potential-based CZMs for problems involving mixed-mode separation and over-closure. We propose an alternative to the well established XN potential-based CZM (the MP model) that improves upon the performance of the XN model under mixed-mode conditions. Specifically, the MP model reduces the zone of repulsive normal tractions when $\phi_t > \phi_n$, so that the computation of such unphysical tractions is reduced under displacement controlled mode mixity. However, it is demonstrated that when $\phi_t > \phi_n$ repulsive normal traction and instantaneous negative dissipation can be computed by the XN and MP models even if an interface subjected to monotonic loading. Additionally, under traction controlled mode mixity when $\phi_t > \phi_n$ the XN and MP models result in normal separation paths for a constant traction-based mode mixity $\psi$ with the exception of pure mode II separation when $\phi_t > \phi_n$. This results in a constant work of separation for all $\psi < 0.5\pi$, which is not in agreement with experimental observation and the theoretical relationship of Hutchinson and Suo (1992).

A number of non-potential-based cohesive zone formulations are also proposed in the present study: Firstly, a non-potential-based model (NP1) that improves upon the BSG model under conditions of mixed-mode over-closure; Secondly, a non-potential-based model (NP2) that provides the option of achieving identical behaviour under mode I, mode II and 45° separation. Similar to NP1, NP2 provides correct penalisation of mixed-mode over-closure; Additionally, a non-potential-based formulation (SMC model) that provides mode-independent behaviour in separation is considered. We demonstrate that under displacement controlled boundary conditions all models provide reasonable mixed-mode behaviour. However, under traction controlled mode mixity the following is demonstrated: (i) BSG model provides a strong bias towards normal separation; (ii) The NP1 model provides a problematic computation of a local minimum in mixed-mode work of separation if $\phi_t = \phi_n$; (iii) The NP1, BSG, and SMC models provide reasonable approximations to the theoretical
relationship of Hutchinson and Suo (1992) if \( \phi_t > \phi_n \) in terms of mixed-mode work of separation. All non-potential models considered in this study provide instantaneous positive dissipation under monotonic loading. A summary of the key findings presented in this paper is provided in Table 1.

In Part II of this study we highlight the practical implications of the findings of the present study by considering three novel case studies: (i) Debonding of an actively contractile cell from a substrate during cyclic stretching simulated using the XN model with \( \phi_t > \phi_n \). It is demonstrated that the computation of non-physical repulsive normal forces significantly influences cell debonding patterns and computed distribution of the actin cytoskeleton (Deshpande et al., 2006; Ronan et al., 2012). Additionally, it is demonstrated that the MP model significantly reduces the computation of such non-physical interface tractions; (ii) Buckling of a stent coating during deployment is simulated using the BSG model. It is demonstrated that failure to penalise mixed-mode over-closure leads to a significant underprediction of coating buckling. It is demonstrated that the NP1 and NP2 models correctly penalise mixed-mode over-closure, leading to significantly increased coating buckling during stent deployment; (iii) Delamination of a bi-layered elastic arch is also simulated, implementing all cohesive zone formulations at the arch interface. This case study represents a practical example of traction controlled interface mode mixity and, following from the findings of the present paper, it is demonstrated that the form of the cohesive zone normal-tangential coupling terms has a pronounced effect on the predicted delamination of the bi-layered arch. It is envisioned that the theoretical analysis of Part I and the finite element implementations of Part II of this study will provide guidance for future development and implementation of potential and non-potential-based CZMs for mixed-mode applications.

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**Conflict of interest**

None
Appendix A

**Figure A1**: Work of separation ($\phi/\phi_n$) as a function of normal ($\Delta_n/\delta_n$) and tangential ($\Delta_t/\delta_t$) components of the interface separation vector for the MP model with $q=0.43$ and $r=0$: (a) $m=0$ (XN model); (b) $m=1$; (c) $m=5$. Dotted line indicates a path comprising of mixed-mode separation followed by normal separation.

MP model potential surfaces for the case of $q < 1$ (work of mode II separation less than work of mode I separation) are presented in Figure A1. Specifically, it is assumed that $q = 0.43$, as is commonly implemented for the XN model. The case of $m = 0$ (the XN model) is presented in Figure A1(a). Once again a separation path is illustrated in which a mixed-mode separation is followed by a normal separation. As detailed in Section 2.1, residual normal tractions must be overcome during the second (normal) phase of the separation despite the preceding full mixed-mode separation. As illustrated in Figure A1(b) and (c) for $m = 1$ and $m = 5$ respectively, the zone in which residual normal tractions are computed is reduced as the parameter $m$ is increased. Hence, for $m = 5$ no residual normal tractions are computed during the second (normal) phase of the separation. Once again it is worth mentioning that the MP model is identical to the XN model in pure mode I and mode II separation.
Figure A2: (a) Tangential traction ($T_t/\tau_{max}$) as a function of tangential displacement ($\Delta_t/\delta_t$) for $q=0.43$ and $r=0$ during a mixed-mode separation where $\tan^{-1}(\Delta_n/\Delta_t) = 20^\circ$. (b) Normal traction ($T_n/\sigma_{max}$) as a function of normal displacement ($\Delta_n/\delta_n$) representing a normal separation subsequent to the mixed-mode separation shown in (a). Curves are shown for the XN model and the MP model ($m=1, 2$ and $5$).

Figure A2(a) shows, for $q = 0.43$, the tangential traction-separation curves for mixed-mode separation ($20^\circ$ to the mode II axis) for the XN model and for the MP model with $m = 1, 2$ and $5$. For all cases, the tangential tractions reduce to zero at a tangential separation of $\Delta_t/\delta_t = 3$. However, it should be noted that an increase in the parameter $m$ leads to an increase in the computed peak tangential traction beyond the peak mode II traction ($\tau_{max}$). For the case of $m = 5$, a peak tangential traction of $T_t/\tau_{max} \approx 1.7$ is computed during the first (mixed-mode) phase of the deformation. The reduction of the residual normal traction zone for high values of $m$ results in a strong influence of the normal work of separation $\varnothing_n$ on mixed-mode separations, even when the mode angle is tending towards mode II. Figure A2 (b) shows the normal traction-separation curves during the second (normal) phase of the separation path when tangential separation is held constant at a value of $\Delta_t/\delta_t = 5$. No residual tractions are computed for the MP model for $m = 5$, as the mixed-mode path followed during the first phase of the deformation extends beyond the residual normal traction zone of the potential surface. However, as $m$ is reduced, the magnitude and region of residual normal tractions is increased. For $m = 1$ a residual normal traction of $T_n/\sigma_{max} = 0.3$ is computed at $\Delta_n/\delta_n \approx 2$. When $\Delta_n/\delta_n \geq 4$, computed residual normal tractions are not significant. However, for the XN model ($m = 0$), residual normal tractions are still evident when the normal separation is increased to $\Delta_n/\delta_n = 6$.
Appendix B

Positive instantaneous dissipation is computed for all paths shown in Figure 13. Figure B1 shows the plot of $d\phi_i$ corresponding to Figure 16(a) (XN model) and Figure 16(d) (NP2 model), demonstrating positive dissipation throughout. Dissipation for the MP model is also shown.

Figure B1: Normalised instantaneous dissipation ($d\phi_i/\phi_n$) during constant traction controlled mode mixity $\psi$ when $\phi_t = 4\phi_n$: (a) XN model; (b) MP model ($m=2$); (c) NP2 model.


