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DETERMINATION OF NOTCH SENSITIVITY CURVES FOR QUASI-BRITTLE MATERIALS USING THE DISCRETE ELEMENT METHOD

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Abstract. The application of polymeric materials is well established in engineering across various fields. Many of these materials exhibit behavior classified as quasi-brittle. The determination of notch sensitivity curves is essential to ensure safety in the design of projects based on such materials. In this study, the Discrete Element Method (DEM) is employed to analyze Expanded Polystyrene (EPS), enabling the representation of both global behavior and the fracture of the material. The model was calibrated using experimental curves obtained from tensile tests. The influence of increasing internal defects on the behavior of EPS under the effect of stress raisers is also investigated. The results indicate that DEM adequately represents the behavior of quasi-brittle materials. Furthermore, the simulations showed that EPS exhibits a predominantly notch-insensitive behavior.

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1 INTRODUCTION

The study of quasi-brittle materials, such as polymers and concrete, has become essential due to their wide range of applications and high susceptibility to abrupt failure. In this context, fracture mechanics plays a fundamental role by analyzing crack propagation and the effect of stress concentrators, factors that decisively determine the structural lifespan of these materials. Among the numerical methods employed for simulation, the Discrete Element Method (DEM) stands out as it enables the inclusion of defects, imperfections, and intrinsic heterogeneities, ensuring a more realistic computational representation of material behavior.

Notch sensitivity curves are essential tools for understanding how materials respond to different notch geometries and stress concentrators. Although well documented for metallic materials, their availability is still limited for quasi-brittle materials, which motivates the present study. DEM allows modeling various notch geometries — including U-shaped, V-shaped, and circular configurations — and analyzing the stress–strain relationship up to failure, making it possible to obtain accurate sensitivity curves.

The overall objective of this work is to perform tensile tests using DEM to validate a methodology for obtaining notch sensitivity curves in quasi-brittle materials. Specifically, the study aims to calibrate the model using experimental tensile data, determine the sensitivity curves, and evaluate the embrittlement effect of EPS along the D/W ratio, thus contributing to a better understanding of the behavior of these materials under different loading conditions.

2 MATERIALS AND METHODS

2.1 Notch sensitivity

As Norton (2013) points out, a notch is defined as any discontinuity that interrupts the flow of forces along a component. Notches can take many forms, such as changes in diameters and grooves. In the literature, it is possible to find parameters that relate the type of notch and dimensions of stress concentration. The factor K_t is widely used and provides charts for steels, for example. The definition of K_t is given by Equation (1), which relates the stress in the notch region to the stress applied to the structure:

$$K_t = \frac{\sigma_{max}}{\sigma_a} \tag{1}$$

Where σ_{max} is the maximum stress at the notch, and σ_a is the stress applied on the specimen. For the specific case of a central circular notch under tensile stress in the specimen, it is possible to analyze the material behavior as a function of the hole diameter.

The analysis is carried out by dividing the fracture stress of the specimens with a central notch, σ_N, by the fracture stress of the specimen without a notch, σ_u. Equations (2) and (3) present the stresses σ_N and σ_u, respectively:

$$\sigma_u = \frac{F}{Wt} \tag{2}$$

$$\sigma_N = \frac{F}{(W-D)t} \tag{3}$$

Where F represents the applied force on the specimen at the moment of fracture; W, the specimen width; t, the specimen thickness; and D, the central hole diameter.

Notch behavior depends on the type of material and can be classified into three groups: ductile, brittle, and quasi-brittle. In the present study, the specific case of a central circular hole under tensile loading is considered, as illustrated in Figure (1).

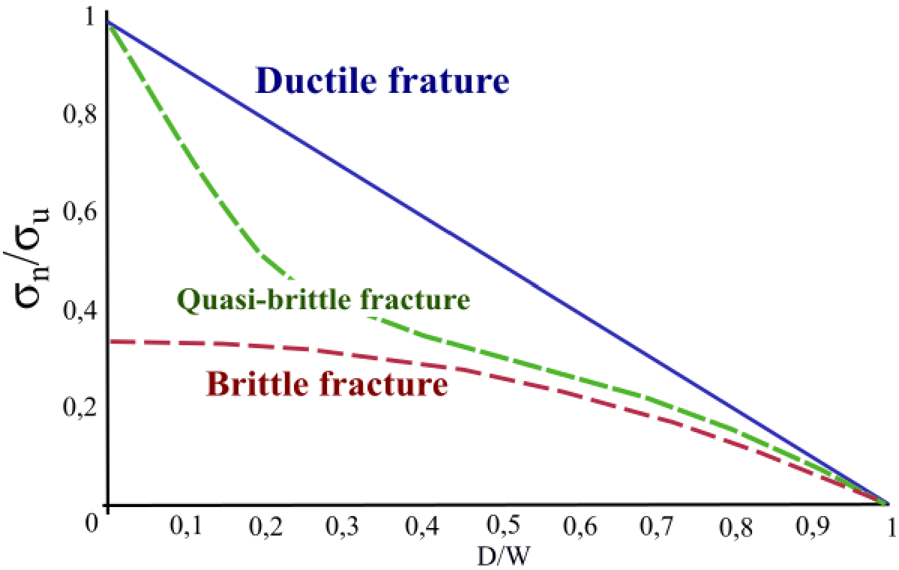


Figure 1: Notch behavior depends on the type of material.

2.2 Discrete Element Method - DEM

The discretization of the materials in the specimens, in DEM, is carried out through points interconnected by bar elements. The points represent mass, while the bars connecting them represent the stiffness of the continuous body Soares and Iturrioz (2016). The basic module consists of 20 bars and 9 nodes, using a Cartesian coordinate system to define the three degrees of freedom of displacements.

The arrangement pattern of the nodes and bars is analogous to the model of a body-centered cubic (BCC) unit cell of length L_{CO}, as illustrated in Figure (2a). The three degrees of freedom associated with each nodal mass are shown in Figure (2b). Considering the nodal masses, the material damping, the three degrees of freedom, and the equilibrium condition between the internal and external forces of each nodal mass, the resultant force at the points and their displacements, within a given time interval, can be determined by Equation (4):

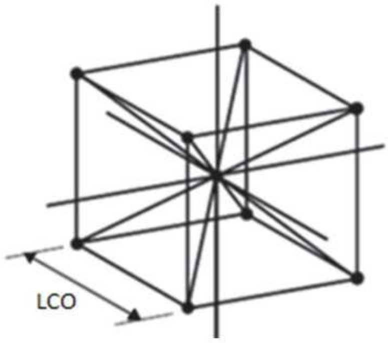
$$M\ddot{x} + C\dot{x} + F(t) - P(t) = 0 \tag{4}$$

Where, M is nodal mass matrix, C is damping matrix, $\ddot{x}$ is nodal acceleration vector, $\dot{x}$ is nodal velocity vector, $F(t)$ is internal nodal force vector and $P(t)$ is external nodal force vector.

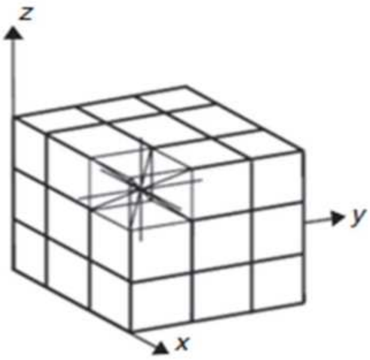
The system can be integrated in the time domain, provided that the condition of the maximum time increment Δt for linear elastic materials is satisfied, so that the integration remains continuous according to Equation (5):

$$\Delta t \leq \frac{0,6LCO}{\sqrt{E/\rho}} \tag{5}$$

Where, ρ is material density and E is elastic modulus.



(a)



(b)

Figure 2: (a) Cubic module of DEM and (b) continuum formed cubic modules.

Proposed by Riera and Rocha (1991), the bilinear constitutive law, or $Hillerborg$ model, allows relating and quantifying the effects of quasi-brittle fracture. The law can be illustrated in Figure (3).

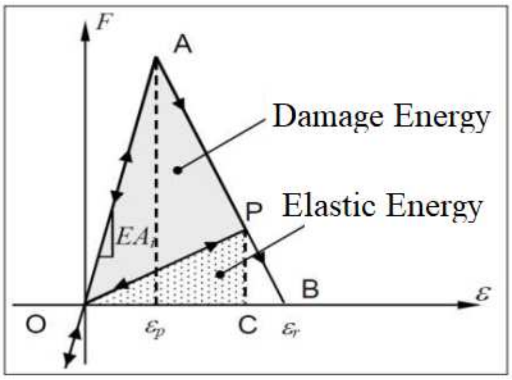


Figure 3: Bilinear constitutive law

Where, F is axial force in the cubic element, ε is strain function in the element, ε_r is fracture strain, ε_p is critical limit strain, E is elastic modulus of the material and A is cross-sectional area of the element.

From the law, it follows that the area under curve OAB represents the minimum energy density required to fracture the bar. The area of triangle OPC represents the energy density stored in the element. Finally, the area of triangle OPA is the energy density dissipated in the fracture of the element. The law states that the energy density dissipated by damage is equal to the fracture energy density; therefore, when the element fails, it will unload this portion linearly $(lineAB)$ until reaching the origin, losing the load capacity.

Thus, when the element reaches the critical limit strain before damage (ε_p), the relationship between the specific fracture energy (G_f) and the elastic modulus of the material can be established by Equation (6), which is modeled based on Linear Elastic Fracture Mechanics. This equation incorporates the material failure factor (R_f), which represents the intrinsic defects and discontinuities of the material.

$$\varepsilon_P = R_f \sqrt{\frac{G_f}{E}} \tag{6}$$

2.3 Expanded Polystyrene

The quasi-brittle material used in this work is the expanded polystyrene (EPS) polymer, a material with several applications, including thermal roof tiles for building insulation, as well as blocks and panels for use in civil construction structures.

The EPS used in this study is characterized by lower density and is also known in the market as 1F. The properties used in the computational model, such as elastic modulus, density, and Poisson's ratio, are presented in Table (1). Some of these properties serve as a basis for the numerical models tested by Cunha 2021.

E[MPa]	ρ[kg/m^3]	ν	G_f[N/m]	CV_{Gfr} [%]
4,88	11,9	0,25	133,4	170

Table 1: EPS material properties

2.4 DEM Model Calibration

To validate the notch sensitivity curve analysis for EPS, the DEM model was calibrated using the experimental tensile test curves obtained in previous works by Cunha (2021) and Colpo (2016). The specimens used for the tests, which were also modeled in DEM, follow the standard defined in ASTM-D638-14 (2014), which regulates tensile test procedures for polymeric specimens. The dimensions of the tested model are shown in Figure (4) and Table (2).

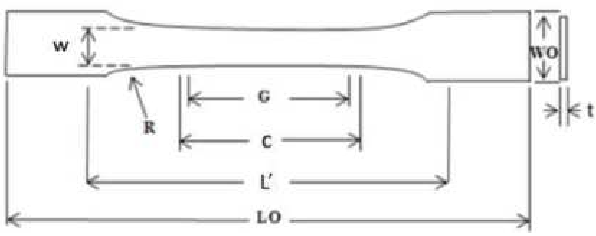


Figure 4: Dimensions specimen used in the tensile test as ASTM-D638-14 (2014).

Dimensions [mm]						
G	L'	c	LO	w	WO	R
50	57	115	246	19	29	76

Table 2: Dimensions of the specimem with measurements in millimeters.

2.5 Notch Sensitivity Analysis

To obtain the sensitivity curve of EPS, rectangular specimens without a hole and with a central hole of diameter D were used. The specimen has dimensions L and W, of $200mm$ and

$50mm$, respectively, as shown in Figure (5). The values of hole diameter D and the ratio D/W are shown in Table (3).

D[mm]	5	10	15	20	25	30
D/W	0,1	0,2	0.3	0.4	0.5	0.6

Table 3: Diameters and D/W ratios analyzed in notch sensitivity for EPS.

The data extracted from the tests were strains and forces, F_u for the specimen without a hole and F_N for the specimen with a hole. Figure (5) shows the specimens without a hole and with holes of $10,$mm, $20,$mm, and $30,$mm diameters generated in the DEM model after fracture. Using the average rupture loads of the specimens without and with a hole, it is possible to plot the characteristic notch sensitivity curve of F_N/F_u as a function of D/W.

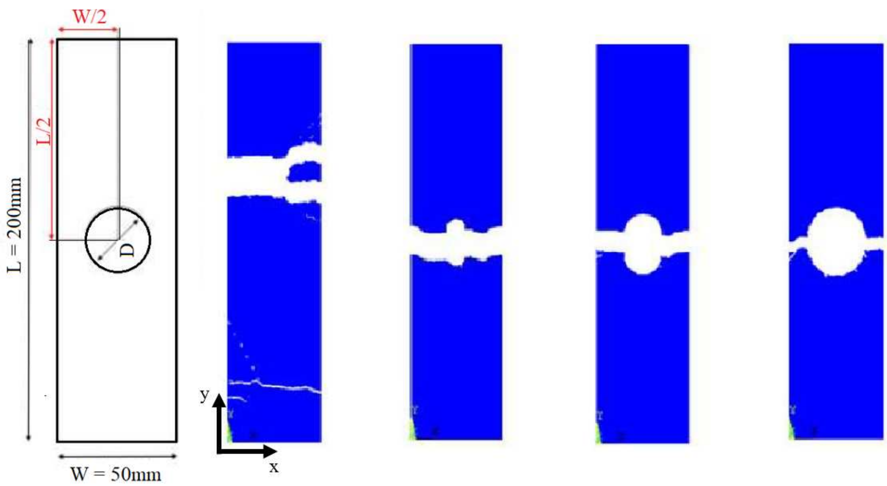


Figure 5: Notch sensitivity fracture

2.6 Brittleness

Brittleness is a common process that can occur in any type of material and is caused by different factors. To analyze the material behavior and the notch sensitivity under the effect of brittleness, the EPS had its failure factor values altered at two levels. The value of R_f (failure factor), represents the intrinsic defects and discontinuities of the material and is present in the application of bilinear constitutive law Riera and Rocha (1991), was increased relative to its original value, as shown in Table (4). By increasing the value of R_f, the DEM model incorporates a greater number of defects, generating material brittleness.

R_f	$[\mathrm{m}^{-1/2}]$
Original	4.3
Brittleness	10
Brittleness	35.8

Table 4: R_f Values

3 RESULTS AND DISCUSSION

This section presents the calibration results for EPS. Next, the material's sensitivity curves as shown as and evaluated.

3.1 Model Calibration

Figure (6) presents the experimental curves (in black) in terms of the normal stress–strain relationship, used for calibration of the numerical model (in red). The experimental curves showed variability in rupture load from $0,78$ N up to $1,08$ N, while strain ranged from $0,024$ mm/mm up to $0,034$ mm/mm, as presented in Table (5). The same figure also shows an example of a fractured specimen in the simulation. Table (6) presents the results obtained in the numerical model developed in DEM. The difference between the mean results was below 10%, for both force and strain.

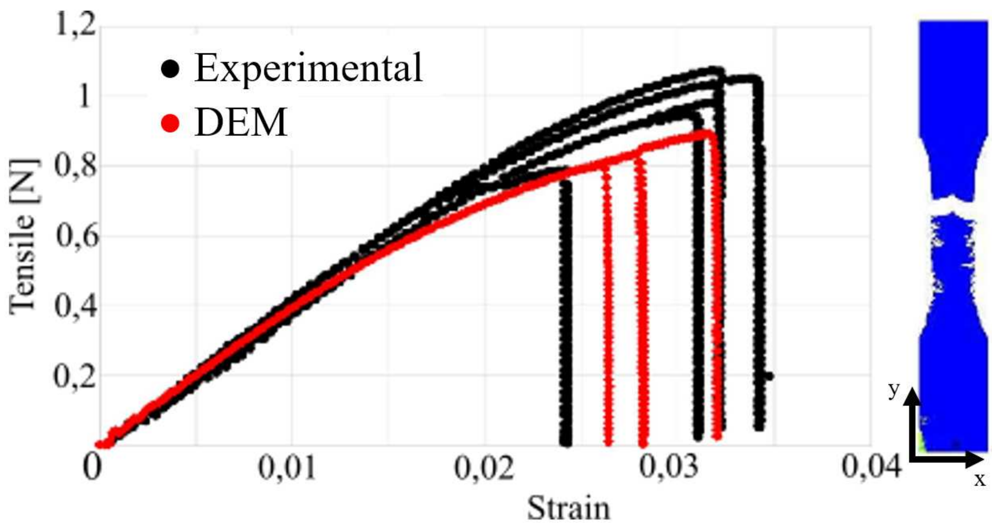


Figure 6: Model calibration results

Curves	1	2	3	4	5	Mean
Tensile [N]	0,78	0,95	0,98	1,08	1,05	0,97
Strain [mm/mm]	0,024	0,031	0,032	0,032	0,034	0,030

Table 5: Experimental values

Simulation	1	2	3	4	5	Mean
Tensile [N]	0,80	0,82	0,83	0,83	0,89	0,83
Strain [mm/mm]	0,026	0,028	0,028	0,028	0,032	0,028

Table 6: Numerical results

3.2 Notch Sensitivity Analysis

To obtain the sensitivity curve of EPS, rectangular specimens without a hole and with a central hole of diameter D were used. The specimen has dimensions L and W, of $200mm$ and $50mm$, respectively, as shown as in Figure (5). The values of hole diameter D and the ratio D/W are shown in Table (3).

Notch [mm]	D/W	Load[N]
No notch	0	5,34
5	0,1	4,46
10	0,2	4,07
15	0,3	3,59
20	0,4	3,14
25	0,5	2,65
30	0,6	2,14

Table 7: Mean value force for EPS

The notch sensitivity curve of EPS is presented in Figure (7) by the red triangular markers. On the horizontal axis, the ratio between the hole diameter D and the specimen width W is shown. On the vertical axis, the ratio between the fracture load with a central hole and without a hole is presented. The limits for ductile materials (in black) and brittle materials (in orange) are also shown in the figure.

It can be observed that EPS is not a notch-sensitive material, although it shows a tendency toward brittleness when D/W is less than $0,2$. Figure (7) also shows specimen models tested with DEM with hole diameters of $10mm$, $20mm$ and $30mm$.

3.3 Brittleness

Upon increasing the value of Rf and consequently adding higher levels of defects and discontinuities to the material, the same previous tests were conducted to obtain a notch sensitivity curve. It's noteworthy that the same random field seeds were used for all the tests. Tables (8) and (9) present the average values of the simulations for the two Rf values tested in the DEM.

The notch sensitivity curves for the two brittleness scenarios can be observed in Figure (8). The curve with a solid line and circular markers represents the material's behavior in a situation with a failure factor equal to $10m^{-1/2}$, while the dashed curve with "X" markers corresponds to an R_f value of $35.8m^{-1/2}$.

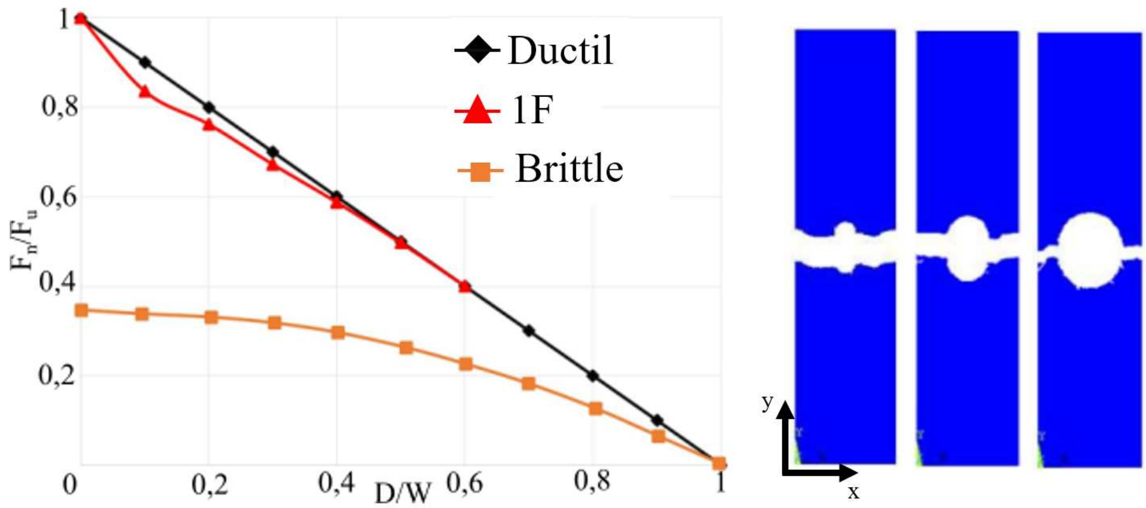


Figure 7: Notch sensitivity curve

Notch [mm]	D/W	Tensile [N]
No notch	0	10,78
5	0,1	6,86
10	0,2	6,44
15	0,3	5,89
20	0,4	5,24
25	0,5	4,56
30	0,6	3,84

Table 8: Mean value for $R_f = 10,0$

Notch [mm]	D/W	Tensile [N]
No notch	0	23,08
5	0,1	13,45
10	0,2	12,34
15	0,3	10,79
20	0,4	9,75
25	0,5	7,84
30	0,6	7,15

Table 9: Mean value for $R_f = 35,8$.

A critical region of notch sensitivity can be observed, located among $D/W = 0$ and $D/W = 0,1$, which shows the most significant increase related to the material's brittleness.

In this area the rate at which the material's strength decreases can be approximated by the slope line, which indicates that within this D/W range, each $1mm$ increase in the notch results in an 8% decrease in the material's strength.

In comparison, for the region from $D/W = 0,2$ up to $D/W = 0,3$ on the R_f $35.8m^{-1/2}$ curve, the slope line indicates that the material's strength decreases by $1,4\%$ with each $1mm$ increase in the hole.

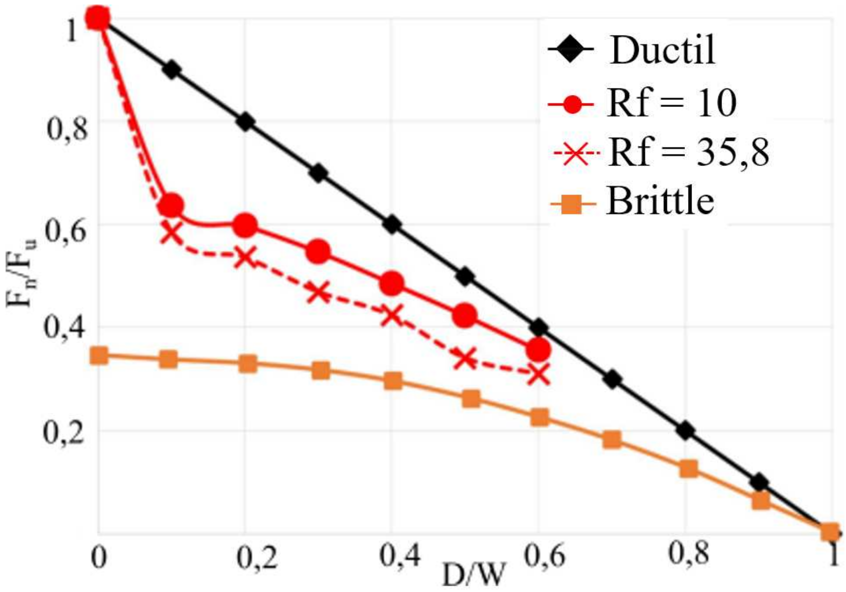


Figure 8: Notch sensitivity curve

4 CONCLUSIONS

This work verified the use of DEM to obtain the notch sensitivity curve for polymeric materials with quasi-brittle behavior, in this case EPS. Based on results found in the literature, it was possible to calibrate the model and then estimate the notch sensitivity response. From the results, the following conclusions can be drawn:

- The DEM model was able to capture with good accuracy the global behavior and fracture of EPS, proving to be an excellent tool to be further explored;
- EPS exhibited behavior practically insensitive to notches across the entire range of D/W;
- Material embrittlement, i.e., the increase of internal defects, changes the material behavior and generates a critical notch sensitivity zone in the range between 0 and $0,1\ D/W$.

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