Cohesive zone laws for void growth – II. Numerical field-projection of elasto-plastic fracture processes with vapor pressure

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Abstract

Modeling ductile fracture processes using Gurson-type cell elements has achieved considerable success in recent years. However, incorporating the full mechanisms of void growth and coalescence in cohesive zone laws for ductile fracture still remains an open challenge. In this work, a planar field projection method, combined with equilibrium field regularization, is used to extract crack-tip cohesive zone laws of void growth in an elastic-plastic solid. To this end, a single row of void-containing cell elements is deployed directly ahead of a crack in an elastic-plastic medium subjected to a remote $K$-field loading; the macroscopic behavior of each cell element is governed by the Gurson porous material relation, extended to incorporate vapor pressure effects. A thin elastic strip surrounding this fracture process zone is introduced, from which the cohesive zone variables can be extracted via the planar field projection method. We show that the material’s initial porosity induces a highly convex traction-separation relationship – the cohesive traction reaches the peak almost instantaneously and decreases gradually with void growth, before succumbing to rapid softening during coalescence. The profile of this numerically extracted cohesive zone law is consistent with experimentally determined cohesive zone law in Part I for multiple micro-crazing in HIPS. In the presence of vapor pressure, both the cohesive traction and energy are dramatically lowered; the shape of the cohesive zone law however remains highly convex, which suggests that diffusive damage is still the governing failure mechanism.

Keywords: Cohesive zone; Gurson model; Void growth; Inverse method; Vapor pressure

1. Introduction

Mechanism-based computational models can link the microscopic fracture process of a material to its macroscopic failure behavior, and are widely used in the prediction of fracture and failure of structural components. One well established model is the cohesive zone law which constitutes the relationship between the cohesive zone tractions in

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equilibrium with the stress fields of the surrounding body and the cohesive zone separations compatible with the deformation fields of the surrounding body. This constitutive law has been highly effective in quantifying the behavior of quasi-brittle materials (e.g. Dugdale, 1960; Barenblatt, 1962).

In ductile fracture, void growth to coalescence becomes part of the crack growth mechanism. Studies have shown that high stress triaxiality coupled with intense plastic straining near a crack-tip could accelerate void growth, leading to the nucleation of new voids, and the subsequent lowering of the peak separation stress (Kopik and Needleman, 1988; Faleskog and Shih, 1997; Chew et al., 2006). By contrast, traditional cohesive zone laws assume that the cohesive strength and energy are material constants. To this end, Tvergaard and Hutchinson (1992, 1994, 1996) examined the regime of applicability of the cohesive zone law in representing ductile fracture, and incorporated the effects of plastic straining in a modified traction-separation relation. A more direct method for modeling ductile fracture was put forth by Xia and Shih (1995) where void growth and coalescence in the material was confined to a single row of void-containing cell elements ahead of the crack-tip. The progressive damage of these computational cells was governed by the Gurson constitutive model (Gurson, 1977). This “cell element approach” has been used to study the vapor pressure assisted failure of electronic packages (Chew et al., 2005a, 2005b, 2008). Unlike the cohesive zone law, the mechanism of void growth and coalescence inherent in the cell element approach could account for the full effects of plastic straining and stress triaxiality on fracture.

Continuing efforts to include the effects of void growth and coalescence in cohesive zone models for ductile fracture were made by Várias (1998), Siegmund and Brocks (1998) and Tvergaard (2001). These studies have proposed the use of special interface elements in the crack plane ahead of the crack to represent the fracture process zone; the cohesive properties of these elements relate to the cell element approach viz. the calibration of the separation energy and maximum cohesive traction using a porous material model. While the global fracture behaviors of some solid structures can be approximately described by calibrating these cohesive zone properties, it has been observed that certain mechanical processes are highly sensitive to details of the cohesive zone law. For example, Chandra et al. (2002) observed that the macroscopic mechanical response of a composite system was highly sensitive to the detailed shape of the cohesive zone model. Li and Chandra (2003) also showed that in addition to the cohesive strength and energy, the functional form of the cohesive zone model plays a vital role in determining the crack growth resistance of ductile materials. Similar conclusions were reached by Murphy and Ivankovic (2005) for the dynamic fracture of polymethylmethacrylate (PMMA), and Olden et al. (2008) for the environmental-assisted failure of ductile metals. To-date, a high resolution extraction of cohesive zone laws from micro-mechanical models of ductile fracture remains elusive, and is an important step towards advancing cohesive zone models for void growth.

One method to identify the crack-tip cohesive zone relations from the elastic far-fields is the inverse-problem solution developed by Hong and Kim (2003). In this method, the general form of the elastic fields of a crack-tip with a cohesive zone in a homogeneous isotropic solid was expressed in terms of an eigenfunction expansion of complex functions in the Muskhelishvili formalism (Muskhelishvili, 1953). Hong and
Kim (2003) showed an effective use of the eigenfunction expansion in an energetically meaningful planar field projection (P-FPM), providing an inversion method based on interaction $J$-integrals (Chen and Shield, 1977). The method was extended by Choi and Kim (2007) to extract the intrinsic nanoscale cohesive zone laws of an interface between two anisotropic elastic solids. The planar field projection methodology was also adopted in our recent experimental studies in Part I to obtain the cohesive zone laws for multiple crazing in high impact polystyrene (HIPS) and single methanol craze formation and growth in PMMA. We showed that the cohesive zone law for HIPS has a convex-shape relationship, while that for PMMA in methanol is highly concave. The former was attributed to toughening enhanced by multiple craze zone broadening, while the latter was due to environmental embrittlement which confined crazing to the crack-tip regime.

In this work, we investigate the crack-tip cohesive zone constitutive relations for void growth and vapor pressure induced damage in elastic-plastic solids using the P-FPM of Hong and Kim (2003). The cell element approach of Xia and Shih (1995) is adopted wherein damage arising from void growth and coalescence in the solid is confined to a single row of void-containing cell elements deployed directly ahead of a crack; the macroscopic behavior of each cell element is governed by the Gurson porous material relation, extended to incorporate vapor pressure effects (Guo and Cheng, 2002, 2003). With regards to inter-particle multiple crazes in polymers, this well-delineated damage zone can be considered as an effective micro-scale voiding zone, in which the volume expansion caused by multiple crazes is included as part of the effective micro-scale void growth. In ductile fracture, substantial plastic dissipation is involved in the background material. Here, extraction of the cohesive zone law is achieved by introducing a thin elastic layer between the process zone and the elastic-plastic background material, within which the framework of the P-FPM remains valid. Finally, we impose an equilibrium field regularization to minimize global errors in the numerical data used for the inversion process.

2. **Problem formulation**

Fig.1a shows the schematic of the small-scale yielding model, consisting of a homogeneous material with a semi-infinite crack loaded remotely by the symmetric mode I $K$-field under plane strain conditions. By taking advantage of symmetry, only one half of the geometry needs to be analyzed. The model can be divided into three distinct regions: (i) process zone ahead of the crack; (ii) elastic strip for planar field projection surrounding the process zone; (iii) elastic-plastic outer region. The elastic properties of these regions are denoted by Young’s modulus, $E$, and Poisson’s ratio $\nu$.

2.1 **Boundary value problem**

The uniaxial tensile stress-strain behavior of the elastic-plastic outer region is described by the true stress-logarithmic strain relation
where $\sigma_0$ is the initial yield stress in tension, and $n$ the strain hardening exponent; $n \to 0$ corresponds to an elastic-ideally plastic solid. Generalization to multiaxial stress states assumes isotropic hardening and Mises yield condition.

Along the remote circular boundary, the elastic asymptotic (in-plane) displacement field

\begin{equation}
\begin{aligned}
u_1(r, \theta) &= K_1 \frac{1 + \nu}{E} \sqrt{\frac{r}{2\pi}} (3 - 4\nu) \cos \frac{\theta}{2}, \\
u_2(r, \theta) &= K_1 \frac{1 + \nu}{E} \sqrt{\frac{r}{2\pi}} (3 - 4\nu) \cos \frac{\theta}{2},
\end{aligned}
\end{equation}

is applied, where $r^2 = x_1^2 + x_2^2$ and $\theta = \tan^{-1}(x_2/x_1)$ for points on the remote boundary. The radius of the circular boundary is set large enough to satisfy the small scale yielding condition for the fracture process of interest. $K_1$ is the mode I stress intensity factor related to the $J$-integral by

\begin{equation}
J = \frac{1 - \nu^2}{E} K_1^2.
\end{equation}

At various loading stages, the value of the $J$-integral is calculated on a number of contours in the outer elastic region around the crack using the domain integral method (Moran and Shih, 1987). The domain integral value was found to be in good agreement with the value given by (2.3) for the prescribed amplitude $K_i$. This consistency check assures that small-scale yielding conditions are satisfied.

Vapor pressure effects are manifested in two different ways: (i) high vapor pressure within cavities accelerates the process of void growth and coalescence; (ii) vapor pressure exerts tractions on crack faces. The former is modeled as an internal void pressure $p$ (described below), while the latter forms a component of the applied $K_i$. As such, $K_i$ stands in for the effective crack driving force from the contributions of both the background stress and the traction vapor pressure on the crack faces.

### 2.2 Fracture process zone

Metallic and polymeric materials which fail by void growth and coalescence typically display a macroscopically planar fracture process zone of one or two void spacings in thickness; away from this zone, little or no void growth is observed. As in Xia and Shih (1995), we idealize the ductile fracture process by confining void growth to a material layer of initial thickness $D$ ahead of the crack-tip. For polymers which exhibit multiple craze zone broadening, such as HIPS, void growth in the well-delineated process zone in our numerical model can be regarded as the effective volume expansion caused by both multiple crazes and micro-scale voids. A single row of 120 uniformly sized void-
containing cell elements, each of dimensions $D/2$ by $D/2$, is embedded in the highly refined mesh region ahead of the crack-tip (see Fig. 1b). The computations are carried out under plane strain conditions using the finite element program WARP3D (Gullerud et al., 2002).

The behavior of each cell element is governed by the Gurson flow potential $\Psi$ (Gurson, 1977; Tvergaard, 1990) extended to take account of vapor pressure $p$ (Guo and Cheng, 2002). It has the form:

$$\Psi = \left( \frac{\Sigma_e}{\hat{\sigma}} \right)^2 + 2q_1f \cosh \left( \frac{3q_1(\Sigma_m + p)}{2\hat{\sigma}} \right) - \left[ 1 + (q_1f)^2 \right] = 0$$  \hspace{1cm} (2.4)$$

where $\Sigma_e$ denotes the equivalent macroscopic stress, $\Sigma_m$ the mean macroscopic stress, $\hat{\sigma}$ the flow stress of the matrix as determined by Eq. (2.1), and $f$ the current void volume fraction. The yield surface for conventional $J_2$ flow theory is recovered by setting $f = 0$ in (2.4). The micromechanics parameters $q_1$ and $q_2$ were introduced by Tvergaard (1990) to improve model predictions for periodic arrays of cylindrical and spherical voids.

The Gurson flow potential has two internal variables, $\hat{\sigma}$ and $f$. The extended form introduces vapor pressure as a new internal variable $p$. Two separate cases are studied. The first represents the case for fully vaporized moisture, given by

$$\frac{p}{p_0} = \frac{T_0 f_0}{T f_0} \frac{1-f}{1-f_0} e^{-3q_1f \alpha \Delta T} ,$$  \hspace{1cm} (2.5)$$

where $\alpha$ is the coefficient of thermal expansion, and $\Delta T$ is the temperature rise relative to the reference temperature $T_0$. Equation (2.5) represents the equation of state for an ideal gas in an incompressible, thermally expanded, spherical shell. The reference state is given by $p_0, f_0, T_0$. In our isothermal analysis, we take $\Delta T = 0$. The second case represents high moisture content, where vapor pressure is assumed to be constant throughout the deformation, i.e.

$$p = p_0.$$  \hspace{1cm} (2.6)$$

The void growth rate $\dot{f}$ obeys the volumetric plastic strain rate relation

$$\dot{f} = (1-f) \text{tr} \mathbf{d}^p$$  \hspace{1cm} (2.7)$$

with nucleation neglected. Here, $\text{tr} \mathbf{d}^p$ implies trace of the plastic deformation rate $\mathbf{d}^p$. The extended Gurson relation (2.4) together with (2.5) – (2.7) describes the process of void growth. The adjustment parameters $q_1$ and $q_2$ in (2.4) are set to be 1.25 and 1 respectively (Faleskog et al., 1998).

2.3 Planar field projection with an embedded elastic strip

The effectiveness of the planar projection method (P-FPM) in extracting cohesive zone laws from elastic far-fields of a cohesive crack-tip (Hong and Kim, 2003) suggests that a similar approach could be utilized to determine the traction-separation relations for void growth. A summary of the procedure is described below.
Planar field projection method  As introduced by Hong and Kim (2003) and Choi and Kim (2007), the cohesive zone representation of a fracture process in a single crack-tip can be inversely determined from the elastic field surrounding the crack-tip process zone. Designating the Greek subscript $\alpha = 1$ or 2 throughout this paper, the distributions of the cohesive traction $t_\alpha(x_\alpha)$ and the separation $\delta_\alpha(x_\alpha)$ in the cohesive zone representation for $0 \leq x_\alpha \leq 2c$ can be expressed as (Hong and Kim, 2003),

$$t_\alpha(x_\alpha) - i\delta_\alpha(x_\alpha) = \sqrt{\frac{x_\alpha}{c}} \sum_{n=0}^{N} A_n U_n(x_\alpha/c) - 1$$  \hspace{1cm} (2.8)

$$\delta_\alpha(x_\alpha) = i\frac{\kappa+1}{2\mu} \sum_{n=0}^{N} B_n c \int_{x_\alpha/c}^{2c} \sqrt{\xi} U_n(\xi - 1) d\xi$$  \hspace{1cm} (2.9)

where $N \to \infty$, $U_n(\cdots)$ denotes the Chebyshev polynomials of the second kind, $i$ the imaginary number $\sqrt{-1}$, $\kappa = 3 - 4\nu$ for plane strain, $\kappa = (3 - \nu)/(1 + \nu)$ for plane stress, $\mu$ the shear modulus, $\nu$ Poisson’s ratio, and $A_n$ and $B_n$ complex coefficients which is determined from the surrounding elastic field as follows.

$$A_n = \frac{2}{\pi c} \left\{ J^\text{int}[S, \hat{S}_{t_\alpha}] + i J^\text{int}[S, \hat{S}_{b_\alpha}] \right\}$$  \hspace{1cm} (2.10)

$$B_n = \frac{2}{\pi c} \left\{ J^\text{int}[S, \hat{S}_{b_\alpha}] - i J^\text{int}[S, \hat{S}_{t_\alpha}] \right\}$$  \hspace{1cm} (2.11)

where the interaction $J$-integral $J^\text{int}[S, \hat{S}^{(n)}]$ between the physical cohesive-crack field of interest $S[\sigma_{\alpha\beta}, u_{\alpha,\beta}]$ and auxiliary proving fields $\hat{S}^{(n)}[\hat{\sigma}_{\alpha\beta}, \hat{u}_{\alpha,\beta}]$ for $n = 0, 1, 2\ldots N$, is defined as

$$J^\text{int}[S, \hat{S}^{(n)}] = \int_{\Gamma} (\sigma_{\alpha\beta} \hat{u}_{\alpha,\beta} n_\alpha - \sigma_{\alpha\beta} \hat{u}_{\alpha,\beta} n_\alpha - \hat{\sigma}_{\alpha\beta} n_\alpha) ds.$$  \hspace{1cm} (2.12)

The auxiliary elastic field $\hat{S}^{(n)}[\hat{\sigma}_{\alpha\beta}, \hat{u}_{\alpha,\beta}]$ with a subscript $t_\alpha$ or $b_\alpha$ stands for a set of stress and displacement fields corresponding to the complex elastic potential,

$$\hat{\Phi}^{(n)}(z) = \frac{i^\alpha \mu}{\kappa + 1} \sqrt{z - 1} U_n(\bar{z})$$  \hspace{1cm} (2.13)

or

$$\hat{\Phi}^{(n)}(z) = -\frac{i^\alpha \mu}{\kappa + 1} \sqrt{z + 1} U_n(\bar{z})$$  \hspace{1cm} (2.14)
respectively, with which the stress and the displacement gradient fields can be derived as

\[
\begin{align*}
\sigma_{22} - i\sigma_{12} &= (z - \bar{z})\Phi'(\bar{z}) + 2\Phi(z), \\
\frac{1}{2}(\sigma_{11} + \sigma_{22}) &= \Phi(z) + \Phi(\bar{z}), \\
u_{1,1} + i\nu_{2,1} &= \frac{1}{2\mu} \left\{ (\bar{z} - z)\Phi'(z) + (\kappa - 1)\Phi(z) \right\}, \\
u_{1,2} + i\nu_{2,2} &= -\frac{i}{2\mu} \left\{ (\bar{z} - z)\Phi'(z) - (\kappa + 1)\Phi(z) + 2\Phi(z) \right\}.
\end{align*}
\]

(2.15)

Here, \( z = x_1 + ix_2 \), \( \bar{z} = x_1 - ix_2 \) and \( \bar{z} = (z - c)/c \). Note that the origin of the coordinate in (Hong and Kim, 2003) is located at the center of the cohesive zone, while the origin of the coordinate in this paper is at the left end of the cohesive zone.

**Embedded elastic strip**

The above procedure was developed within the framework of continuum deformation kinematics of linear elasticity. In ductile fracture, however, substantial plastic dissipation and nonlinear deformation is involved in the background material. To extend the validity of the P-FPM for fracture processes surrounded by nonlinear deformation, we introduce a thin elastic strip of thickness \( e_h \), sandwiched between the porous cell element layer described in Section 2.2 and the elastic-plastic background material. See shaded region in Fig. 1b. The interaction \( J \)-integral in (2.12) is then taken along the fixed contour \( \Gamma \) within the elastic strip, which encompasses the process zone.

Before proceeding further, we examine the effects of the elastic strip on the extent of plastic dissipation in the solid. To better demonstrate the validity of the elastic strip assumption that a thin elastic strip would minimally disturb the surrounding elasto-plastic deformation, we adopt the material parameters \( \sigma_0/E = 0.001 \), \( \nu = 0.3 \), \( n = 0 \), \( f_0 = 0.001 \), which are representative of metallic materials exhibiting severe plastic behavior. The plastic strain contours, operationally defined by \( \varepsilon^p > 0.001 \), at fixed load of \( J/(\sigma_0 D) = 0.75 \) are shown in Fig. 2 for several elastic strip thicknesses \( e_h \). The solid curve denotes the actual numerical solution without the elastic strip. Observe that the plastic strain contour for \( e_h = D \) remains remarkably close to the actual solution even when the extent of plastic deformation in the background material is large. For \( e_h = 2D \) or \( 3D \), however, deviation from the exact solution becomes more significant. Careful examination further reveals that the plastic dissipation within the process zone for \( e_h = 2D \) and \( 3D \) can be about 1.5- and 2-fold larger than the actual solution. For \( e_h = D \), plastic dissipation within the process zone remains almost identical to the exact solution. This suggests the validity of the embedded elastic strip assumption for small \( e_h \) values. Unless otherwise stated, we assume \( e_h = D \) in the computations to follow. An evaluation of the elastic strip thickness effects on the cohesive zone relationship extracted by P-FPM is presented later in Fig. 7.

**2.4 Cohesive zone length and model parameters**
Prior to the application of the P-FPM, the size of the cohesive zone (width $2c$) remains an unknown parameter which has to be determined. This can be derived from far-field information using $J$ and $M$ conservation integrals (Hong and Kim, 2003), or directly from the porosity and mean stress distribution within the cell element layer representing the process zone (Chew et al., 2005a). However, the size of the cohesive zone is a strong function of the initial porosity, vapor pressure, and loading level, among other parameters. Any changes in the cohesive zone length should be accompanied by redefining the interaction $J$-integral contour $\Gamma$, and hence the elastic strip, since the errors introduced in the inversion scheme become significantly larger with increasing distance between the cohesive zone and $\Gamma$. Numerical experiments by Hong and Kim (2003) showed that the P-FPM works well as long as the estimated region of the cohesive zone encloses the true region of the cohesive zone. If the estimated zone size is too large compared to $2c$, the polynomial expansion requires a much higher order to have the same accuracy of approximation as that with the correct cohesive zone size. To avoid the onerous task of redefining the cohesive zone length (and hence $\Gamma$ and the elastic strip surrounding the cohesive zone), we adopt a high order polynomial expansion and assume a fixed cohesive zone length of $2c = 60D$ in our computations, which corresponds to the 120 cell elements representing the process zone.

The focus of this study is on void growth in polymeric materials. The estimated void volume fraction $f_0$ for polymeric materials used in plastic packages, like bimaleimide triazine epoxy, ranges from 1–5%; the initial porosity for cavitated rubber particles combined with inter-particle multiple crazing in glassy polymers can be much higher ($f_0 > 0.1$). For most of the computations, we assume $f_0 = 0.05$, with the material properties of the solid specified by $\sigma_0/E = 0.01$, $\nu = 0.4$ and $n = 0.1$.

3. Cohesive zone law for void growth

The critical porosity governing the onset of void coalescence in metals ranges from $f_e = 0.15$–0.25 (Tvergaard 1990; Needleman et al., 1992). In glassy polymers, $f_e$ can be much higher since the fibrils spanning the craze zones are load-bearing. The material’s $f_e$ has a strong correlation with the development of a crack-tip cohesive zone – the crack-tip cohesive zone becomes fully developed when the peak porosity at the crack-tip $f_{\text{tip}}$ reaches $f_e$.

Fig. 3a displays the evolution of $f$ ahead of the crack under pure remote loading. The discrete points in the figure represent the actual numerical values. At applied load of $J/(\sigma_0D) = 0.26$, results show voids adjacent to the crack-tip growing rapidly with near-tip $f$ reaching about 0.15. At higher load levels of $J/(\sigma_0D) = 0.35$, 0.44 and 0.56, the near-tip porosity reaches $f_{\text{tip}} = 0.2$, 0.25 and 0.3. The corresponding mean stress profiles ahead of the crack are shown in Fig. 3b. As $J/(\sigma_0D)$ increases from 0.26 to 0.56, the stress relaxation associated with the zone of voiding emanating from the crack in Fig. 3a shifts the peak mean stress location further ahead of the crack from $x_1 = 2D$ to $x_1 = 7D$. Observe that this peak mean stress location, which denotes the transition between stress elevation due to material hardening and softening due to void growth, coincides with the onset of rapid void growth. For polymers, the peak mean stress level is strongly influenced by the initial porosity, pressure-sensitivity level, and the effects of vapor pressure (Chew et al., 2006).
Investigations on ductile fracture based on the cohesive zone law have largely assumed a traction-separation relation where the failing layer undergoes uniaxial straining in the direction normal to the plane (e.g. Tvergaard and Hutchinson, 1992). As shown in Fig. 3, hydrostatic stress strongly controls the growth of voids in ductile fracture. For cohesive zone laws of void growth to better fit the physical reality, this hydrostatic stress component should be incorporated as an in-plane $T$-stress term in the two-parameter expansion of the remote elastic stress field.

The P-FPM with a high-order polynomial representation of $N = 6$ is used to trace the development of the normalized traction $t_2/\sigma_0$, separation-gradient $\tilde{b}_2(= 2\mu b_2 / \sigma_0(\kappa + 1))$, and separation $\delta_2/D$ ahead of the crack in Fig. 4a–c. The corresponding traction-separation relationship is provided in Fig. 4d. For verification purposes, we note that the difference between these values increases with loading, which is reflective of the increasing plastic dissipation in the background material. Hence, the methodology adopted in this paper allows one to segregate the individual contributions of the separation energy and background plastic dissipation from the overall fracture toughness. Results show a slight dip in the peak traction from $t_2/\sigma_0 = 2.2$ to 2.0 as the loading increases from $J/(\sigma_0D) = 0.26$ to 0.44. At higher loads of $J/(\sigma_0D) = 0.26$ and 0.35 occur in the vicinity of the crack-tip ($x_1 \leq 2D$); the larger numerical errors near the crack singularity may explain the discrepancies in the calculated peak tractions at these loads (as compared to higher loadings). This notwithstanding, the curves for $f_{tip} = 0.15, 0.2$ and 0.25 (represented by $J/(\sigma_0D) = 0.26, 0.35$ and 0.44) follow quite closely to the main envelope of $f_{tip} = 0.3$ (at $J/(\sigma_0D) = 0.56$) but individually fall off at higher separation levels. These trends show the correct development of the cohesive zone. Henceforth, we assume the cohesive zone to be fully developed when $f_{tip} = f_e = 0.3$.

Interestingly, our inverse approach shows that the cohesive zone law for void growth has a convex shape (Fig. 4d): the traction reaches its peak almost instantaneously and decreases gradually during void growth; as $f$ approaches $f_e$, the sustainable traction drops rapidly. The highly convex cohesive zone law is in sharp contrast to the trapezoidal-shaped cohesive zone law assumed by Tvergaard and Hutchinson (1992, 1994, 1996) and the exponential form adopted by Xu and Needleman (1994), both of which fail to account for rapid softening behavior observed in our simulations during void coalescence.

Fig. 5 examines the convergence of the cohesive zone law measurements with the order of the polynomial representation $N$ for $f_0 = 0.05$. As shown in Fig. 5a, the second order representation $N = 2$ does not have enough degrees of freedom to fit the cohesive traction $t_2$. As the order increases from $N = 2$ to 4, the Chebyshev-polynomial series for $A_n$ in (2.10) converges rapidly, and an exact agreement is reached between the cohesive traction distributions for $N = 4$ and 5. With a higher polynomial order of $N = 6$, the solution diverges slowly. Thus, there appears to be an optimal order $N$ with which the cohesive zone law can be determined: while a small order representation will have insufficient terms to fit the actual distribution, a larger $N$ increases the singularity of the inversion scheme. Focusing on the cohesive separation in Fig. 5b–c, we observe that a 5-order polynomial representation for $B_n$ in (2.11) is required for convergence of $\tilde{b}_2$, and
hence $\delta_2$ – see exact solution match between $N = 5$ and 6. As such, we use a 5-order polynomial representation to obtain an accurate traction-separation relation for $f_0 = 0.05$ (Fig. 5d). This procedure is repeated to determine the optimal $N$ in subsequent computations.

We have also conducted computations for different assumed cohesive zone lengths ranging from $2c = 30D$ to $60D$. With each predetermined value of $c$, we redefined the width of the interaction $J$-integral contour $\Gamma$, such that $\Gamma \approx \Gamma_0$, to minimize global errors in the inversion scheme. The extracted distributions of tractions and separation gradients were found to be somewhat insensitive to the assumed cohesive zone size, as previously noted by Hong and Kim (2003). However, a more accurate estimation of $c$ would reduce the order of $N$ required to obtain convergence of the extracted cohesive zone parameters. For example, with an assumed cohesive zone width of $2c = 30D$ which is a closer estimate to the actual cohesive zone size, a third-order polynomial representation is sufficient to obtain accurate distributions of $t_2$ and $\delta_2$ as compared to $N = 5$ for $2c = 60D$ in Fig. 5.

4. Vapor pressure assisted void growth

The physical and mechanical properties of many ductile engineering materials can deteriorate under the deleterious effects of environmentally assisted degradation such as moisture swelling and stress corrosion cracking. An important example is the failure of polymeric molding compound and adhesives during the surface mounting of electronic packages onto printed circuit boards under reflow (slightly above glass transition) temperatures of 220–260°C. Prior to reflow soldering, moisture diffuses through the hygroscopic polymeric materials and condenses within the micro-pores. At high reflow temperatures, the condensed moisture rapidly vaporizes into steam, creating high internal pressures on pre-existing voids and particle/matrix interfaces. The rapidly expanding water vapor exerts internal pressures on the voids that could reach 3–6 MPa (Liu and Mei, 1995). Such stress levels are comparable to the yield strengths of epoxy molding compounds and epoxy adhesives whose glass transition temperatures $T_g$ range between 150 and 300°C. Guo and Cheng (2002) showed that the vapor pressure $p$ for fully vaporized moisture can be derived from the ideal gas law in (2.5) and is dependent on the current void volume fraction $f$. This holds true for low moisture content. If the void contains high moisture content, the moisture may not fully vaporize leaving a two-phase mixture of water and vapor gas. In such cases, a constant level of high vapor pressure can be sustained for a considerable amount of void growth, Eq. (2.6).

Fig. 6a shows the traction-separation relationships for fully vaporized moisture, with $f_0 = 0.05$ and $N = 5$. Observe that increasing $p_0$ lowers both the peak traction and work of separation, and hence the fracture toughness of the material. When $p_0/\sigma_0$ increases from 0 to 0.5, the $t_2$–$\delta_2$ relationship is proportionally lowered. At higher vapor pressure levels of $p_0/\sigma_0 = 1.0$ and 1.5, the reduction in $t_2$ becomes most dramatic at small $\delta_2$; at larger $\delta_2$, the damaging effects of vapor pressure weakens. This observation can be anticipated from the ideal gas law in (2.5). When $\delta_2$ is small, the void porosity $f$ remains close to $f_0$. High pore pressure acting over a relatively small area substantially lowers the sustainable traction. At larger $\delta_2$, the high hydrostatic stress ahead of the crack triggers the unstable
growth of voids (see Fig. 3b). The fully vaporized moisture now acts over a larger void surface, and the current pressure $p$ in (2.5) decreases. The resulting shape of the cohesive zone law under high $p_0$ levels is highly convex.

Next, we examine the high moisture content case in Fig. 6b, where vapor pressure is assumed to be constant during the deformation. Compared to Fig. 6a, the reduction in the cohesive traction and energy is much greater for constant vapor pressure $p$. Results also show a significant drop in $t_2$ with vapor pressure at all separation distances. To characterize the convexity changes of the cohesive zone laws, we reintroduce the cohesive zone softening shape factor $G/G_c$ defined in Part I, where $G$ is the overall separation energy, $G = \sigma^* \delta^* / 2$ the linear softening separation energy, and $\sigma^*$ and $\delta^*$ the peak cohesive traction and total separation respectively. As the constant vapor pressure level increases from $p/\sigma_0 = 0$ and 0.9, the softening shape factor is slightly lowered from $G/G_c = 1.50$ to 1.44 which indicates a slight drop in the convexity of the $t_2-\delta_2$ relationship. While our experimental studies in Part I for PMMA also show substantial lowering of the peak cohesive traction and separation energy under methanol environment, the corresponding convexity reduction of $t_2-\delta_2$ in PMMA under methanol environment is substantially more severe (with $G/G_c = 0.32$) than in our numerical study on vapor effects in Fig. 6b. This discrepancy can be explained by the different micro-mechanisms involved in these separate fracture processes. During embrittlement of the methanol craze in PMMA, the softening agent diffuses from the crack surface, resulting in concentrated tractions (and very rapid craze voiding) at the craze-tip, trailed by rapid softening cohesive tractions (and lower craze void growth rate) some distances behind the craze-tip. Vapor pressure induced embrittlement in our present analysis, however, is caused by void pressure in which the pressure inducing vapor diffuses mostly in the bulk; the more diffusive void growth therefore explains the smaller convexity reduction of the cohesive zone law in this study. This scenario is representative of the vapor pressure assisted popcorn cracking phenomenon in electronic packages during reflow soldering (Gallo and Munamarty, 1995).

Fig. 7a displays the effects of initial porosity on the traction-separation relationship, with $f_0$ ranging from $f_0 = 0.01$ for partial decohesion of filler particles from particle/polymer matrix interfaces, to $f_0 = 0.1$ for cavitated rubber blends. The effects of $f_0$ under constant vapor pressure $p = 0.9\sigma_0$ are displayed in Fig. 7b. Results show that increasing $f_0$ reduces both the peak traction and work of separation. These effects are further exacerbated under high levels of vapor pressure. For example, the presence of constant vapor pressure $p = 0.9\sigma_0$ reduces the peak traction for $f_0 = 0.01$ by 35%; the reduction becomes 63% for $f_0 = 0.1$. From Fig. 7a, we also observe that as $f_0$ increases from 0.01 to 0.1, the shape of the $t_2-\delta_2$ relationship becomes slightly more convex, with $G/G_c$ increasing from 1.49 to 1.56. For highly porous damage zones ahead of the crack ($f_0 = 0.1$), the rapid softening regime dominates the cohesive zone law, which suggests that limited voiding occurs before the onset of coalescence. This highly convex $t_2-\delta_2$ profile closely resembles the experimentally determined cohesive zone law in Part I for inter-particle multiple crazes in HIPS ($G/G_c = 1.36$).

At this juncture, we turn our attention to the effects of vapor pressure and porosity on the hydrostatic stress development ahead of the crack. As noted from the self-similar mean stress profiles in Fig. 3b, the peak mean stress level is responsible for the onset of
rapid voiding. This critical stress $\Sigma_m^c / \sigma_0$ is summarized in Table 1 for various initial porosities and vapor pressure levels. Observe that an increase in $f_0$ significantly reduces $\Sigma_m^c$. When coupled with high vapor pressure levels, $\Sigma_m^c$ is dramatically lowered to levels below $\sigma_0$.

Recall from Fig. 2 that the embedded elastic strip has no discernable influence on the plastic dissipation in the material when the elastic strip thickness $e_h$ is small. For completeness, we compare the effects of $e_h$ on the cohesive zone measurements in Fig. 7. For initial porosities of $f_0 > 0.05$ or in the presence of vapor pressure, the $t_2-\delta_2$ relationships between $e_h = D$ (solid curves) and $e_h = 3D$ (dashed curves) are almost identical. For $f_0 \leq 0.05$, some differences are observed due to the larger plastic dissipation in the background material for small $f_0$. For larger $f_0$ or in the presence of vapor pressure, the voids grow rapidly with little or no plastic dissipation in the background material.

5. Equilibrium field regularization

The cohesive zone characteristics in Sections 3 and 4 are evaluated by the P-FPM with interaction $J$-integral along the contour $\Gamma$ within the embedded elastic strip. The accuracy of this inversion scheme is therefore limited by the number of available gauss points offered by the finite-sized mesh along $\Gamma$. In this section, an equilibrium field regularization technique is introduced to increase the number of accurate data points along $\Gamma$ from which the interaction $J$-integral can be calculated, without physically increasing the actual finite element mesh density.

5.1 Method and implementation

We consider an element refinement approach in which each quadrilateral finite element within the domain of the embedded elastic strip $\Omega$ is divided into $\eta \times \eta$ virtual elements (Fig. 8). The displacement field of these virtual elements, denoted by $\tilde{u}_i(\mathbf{x})$, is obtained by linear interpolation from the numerical displacements at the original nodal points using finite element shape functions. Except at these original nodal points, the approximate displacement field $\tilde{u}_i(\mathbf{x})$ does not necessarily satisfy the equilibrium equation, and may include a small amount of interpolation error $\delta_i(\mathbf{x})$, i.e.

$$\tilde{u}_i(\mathbf{x}) = u_i(\mathbf{x}) + \delta_i(\mathbf{x}) \quad (5.1)$$

where $u_i(\mathbf{x})$ denotes the actual displacement field. This interpolation error can be quantitatively characterized by the Euclidian norm of error

$$E[u_i(\mathbf{x})] = \frac{1}{2} \int_\Omega \| u_i - \tilde{u}_i \|^2 d\Omega. \quad \mathbf{x} \in \Omega \quad (5.2)$$

Thus, equilibrium smoothing can be achieved by minimizing (5.2) subject to the equilibrium equation

$$C_{ijkl} u_k,\mathbf{j} = 0 \quad (5.3)$$
in $\Omega$, where $C_{ijkl}$ denotes the fourth-order elasticity tensor. The displacement fields $u_i(x)$ and $\tilde{u}_i(x)$ are approximated by the finite element shape function for quadrilateral elements $M^{(k)}(x)$ as follows

$$u_i(x) = \sum_{k=1}^{4} M^{(k)}(x) u^{(k)}$$

$$\tilde{u}_i(x) = \sum_{k=1}^{4} M^{(k)}(x) \tilde{u}^{(k)}$$

where $u^{(k)}$ and $\tilde{u}^{(k)}$ denote the actual and approximate arrays of nodal displacement values in the finite element mesh. Inserting (5.4) into (5.2), we obtain

$$E[u] = \frac{1}{2} u \cdot Pu - u \cdot \tilde{P}u + \frac{1}{2} \tilde{u} \cdot \tilde{P}u$$

where $P = [P_{ij}]_{4x4} = \int_{\Omega} M^{(i)}(x) M^{(j)}(x) d\Omega$ and $u$ and $\tilde{u}$ are the arrays of nodal displacement values in the equilibrium field and approximate field.

A linear algebraic form of the equilibrium equations in (5.3) can be written as

$$\begin{bmatrix} K_{11} & K_{12}^T \\ K_{12} & K_{22} \end{bmatrix} \begin{bmatrix} u_b \\ u_i \end{bmatrix} = \begin{bmatrix} p_b \\ 0 \end{bmatrix}$$

where $u$ and $p$ represent arrays of nodal displacements and nodal forces, and subscripts of $b$ and $i$ indicate boundary and internal nodes in $\Omega$, respectively. The nodal forces on the internal nodes vanish from equilibrium conditions, while the nodal forces on the boundary are unknown in the equilibrium smoothing. As such, a linear algebraic form of the equilibrium constraints in the internal domain can be written as

$$K u = 0$$

where the stiffness matrix $K = [K_{12} \quad K_{22}]$.

Using the Lagrange multiplier method, we achieve equilibrium smoothing by minimizing

$$E[u, \lambda] = \frac{1}{2} u \cdot Pu - u \cdot \tilde{P}u + \frac{1}{2} \tilde{u} \cdot \tilde{P}u + \lambda \cdot Ku$$

where $\lambda$ is an array of Lagrange multipliers. In other words, we impose

$$\frac{\partial E}{\partial u} = Pu - \tilde{P}u + K^T \lambda = 0$$

$$\frac{\partial E}{\partial \lambda} = Ku = 0.$$  

In matrix form, Eq. (5.9) can be expressed as
\[
\begin{bmatrix}
P & K^T \\
K & 0
\end{bmatrix}
\begin{bmatrix}
u \\
\lambda
\end{bmatrix} = \begin{bmatrix}
P\tilde{u} \\
0
\end{bmatrix}.
\tag{5.10}
\]

Inverting (5.10), we obtain
\[
\begin{bmatrix}
u \\
\lambda
\end{bmatrix} = \begin{bmatrix}
P^{-1} + p^{-1}K^T\Delta^{-1}Kp^{-1} & -P^{-1}K^T\Delta^{-1} \\
-\Delta^{-1}Kp^{-1} & \Delta^{-1}
\end{bmatrix}\begin{bmatrix}
P\tilde{u} \\
0
\end{bmatrix}.
\tag{5.11}
\]

where \(\Delta = -KP^{-1}K^T\).

Finally, the regularized displacement field \(u\) satisfying the equilibrium conditions can be expressed as
\[
u = (I + P^{-1}K^T\Delta^{-1}K)\tilde{u}.
\tag{5.12}
\]

By controlling the element refinement level \(\eta\) (see Fig. 8), the above equilibrium field regularization technique allows us to obtain converged inverse solutions, without going through the arduous task of finite element mesh refinement.

5.2 Regularized cohesive zone law

We first examine the effects of field regularization on the cohesive zone law measurements for \(f_0 = 0.05, N = 5\) in Fig. 9, under \(p = 0\) and constant vapor pressure \(p = 0.9\sigma_0\). Four levels of element refinement \(\eta = 1-4\) shown in Fig. 8 are considered. Observe that the effects of \(\eta\) remain small for \(p = 0.9\sigma_0\). For \(p = 0\), some quantitative changes in \(t_2\) are noted, and the \(t_2-\delta_2\) relationship converges rapidly as \(\eta\) increases from 1 to 4. These small quantitative differences between the regularized and non-regularized solution demonstrate the numerical accuracy of our previous calculations in Sections 3 and 4.

The computations thus far have assumed a fixed cohesive zone width, with the interaction \(J\)-integral in (2.12) taken along a fixed contour \(\Gamma\) around the embedded elastic strip encompassing the process zone. The close proximity of \(\Gamma\) to the cohesive zone region infers that \(\Gamma \approx \Gamma_0\), where \(\Gamma_0\) is the interaction \(J\)-integral contour along the cohesive zone faces. The path independence property of (2.12) proves the theoretical equivalence between the interaction \(J\)-integrals along a far-field contour \(\Gamma\) and \(\Gamma_0\). As Hong and Kim (2003) noted, however, the interaction integral yields a small number by adding and subtracting large numbers. Since the integrand of the interaction integral has terms of very large numbers of order \(2^N(r/c)^{N+1/2}\) multiplied to the displacement field, the inversion scheme therefore becomes more singular with increasing \(2^N(r/c)^{N+1/2}\). As such, errors introduced in the inversion scheme become significantly larger with increasing distance between the cohesive zone and \(\Gamma\) for high-order polynomial representations. The effectiveness of equilibrium field regularization in minimizing these errors is next examined.

Figs. 10 and 11 display the distributions of tractions and separations in the cohesive zone for \(f_0 = 0.05\) with fixed cohesive zone width of \(2c = 40D\). The solid lines represent the profiles obtained by P-FPM with the interaction integral taken along the same contour \(\Gamma\) used in our earlier computations for \(2c = 60D\), i.e. \(\Gamma \approx 1.5\Gamma_0\). The open circles and crosses denote the profiles obtained by redefining the interaction integral contour to
within close proximity of the presumed crack-tip cohesive zone, such that $\Gamma \approx \Gamma_0$. We first discuss the results for $\Gamma \approx \Gamma_0$. Observe that a lower-order polynomial representation of $N = 3$ is sufficient to obtain a converged set of $t_2$ and $\delta_2$ distributions (compared to $N = 5$ in Fig. 5). Effects of field regularization are also found to be small, and a converged solution is maintained even for higher order polynomial representation of $N = 4$. By contrast, the non-regularized traction distributions extracted along $\Gamma \approx 1.5\Gamma_0$ diverges rapidly for $N = 4$ and beyond (Fig. 10c). The non-regularized separation distribution begins to oscillate for $N = 3$ (Fig. 11b). For $N = 4$, the $\delta_2$ distribution oscillates wildly about $\delta_2 = 0$ and the solution diverges (Fig. 11c). As $\eta$ increases from 1 to 2, however, the degree of oscillations for both traction and separation distributions dramatically decreases. By further increasing the number of elemental subdivisions to $\eta = 8$, the regularized solution extracted from the far-field contour $\Gamma \approx 1.5\Gamma_0$ closely approaches that for $\Gamma \approx \Gamma_0$. These results show that the equilibrium field regularization can overcome some of the singularity issues associated with the inversion scheme.

6. Concluding remarks

This work is aimed at establishing the crack-tip cohesive zone constitutive relations for void growth and vapor pressure induced damage in elastic-plastic solids. With this in mind, the computational study deploys a single row of void-containing cells directly ahead of a crack in an elastic-plastic material to model the fracture process zone. The process zone is surrounded by an embedded elastic strip, from which the distributions of tractions and separations in the process zone are extracted using the planar field projection method (Hong and Kim, 2003). The influence of the elastic strip on the plastic dissipation and the measured cohesive tractions and separations was found to be small. Equilibrium field regularization was also employed to validate the accuracy of the inverse solution.

We show that the cohesive zone law for void growth has a distinctively convex shape: the traction reaches its peak almost instantaneously, and decreases gradually during void growth; when void coalescence occurs, the sustainable traction rapidly decreases. The latter’s rapid softening behavior is not captured by the trapezoidal-shaped cohesive zone law assumed by Tvergaard and Hutchinson (1992, 1994, 1996) and the exponential form adopted by Xu and Needleman (1994). The functional shape of this numerically extracted cohesive zone law (cohesive zone softening shape factor of $G/G_c = 1.49 – 1.56$) is close to our experimentally determined cohesive zone law in Part I for inter-particle multiple micro-crazing in HIPS ($G/G_c = 1.36$). For fully vaporized moisture, vapor pressure effects are mainly confined to the early separation stages, and the resulting traction-separation relationship is highly convex. With high moisture content, constant vapor pressure reduces both the cohesive traction and energy, particularly when the material’s initial porosity is high; the shape of the cohesive zone law, however, remains distinctively convex. The effects of vapor pressure induced embrittlement are different from that of methanol craze embrittlement in PMMA where the experimentally extracted cohesive zone law was highly concave (Part I). The functional shape of the cohesive zone law therefore depends on the involved embrittlement mechanism: diffusion of moisture-induced vapor pressure in the bulk causing more diffusive damage in the material, versus methanol diffusion from the crack surface leading to concentrated near-tip damage.
A strong correlation between the peak hydrostatic stress and the unstable growth of voids has also been established. For cohesive zone laws of void growth to better fit the physical reality, this hydrostatic stress component should be incorporated as an in-plane $T$-stress term in the two-parameter expansion of the remote elastic stress field. When taken together with the extracted convex traction-separation relation from planar field projection, the regime of applicability of traditional cohesive zone laws can be suitably extended to ductile fracture.

Acknowledgements

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References


Figure Captions

Figure 1: (a) Small-scale yielding model of a crack with a single row of void-containing cell elements in the process zone, surrounded by an embedded elastic strip, in an elastic-plastic body. (b) Close-up view of the finite element mesh near the crack-tip.

Figure 2: Plastic zone shape and size for several elastic strip thickness $e_h$.

Figure 3: Distribution of (a) porosity $f$ and (b) mean stress $\Sigma_m/\sigma_0$ ahead of crack for $f_0 = 0.05$.

Figure 4: Development of cohesive zone variables and a cohesive zone law extracted by the planar field projection method for $f_0 = 0.05$, $N = 6$; (a) traction; (b) separation gradient; (c) separation; (d) cohesive zone law.

Figure 5: Cohesive zone variables and a cohesive zone law extracted by the planar field projection method with a polynomial of order $N$ for $f_0 = 0.05$; (a) traction; (b) separation gradient; (c) separation; (d) cohesive zone law.

Figure 6: Effects of vapor pressure on the cohesive zone law for $f_0 = 0.05$, $N = 5$; (a) vapor pressure $p_0$ governed by the ideal gas law; (b) constant vapor pressure $p$.

Figure 7: Effects of initial porosity $f_0$ and elastic strip thickness $e_h$ on the cohesive zone law; (a) $p = 0$; (b) constant pressure $p = 0.9\sigma_0$.

Figure 8: Close-up view of the elastic strip with four levels of equilibrium field regularization (a) $\eta = 1$; (b) $\eta = 2$; (c) $\eta = 3$; (d) $\eta = 4$.

Figure 9: Effects of equilibrium field regularization on cohesive zone variables and cohesive zone law for $f_0 = 0.05$, $N = 5$ with $p = 0$ and constant pressure $p = 0.9\sigma_0$; (a) traction; (b) separation gradient; (c) separation; (d) cohesive zone law.

Figure 10: Effects of equilibrium field regularization on traction distributions in the cohesive zone for $f_0 = 0.05$, $2c = 40D_i$; (a) $N = 2$; (b) $N = 3$; (c) $N = 4$. The solid lines represent the extracted solution along $\Gamma = 1.5\Gamma_0$; the open circles and crosses denote the extracted solution along $\Gamma = \Gamma_0$.

Figure 11: Effects of equilibrium field regularization on separation distributions in the cohesive zone for $f_0 = 0.05$, $2c = 40D_i$; (a) $N = 2$; (b) $N = 3$; (c) $N = 4$. The solid lines represent the extracted solution along $\Gamma = 1.5\Gamma_0$; the open circles and crosses denote the extracted solution along $\Gamma = \Gamma_0$. 
Table 1: Critical mean stress for cells ahead of the crack

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<th>Initial porosity $f_0$</th>
<th>Critical stress $\Sigma_m^c / \sigma_0$</th>
<th>$p = 0$</th>
<th>$p = 0.9\sigma_0$</th>
<th>$p = p_0 = \sigma_0$</th>
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</tbody>
</table>
Figure 2

- $\sigma_0/E = 0.001$
- $n = 0$
- $f_0 = 0.001$
- $e_n = 3D$
- $2D$
- $D$
- $\epsilon^p > 0.001$
- $J/(\sigma_0 D) = 0.75$
Figure 3

- $f_0 = 0.05$
- $J/(\sigma_0 D) = 0.26$
- $J/(\sigma_0 D) = 0.35$
- $J/(\sigma_0 D) = 0.44$
- $J/(\sigma_0 D) = 0.56$

Figure 3a

$\Sigma_{E}/\sigma_0$

Figure 3b

$x_1/D$

Figure(s) 3
Figure 8

(a) \[ \eta = 1 \]

(b) \[ \eta = 2 \]

(c) \[ \eta = 3 \]

(d) \[ \eta = 4 \]
Figure 9c

Figure 9d
Figure 10

(a) $N = 2$

- $\eta = 1$
- $\eta = 3$

$\Gamma = \Gamma_0$

(b) $N = 3$

- $f_0 = 0.05$
- $2c = 40D$

(c) $N = 4$

$t_2/\sigma_0$ vs. $x_1/D$

Figure 10