PREDICTIVE FRACTURE MODELLING IN TOUGH POLYETHYLENES USING EXPERIMENTALLY MEASURED COHESIVE ZONE TRACTION CURVES

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ABSTRACT
Difficulties in the assessment of extremely tough materials have recently led to the use of cohesive zone modelling techniques in fracture mechanics which incorporate a local fracture criterion at the notch tip. The model describes the fracture process through a law which relates the separation of the two surfaces within the damage zone to the corresponding holding tractions. A successful method utilising deep notched tensile specimens has been described previously as a means of measuring 'traction – separation' properties experimentally in tough polyethylenes.

Here a predictive fracture model is described using a Finite Volume formulation. A three point bend geometry is modelled under a loading rate of 0.1 mm/min with an experimentally measured single rate traction-separation curve used as the fracture criterion for all computational cells along the crack plane. Load – time and crack growth predictions for two tough grades of polyethylene, PE80 and PE100, are shown to be in reasonable agreement with experimental results for three point bend specimens at the same loading rate. The study highlights some of the difficulties in applying a single rate traction curve to a situation in which the rate of cell opening changes continuously with time for any given cell and is different for all cells along the crack plane. The effect of variations in the cohesive zone parameters on the load – time results for PE80 is also discussed. This limited parametric study highlights the importance of having knowledge of the complete shape of the traction curve in the prediction of failure.

1. INTRODUCTION
Problems associated with the characterisation of very tough materials have increasingly led to the development of computational methods and analytical techniques in which a local 'traction – separation' type fracture criterion, distinct from the properties of the bulk material, is used to describe the material behaviour within the crack tip damage zone. To maintain the validity of the model it is important that the traction – separation relationship chosen to represent the cohesive zone is either linked closely to experimental measurements or has a firm theoretical basis. Hutchinson (5) has provided a useful discussion on the linking of the macroscopic scale to the microscopic, discussing the embedded process zone in the context of a near tip fracture criterion. Broberg (2) has discussed the physical basis for the cell modelling of materials in general terms. The behaviour of a cell was described in terms of a phenomenological cohesion-decohesion property, which should contain within it sufficient information regarding the crack growth characteristic of the material. Problems in many cases do not derive from the computational method, but more from the inappropriate representation of the physical processes at the crack tip [Broberg (2)].

Hillerborg (4) has discussed the application of the fictitious crack model to a range of materials including fibre reinforced plastics and metals. Much of the contemporary interest in this approach now arises from the increasing need to have a local and all inclusive energy based fracture criterion to obviate the need for a stress intensity based approach. A number of recent predictive numerical models have been developed through the incorporation of traction-separation curves as a local fracture criterion within a continuum [Tvergaard and Hutchinson (10), Wei and Hutchinson (11), Xu and Needleman (12)]. Along with the use of finite element techniques, finite volume (FV) is also being used increasingly in the modelling of solid mechanics problems. Some of the advantages of using FV are conservativeness, stability, accuracy and low requirements of computer resources. Murphy and Ivankovic (7) have modelled the evolution of dynamic fracture in brittle PMMA using a FV formulation. Ivankovic (6) has presented a detailed description of the development of FV techniques for the assessment of dynamic fracture.

It is now well established that crazing is the precursor to slow crack growth in tough polyethylene [Bhattacharya and Brown (1), Friedich(3)] and that the nature and rapidity of craze breakdown governs the overall resistance to slow crack growth. Micromechanical modelling of crack growth in tough polyethylene is likely to be complicated by the number of possible processes such as voiding (both at inclusion sites and sites of free volume), fibrillation, fibril disentanglement and chain scission that may occur within the damage zone prior to crack growth. An experimental method to characterise the toughness of PE80 and PE100 using circumferentially deep notched tensile (CDNT) specimens has been described previously by Pandya and Williams (8). In this paper, simulations based on an elastic plastic FV formulation are presented using experimentally measured single rate cohesive traction curves as a local fracture criterion. An initial description of this method was given earlier by Pandya et. al. (9). The use of experimentally measured traction - separation curves retains the vital aspect of physical validation in the modelling of the material which may be lacking in other micromechanical models.

2. MODELLING APPROACH

The CDNT experimental procedure, test specimen and a typical experimental result are illustrated in figure 1. The load was measured by a standard 10 kN load cell and the extension of the damage zone was measured by an extensometer mounted on the specimen as shown. The gauge length of the extensometer was 25 mm and the range was 2.5 mm. In order to minimise the effects of misalignment the load train incorporated universal joints at both ends. A standard result from the test was a traction – separation curve. Measurements over a range of speeds have shown the traction–separation curves to be considerably rate dependent [Pandya and Williams (8)].

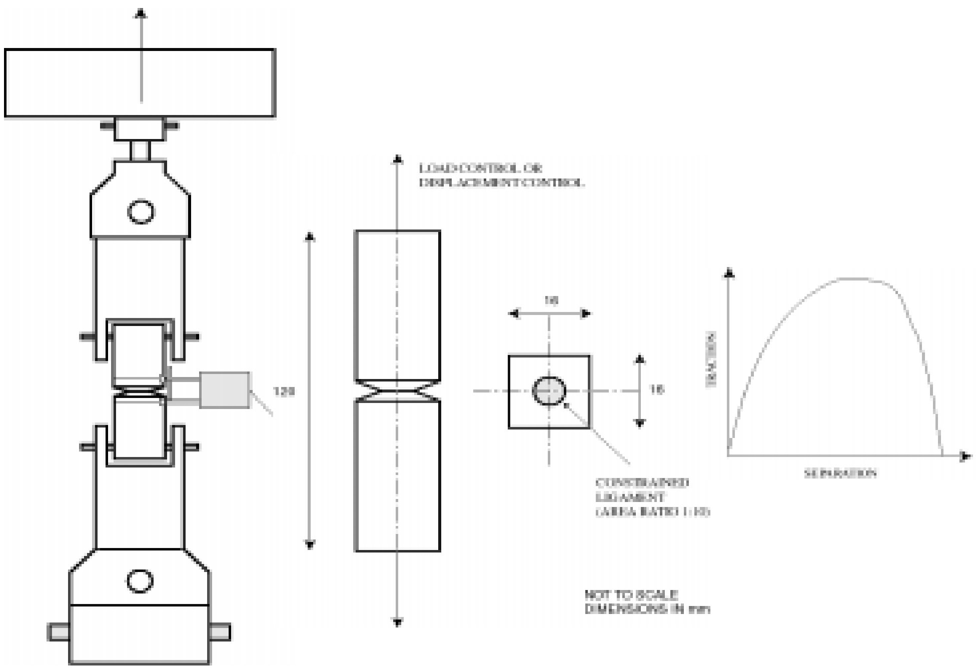

Figure 1: Experimental Procedure for the Measurement of Traction - Separation Properties of Tough Polyethylene

Results are presented for two polyethylene copolymers, PE80 and PE100, the densities for which were respectively 940 kgm^{-3} and 947 kgm^{-3} and each had a Poisson's ratio of 0.3. A schematic illustration of the approach to cohesive zone modelling using a TPB geometry is given in figure 2.

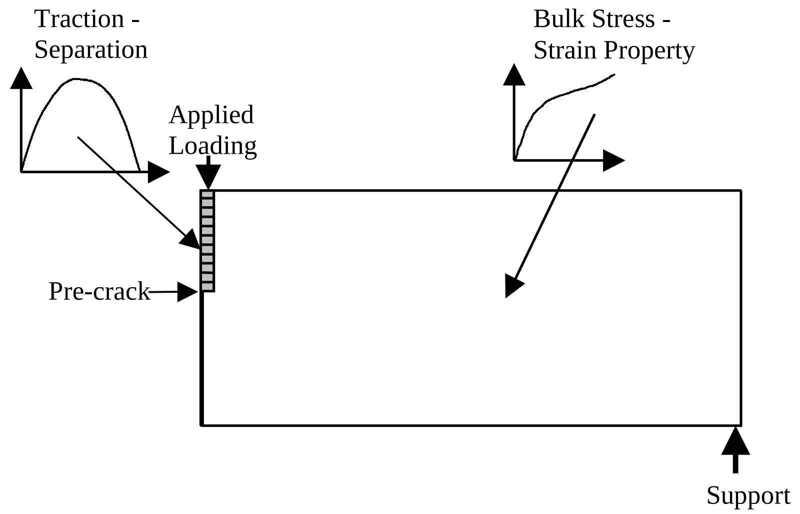

Figure 2: Schematic Illustration of the Cohesive Zone Method in a TPB Geometry

In order to verify numerical predictions of fracture, tests were performed on a TPB specimen at a loading rate of 0.1 mm/min. At this loading rate from a simple rotational analysis the initial notch tip cell opening displacement rate was estimated as 0.006 mm/min. As a first estimate of the fracture criterion, a traction - separation curve measured experimentally at 0.006 mm/min rate was prescribed for all cells along the uncracked ligament while the initial precrack was modelled as a traction free surface, as shown in figure 2. The specimen dimensions were span = 100 mm, width = 25 mm, thickness = 15 mm and the notch to width ratio = 0.55. Making use of geometrical symmetry only half the specimen needed to be modelled. A true stress - strain curve measured experimentally using standard dog bone specimens was specified as the material property.

3. NUMERICAL RESULTS AND DISCUSSION

Figure 3a shows a traction - separation curve for PE80 measured at 0.006 mm/min along with two theoretical curves labelled curve 1 and curve 2 with lower cohesive strengths but the same break separation as the experimentally measured curve. The cohesive strength for curve 1 and curve 2 corresponds to experimental tests run on specimens at displacement rates of 0.004 mm/min and 0.0006 mm/min respectively. The experimentally measured load - time trace for a TPB specimen tested at 0.1 mm/min along with the numerical predictions for each traction curve from figure 3a are shown in figure 3b.

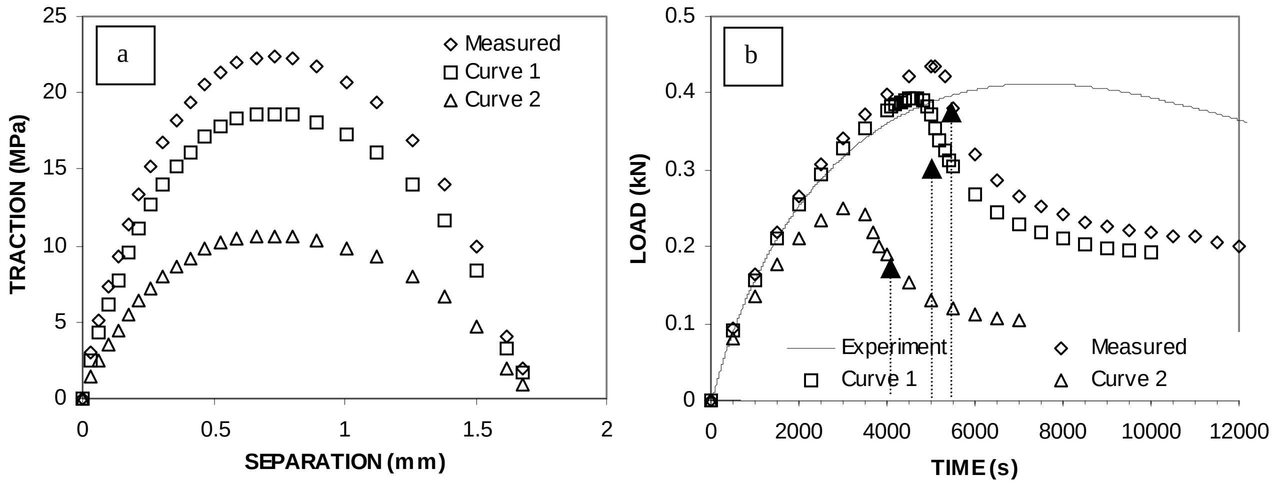

Figure 3: Prediction of Crack Growth in PE80 using Measured and Theoretical Traction - Separation Curves

In figure 3, using curve 1 good agreement is achieved up to the peak load between the experiment and predicted load - time trace. However the numerical prediction using the traction curve measured at 0.006 mm/min was found to over predict the peak load. The predicted initial fall in load is due to cells entering the decohesive state prior to the onset of crack growth. Crack growth is taken to have occurred once the opening of the notch tip cell pair reaches the value of the break separation, the position of which is indicated in each case by the arrows. For each traction curve the numerical model over predicts the fall in load after the peak. The possible reasons for this are discussed shortly by examining the manner in which the rate of cell opening varied for cells along the crack plane during the simulation. First results are shown for PE100. In figure 4a a traction curve measured experimentally at rates of 0.006 mm/min and 0.0003 mm/min are presented. Figure 4b shows the numerical prediction for PE100 using the curve measured at 0.0003 mm/min as the local fracture criterion.

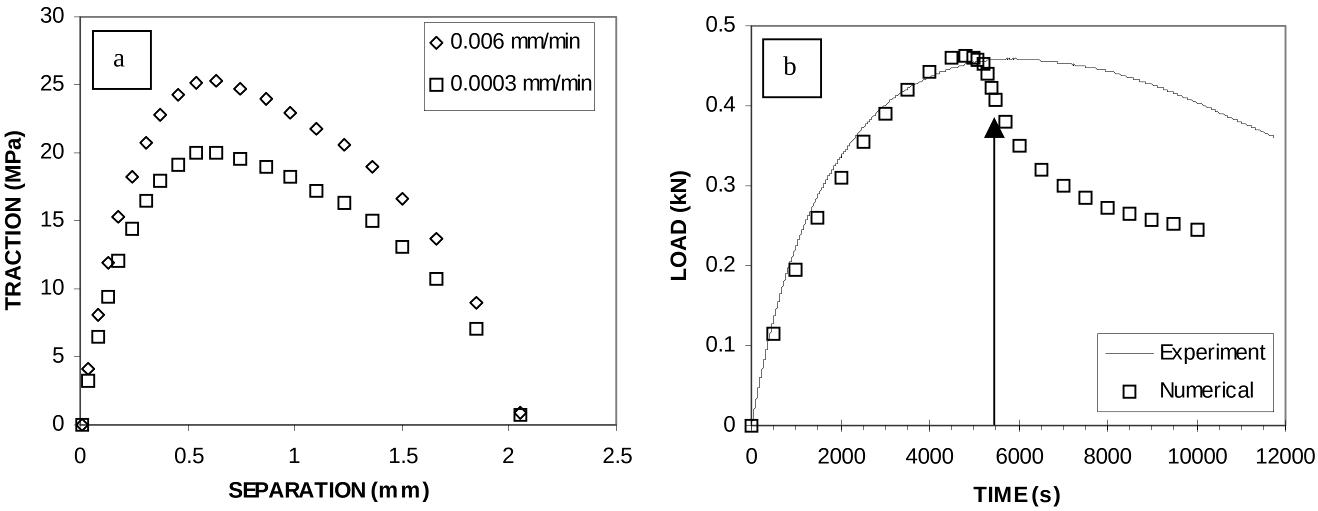

Figure 4: Prediction of Crack Growth in PE100

As with PE80 it was necessary in the modelling of PE100 to use a traction curve measured at a lower speed than that suggested by the rate calculation in order to correctly predict the peak load. It is important here to note the limitations in the current procedure. A single fixed traction curve was applied to all cells along the uncracked ligament. Clearly in reality the notch tip cell opens at the fastest rate while subsequent cells open at progressively lower rates up to the stationary cell at the neutral axis at which point the tensile zone ends. A single traction curve thus represents an average property for all cells across the uncracked ligament. Given that the shape of the traction curve is known to be rate dependent, choosing to use a single curve presupposes that differences in the rate of cell opening can be assumed to have a negligible effect on the cohesive zone parameters of the traction curve. As this is unlikely to be the case in reality, the question remaining to be answered is the extent to which changes in cohesive zone parameters affect the load predictions. This will be shown shortly in a parametric study on the traction – separation properties for PE80. Also with reference to the test method illustrated in figure 1 the quoted measured rate of opening is clearly the applied rate as opposed to the actual notch opening. In reality, for any given cell pair, the opening rate would not be a constant but would be expected to increase with time until final separation.

Figure 5a shows the variation of cell opening at 0.5 mm intervals along the ligament for PE80 using curve 1 in figure 3a as the traction curve for all cells. Crack growth occurs at a cell opening of 0.87 mm which corresponds to a total separation of 1.74 mm. It is clear that the displacement rate for any given cell pair is not constant but changes with time. There is also a change in gradient when crack growth occurs in the notch tip cell, at around 5000s, which affects the displacement rate of not only the notch tip cell but all cells along the ligament. Also from figure 5a there is a significant difference between the rate of opening at the notch tip and cells further away from the notch tip along the ligament. Figure 5b compares the initial gradients for the curves shown in figure 5a.

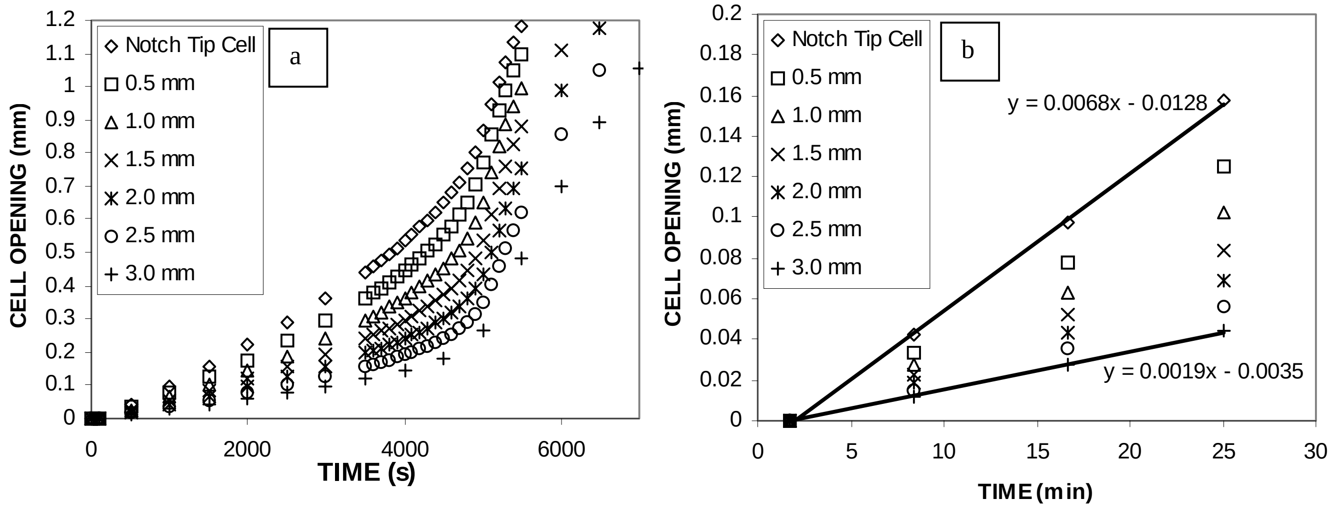

Figure 5: Variation in Cell Opening as a Function of Time for PE80

The initial gradients in figure 5b are given by linear curve fits for the notch tip cell and for a cell at 3.0 mm from the notch tip. The opening rate of the notch tip cell is in good agreement with the displacement rate of 0.006 mm/min for which the traction - separation curve was originally chosen. However subsequent cells all opened at lower rates and it was therefore not strictly correct to apply a single rate traction curve to these cells. Investigation of the numerical results showed that as the solution proceeded in time the notch tip cell was the first cell to reach the decohesive state. Examination of the state of cells adjacent to the notch tip cell along the interface showed that a large number of cells were close to the decohesive state. It is likely that the greater than expected increase in compliance, as indicated by the greater fall in the numerically predicted load compared to the experiment, occurred not only because many cells reached the decohesive state in succeeding time steps, but because the decohesive branch of the traction curve applied to these cells was too steep. Figure 6 shows the cell opening rate calculated from the cell displacement profiles of figure 5, crack growth occurring at 5000s.

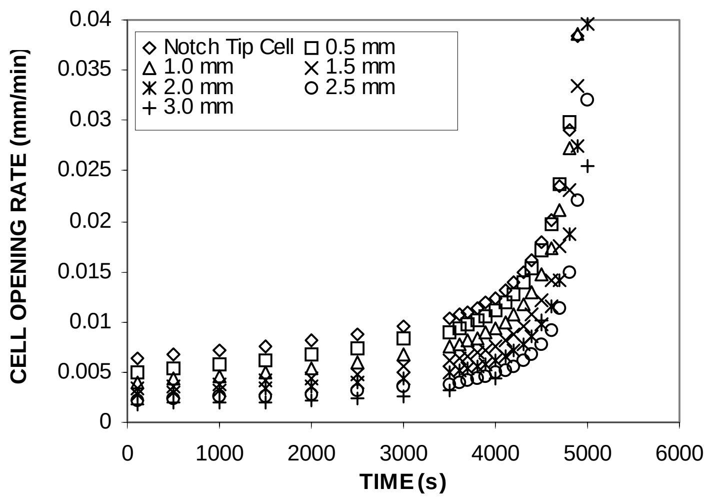

Figure 6: Variation in Cell Opening Rate for a PE80

From figure 6 there is clear evidence of the inappropriateness of using a fixed single rate traction curve for the modelling of a physical situation in which rates of cell opening are changing so significantly. Notwithstanding the comments of the preceding paragraph the comparisons of experimental and numerical results shown earlier for each grade do represent a good indication of how a cohesive zone modelling technique may be used to make crack growth predictions in tough materials. A limited parametric study is now presented on the effects of changing the cohesive zone parameters on the load – time predictions for PE80.

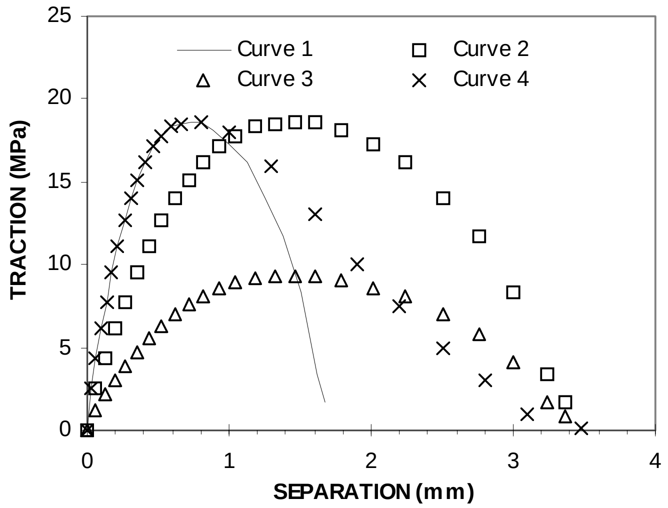

Figure 7: Traction - Separation Curves with Different Cohesive Zone Parameters used to Model Crack Growth in PE80

In figure 7 the original traction curve 1 from figure 3a is shown along with three theoretical curves. In curve 2 the cohesive strength is kept the same and the break separation is doubled thus doubling the area under the curve. In curve 3 the cohesive strength is halved and the break separation doubled leaving the area under the curve the same. In curve 4 the cohesive part of the traction curve was kept the same as in curve 1 and only the displacement values beyond the cohesive strength were doubled. The numerical predictions for the tractions curves of figure 7 are shown in figure 8.

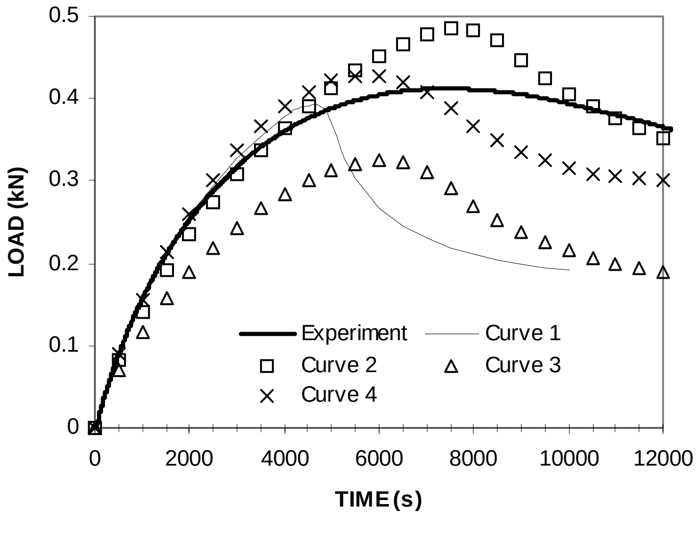

Figure 8: Numerical Load – Time Predictions in PE80 for Different Cohesive Zone Parameters

A number of observations can be made regarding the load - time traces. Firstly the predicted peak load for curve 2 is higher than that predicted by any other curve and also the peak occurs at a longer time. The value of the predicted peak load and the time at which it occurs is thus seen to be dependent not only on the value of the cohesive strength (which are equal in curves 1 and 2) but also on the path taken by the traction curve in getting to that stress. Clearly a longer time is taken and more energy is dissipated when curve 2 is used as the local fracture criterion rather than curve 1. The nature of unloading prior to crack growth is seen to be dependent on the value of the break separation. A steep decohesive branch of the traction curve leads to the prediction of a sharp drop in load after the peak prior to crack growth. However, when the value of break separation is doubled for the same cohesive strength (as in curve 2), the reduction in load is less sudden due to the more gradual decohesion path prior to cell separation. The slope of the unloading portion of the load -

time trace is thus dependent on the degree of steepness of the decohesive branch of the traction - separation curve. As expected, when traction curve 3 is used both the peak load and the rate of unloading are lower than that for either curve 1 or curve 2. One can thus look at the results in two parts: (1) the cohesive branch of the traction curve and the associated load rising portion of the predicted load - time trace and (2) the decohesive branch of the traction curve and the associated unloading portion of the predicted load - time trace. The numerical prediction for curve 4 shows good agreement with the experimental curve up to the peak load and there is also much closer agreement with the unloading portion of the curve than obtained through the use of any of the other curves. It must be noted again that the traction curve has been applied to all cells along the interface and thus models a situation in which the cohesive parameters for leading cells do not change with time as softening and/or crack growth occurs. The good agreement between the experimental and numerical result for curve 4 may therefore be because this traction curve represents a good approximation to the curve that would have been obtained had it been possible to average the traction - separation curves between the high rate notch tip cell and cells further along the uncracked ligament. The above parametric study shows conclusively that the numerical predictions are dependent not only on the area under the traction – separation curve but on the actual cohesive zone parameters. Both the values of the cohesive zone parameters and the entire path of the traction – separation curve are required for a proper fracture assessment. The distinction between the numerical predictions for curves 1 and 3 in figures 7 and 8 is evidence of this.

A possible extension to the model would be to build up a database through experimental measurements of traction - separation curves measured at a number of displacement rates and temperatures, although for the rates considered here temperature effects are considered insignificant. With a database in place, as the simulation proceeded there could then be a process of switching between curves depending on the current state at any given time i.e. for any cell, for a given separation and rate a corresponding traction would be found from the family of curves. A degree of generality currently not present in the simulation could then be introduced. Figure 9 illustrates this.

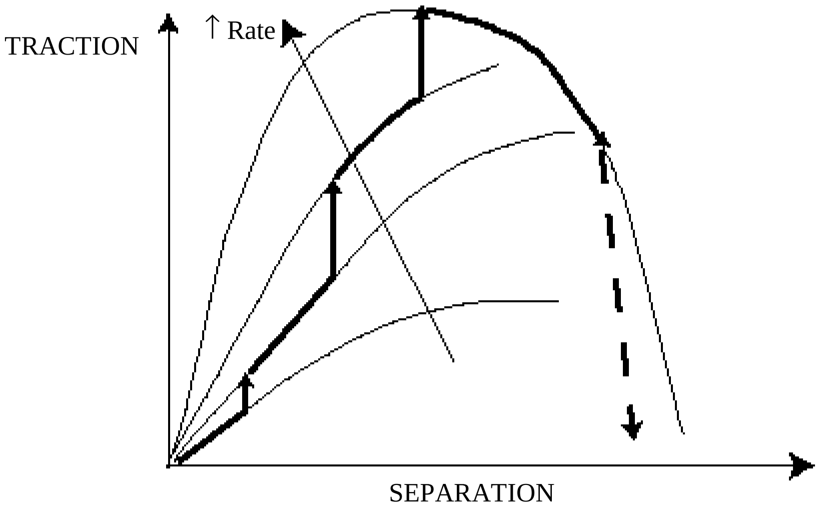

Figure 9: Schematic Representation of Possible Switching Between Traction Curves during Numerical Simulation

4. CONCLUSIONS

A single rate traction curve was found to be an unsuitable representation of physical reality at the notch tip. A single traction curve represents an average property and is unable to take into account the significant rate effects present at the notch tip. Within the limitations of using a single rate curve it was possible to make some preliminary assessments of crack growth predictions in PE80 and PE100. In future a generalised fracture assessment may be achieved by incorporating a family of rate dependent traction curves into the model and switching between them during the simulation. Alternatively a fully integrated mathematical material model could be developed which would cater for any possible changes in rate or temperature as the simulation proceeded. Parametric studies revealed the dependence of load and crack growth predictions on the choice of cohesive zone parameters. The results showed that no single fracture parameter can adequately characterise fracture, and that the entire curve is required for the prediction of failure in tough polyethylenes.

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