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Numerical and experimental results on Charpy tests for blends polypropylene + polyamide+ ethylene propylene diene monomer (PP+PA+EDPM)

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Abstract: This paper presents results from numerical and experimental investigation on Charpy tests in order to point out failure mechanisms and to evaluate new polymeric blends PP+PA6+EPDM. Charpy tests were done for initial velocity of the impactor of 0.96 m/s and its mass of 3.219 kg and these data were also introduced in the finite element model.

The proposed model take into account the system of four balls, including support and the ring of fixing the three balls and it has a finer discretization of the impact area to highlight the mechanisms of failure and their development in time. The constitutive models for four materials (polypropylene with 1% Kritilen, two blends PP+PA6+EPDM and a blend PA6+EPDM) were derived from tensile tests. Running simulations for each constitutive model of material makes possible to differentiate the destruction mechanisms according to the material introduced in the simulation, including the initiation and the development of the crack(s), based on equivalent plastic strain at break (EPS) for each material. The validation of the model and the simulation results was done qualitatively, analysing the shape of broken surfaces and comparing them to SEM images and quantitatively by comparing the impact duration, energy absorbed by the sample, the value of maximum force during impact. The duration of the destruction of the specimen is longer than the actual one, explainable by the fact that the material model does not take into account the influence of the material deformation speed in Charpy test, the model being designed with the help of tests done at 0.016 m/s (1000 mm/min) (maximum strain rate for the tensile tests). Experimental results are encouraging for recommending the blends 20% PP+42% PA6+28% EPDM and 60% PA6+ 40%EPDM as materials for impact protection at low velocity (1m/s).

Simulation results are closer to the experimental ones for the more brittle tested materials (with less content of PA6 and EPDM) and more distanced for the more ductile materials (with higher content of PA6 and EPDM).

Keywords: Charpy test, PA6, PP, EPDM, simulation, FE analysis, constitutive model, tensile test

1. Introduction

Charpy tests have been characterized materials for impact resistance till the XIX century [1-5], but relevance had been initiated by Charpy [6] the test keeping his name till nowadays.

Reviewing the available literature on this type of tests [7-10] and on Charpy impact modeling [11-17] pointed out the following aspects:

- models are using very different mesh web rougher or finer (especially near the notch) [18-20], on a quarter or half of the sample, from 2D to 3D [21], but new achievement in hardwares and dedicated softwares allows for using finer mesh, all the sample, investigation on strain and stress, simulation in actual time etc.,
- first models did not take into account friction, but recent ones have included condition for friction, usually with a constant friction coefficient,
- at the beginning, constitutive models were simpler, implying only a failure criterion, usually the strength limit in tensile and there has been interest in performant materials like steel, titanium and aluminum alloys [22], [23]; for polymers and especially for blends fewer research reports being [24-27].
- each model has simplifying hypotheses that could alter the sample behavior as compared to the actual one.

Many engineers were interested in Charpy test for metallic materials [11], [28-30], but nowadays this test, in classical or modified configuration, becomes useful to be done for other materials, including polymers, composites [31] and ceramics [32]. Simulation of such a test is useful for understanding the material behavior under impact load, and when knowing mechanical characteristics at impact, to assess the first step in designing structures with tested materials under such conditions.

Tanguy [11] proposed a simulation with a detailed description of the material viscoplastic behavior over a wide temperature range. The Charpy test is simulated using a full 3D mesh and accounting for adiabatic heating and contact between the specimen, the striker and the anvil. This research team stipulated that 2D plane strain simulations instead of 3D ones offer a significant reduction of running time, but an overestimation of load and, consequently, the crack advance. The model is well suited to represent ductile tearing. Among material factors affecting the material model to be introduced for simulating Charpy test are: the simplifying concept for the model (2D or 3D, recent works being in the favor of the last, including the simulation here presented), accepting quarter or half of the actual test system (imposing symmetrical planes that are not supported by the results of this work), conditions for constraints among parts of the systems (no contact with anvils can be done by imposing a fixed displacement on the opposite side of the notch and a zero displacement on the initial contact line between the anvil and the specimen, but this approach develops higher stresses in the notch, causing earlier ductile crack start), adiabatic heating and heat diffusion, the viscoplastic behavior of the material (at higher impact velocities, ultimate strength is increased, which causes earlier failure).

Smith et al. [Smith, 2018] [33] did a FE analysis of Charpy specimen (both quasi-static and dynamic loading), using a symmetrical quarter model and an original mesh. The notch was modeled with a radius of 0.25 mm and internal angle of 45° and, at the tip of the notch, 30 concentric rings of elements were defined. The model was validated by comparing the load vs. clip gauge opening values from the simulation to experimental values. The plastic behaviour of this material was modeled using von Mises plasticity with isotropic hardening. The dynamic loading condition was achieved by altering the maximum applied ΔY value in conjunction with the simulating time to achieve an initial velocity of 5.23 m/s, as in actual test. The anvil and its contact with the specimen was modeled to incorporate its effect on global behavior of the system. Dynamic tensile properties were implemented using the curve fitting procedures. Separate power law curves were used to include dynamic flow properties over the strain rate range $10^{-5} < \dot{\epsilon} < 2000 \text{ s}^{-1}$. Heat generation due to plastic deformation was not taken into account as the temperature increase was found to be less than 20 °C, when cleavage was initiated.

Banerjee et al. [14] included a model of Charpy test for characterizing the behavior of an armor steel under high strains and strain rates, at elevated temperatures. In their work, model constants of Johnson-Cook constitutive relation [34], [35] and damage parameters have been determined experimentally from four types of uniaxial tensile test and they were used a modified constitutive model, introduced as user material sub-routine. There was used a half of the specimen and the impactor, for reducing the computing time. The impactor was modeled as elastic body and the specimen as being made of an elasto-plastic material. The nodes on the impactor were constrained to

move only in the vertical direction, impactor velocity being as the initial condition. Johnson–Cook failure criterion was applied only to a narrow region including the notch, along the specimen height. The constants of constitutive and failure model were deduced from tensile tests. This simulation used explicit time integration and was run for a total time of 2×10^{-3} s. The simulation results are validated by experimental ones. those being in reasonable agreement.

Recent tests provided complex data on the behavior of polymeric materials, with increasingly complex constitutive models, which take into account several factors (temperature, deformation rate, structure, stress).

The importance of modeling the behavior of the material, regardless of its nature, is emphasized by valuable works[23], [34-36]. Recent studies, experimental and obtained by simulation, have emphasized the importance of modeling the material at high deformation rate, [22], [37-40]. But most studies refer to metal alloys, used in aero, space and military applications. Equipment for testing materials at high deformation rates does not reproduce the conditions encountered in practice and the obtained results, although realistic, cannot be extrapolated to actual applications without accepting a higher degree of risk than in the case of low deformation rates. Hence, the usefulness of numerical simulations, along with experiments, because it presents an alternative for studying of damage processes.

As the temperature increases, yielding may occur and its limits decreases with increasing temperature. The deformation at break, increases with increasing temperature, the polymer becoming a brittle material at low temperature, but a ductile material at higher temperature. The effect of the loading rate on the stress-strain curve is opposite to that caused by temperature. At low loading rates, the polymer may behave ductile, with a more pronounced hardening but at high loading rates, the same polymer behaves as a more brittle material.

For polymeric materials, simulation of Charpy tests are few, but the interest in using them as shock absorbers and protective materials makes this subject to be the treated in this study.

2. Materials and Constitutive Models

Samples were obtained by injection molding at Monofil Savinesti SA, Romania, the compositions being given in Table 1 [41], [42]. Details of the laboratory scale process for obtaining them are given in] [27].

Based on the documentation [43-46], the authors modeled the four materials with the help of multilinear elasto-plastic curves.

The results reported in the literature show that polymers also have a stress-strain curve dependent on the strain rate (if other test parameters are kept constant) [24], [47].

Table 1. Recipes for the formulated polymer blends

Material	PA6	PP	EPDM	Polybond 3200	Kritilen
PPm	-	99	-	-	1
H	12	60	8	20	-
G	42	20	28	10	-
PA6m	60	-	40	-	-

The tested polymeric blends are based on polyamide 6 (PA6), polypropylene (PP) and EPDM (ethylene propylene diene monomer rubber), polybond 3000 și kritilen, the blend concentration being given in Table 1.

The material model was obtained based on experimental data obtained at traction for the highest speed ($v=1000$ mm/min) [27] because it was estimated that for these materials the influence of the test rate, except for the lowest test strain rate ($v=10$ mm/min), is very low for the shape of the stress-strain curve and the characteristic values obtained from the tensile tests [Musteata, PhD 2020] For instance, Musteata [42] reported small differences in strain-stress curves obtained in tensile tests for PA6 and PP, under test rate of 250...1000 mm/min (aprox. 35×10^{-3} s⁻¹... 150×10^{-3} s⁻¹), but different

shape and characteristic values at the lowest test rate of 10 mm/min (approx. 10^{-3} s^{-1}). Charpy test with 1 m/s could have 10...25 s^{-1} (taking into account the possible span between anvils). Figure 1 presents the results from tensile tests (first column of plots), the selected curve for introducing as constitutive model (second column) and the ten-point true stress-true strain curve used as constitutive model for each material. From these experimental results, the four materials have different values for EPS (echivalent plastic strain at break) (Table 2).

Table 2. Characteristics of modeled materials

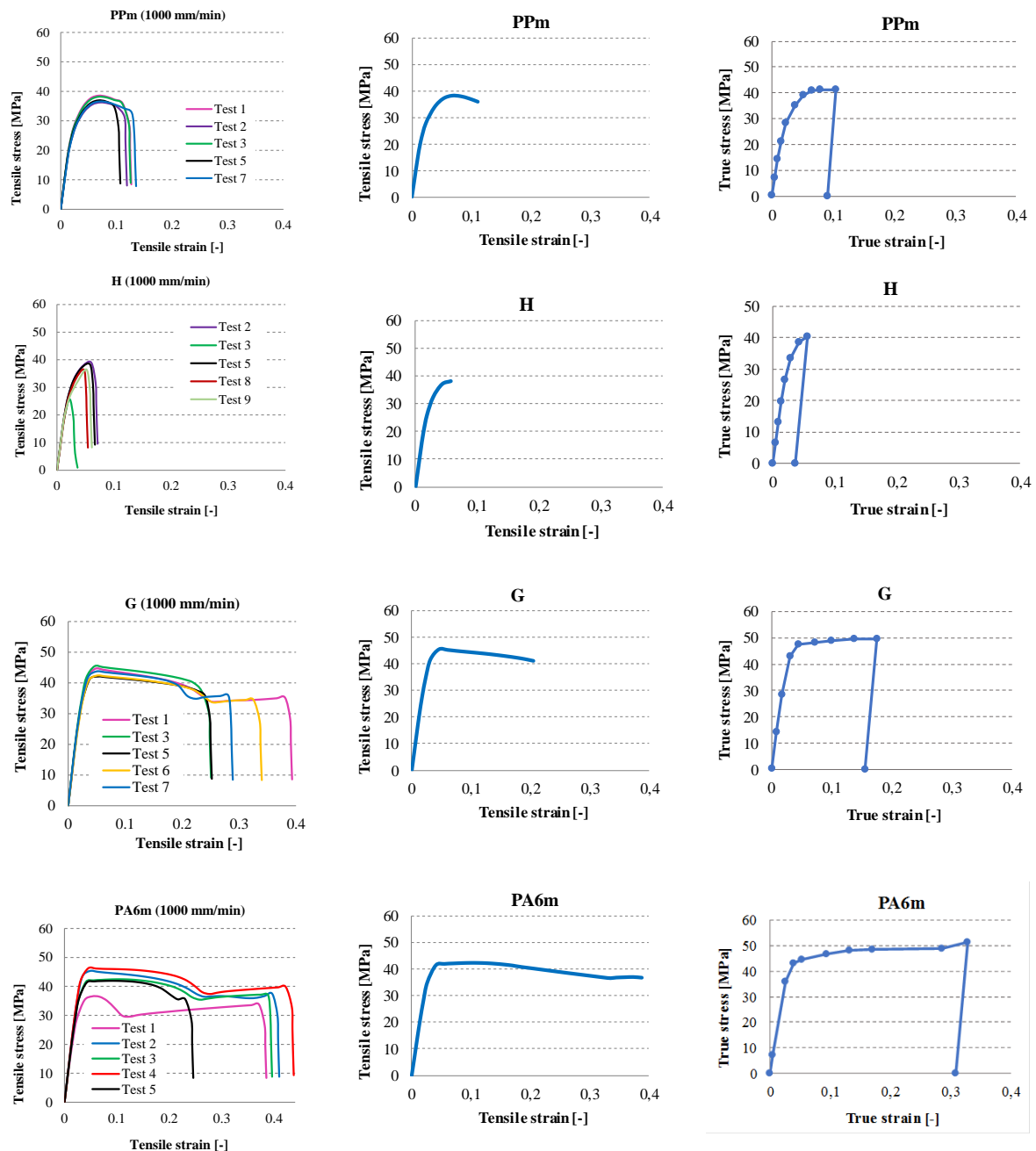
Characteristic	PPm	H	G	PA6m
Density, kg/m^3	915	915	915	915
Longitudinal modulus of elasticity, E, MPa	1466	1582	1625	1595
Poisson's ratio, ν	0,4	0,4	0,4	0,4
The volume module, MPa	2443.3	2636,7	2708,3	2658.3
Shear modulus, MPa	523.57	565	580,36	569.6
EPS at break	0.09	0.036	0.156	0.308

3. The Model

For this model, the impactor and the anvils were considered as rigid bodies as the differences in material properties between those and tested materials is more than one order of magnitude (around 60, considering the tensile strength limit). Analyzing the fracture in this model, for all materials, one may notice that, even if, at crack initiation, a symmetry of the stress & strain fields is visible, this is disturbed by the occurring of high stress and strain. To use the whole sample volume in the simulation seems to be more reasonable for having a more realistic model.

The issue of the mesh network for the Charpy model is the big difference between the dimensions of the specimen and the dimensions of the notch. Choosing a uniform mesh network would increase the time required for the simulation, without bringing significant improvements in the results of interest (stress and strain distributions etc.). In [16], [18-21], there are given several solutions of mesh networks for modeling and simulating the Charpy test.

The mesh network was selected to simulate the Charpy test as presented in Fig. 2. The size of the sides of the elements is between 0.25 mm and 0.75 mm. Growth ratio between elements 1.2, relatively lower than in the discretisations of other works [Haušild, 2005]. In addition, the model was formed entirely, because in the first simulations with a coarser mesh, it was observed that, although the application of the load and the geometry of the model are symmetrical to a vertical plane, stress distributions and the tendency to zigzag under the notch appeared, a fact also observed on the surfaces of broken specimens..



a) Tensile test results

b) typical stress-strain curve
(selected by the authors)c) True stress-strain curve,
approximated by 10 points**Fig. 1.** Tensile tests and models for the materials

The assumptions considered in these models are as follows.

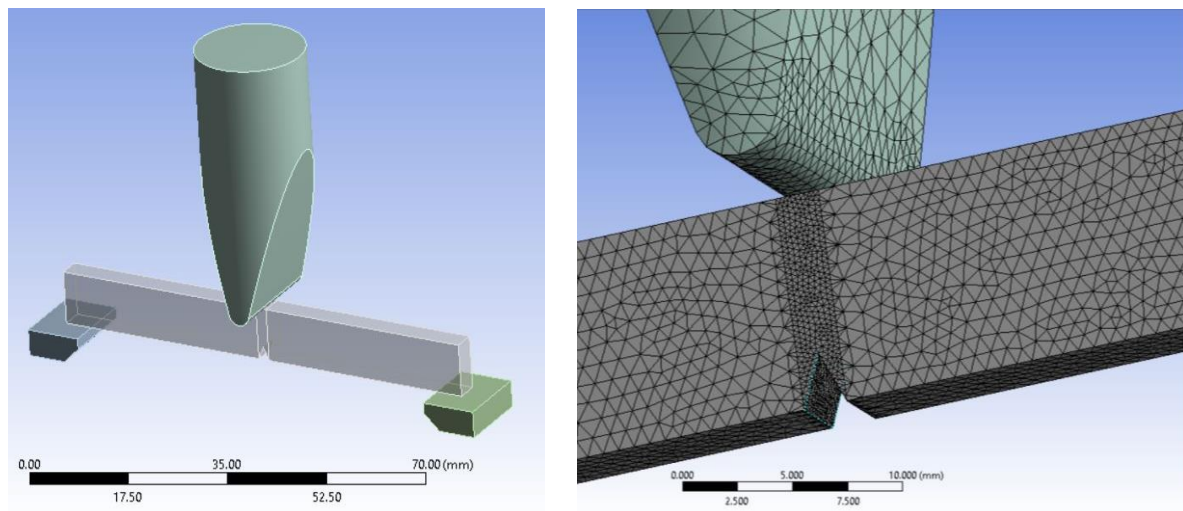
- The supports and the impactor are considered rigid, given the difference in properties; impactor and rigid supports were also considered in the works [16],[18], [19], [48] but in the work of Sainte Catherine [21] the impactor and supports they were considered perfectly elastic, given the testing of steel specimens.

- The initial velocity (just before impact) is $v_0=0.96$ m/s (impact velocity, with which the actual tests were performed).

- Boundary conditions: friction between specimen and supports, friction between specimen and impactor (COF=0.3) for all analyzed cases; Poussard et al. [19], Haušild [17] and Sainte Catherine [21] did not consider friction, but the friction between impactor and sample and sample and supports was taken into account in the models from [42].

- Failure criterion was selected for equivalent plastic strain at break (EPS): when the critical value of EPS (at break) is reached in the model, the crack is initiated.

From the experimental results, it was found that the four materials for which the impact behavior was simulated with an impactor having linear trajectory, have different values for EPS at break, as calculated from the diagram true stress - true strain (Table 2).



a) Arrangement of the parts involved in this model

b) Detail of the mesh for the notch zone

Fig. 2. Mesh network of the model

Table 3

Body	Numbers of nodes	Numbers of elements
Impactor	4259	20738
Support 1	3996	3146
Support 2	4212	3354
Sample	20811	106591
Total model	33278	133829

The size of the elements varies between a minimum of 0.25 mm and 0.75 mm and the number of nodes and elements for each part of the test system is given in Table 3

Hypotheses are the followings:

- the supports for the sample and the impactor are considered perfectly rigid, this hypothesis being reasonable if the large differences in material properties are considered (sample are made of polymeric blends that have tensile limit even 10 times and more lower than that of the impactor and supports),

- initial velocity (just before the impact) $v_0=0,96$ m/s (it is the same value as that used for the experimental work),

- boundary conditions include: contact with friction between sample and support and between sample and impactor, the friction coefficient being constant for all cases (COF=0.3),

- the equivalent plastic strain at break was the failure criterion selected in this work (see values for each material in the last line of Table 2).

4. Experimental Results of Charpy Tests

In this paper, the tests were performed on the CEAST 9340 impact test machine within the materials strength laboratory at "Politehnica" University of Bucharest. The tests were performed with a hemispherical impactor, with a speed of 0.96 m/s and the mass of the impactor 3.219 kg. The specimen has the drawing shown in Fig. 3, and Fig. 4 shows the geometry of the impactor.

According to the SR ISO 179 standard, ten tests were chosen for each material considered to be typical for the respective material (the tests that gave results far from the typical values were eliminated).

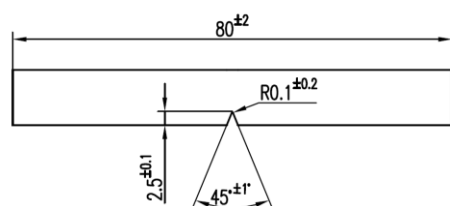


Fig. 3. Specimen dimensions

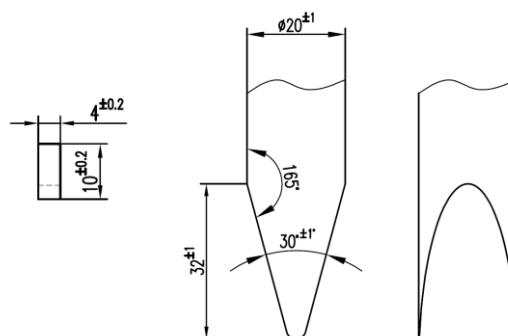


Fig. 4. Impactor geometry

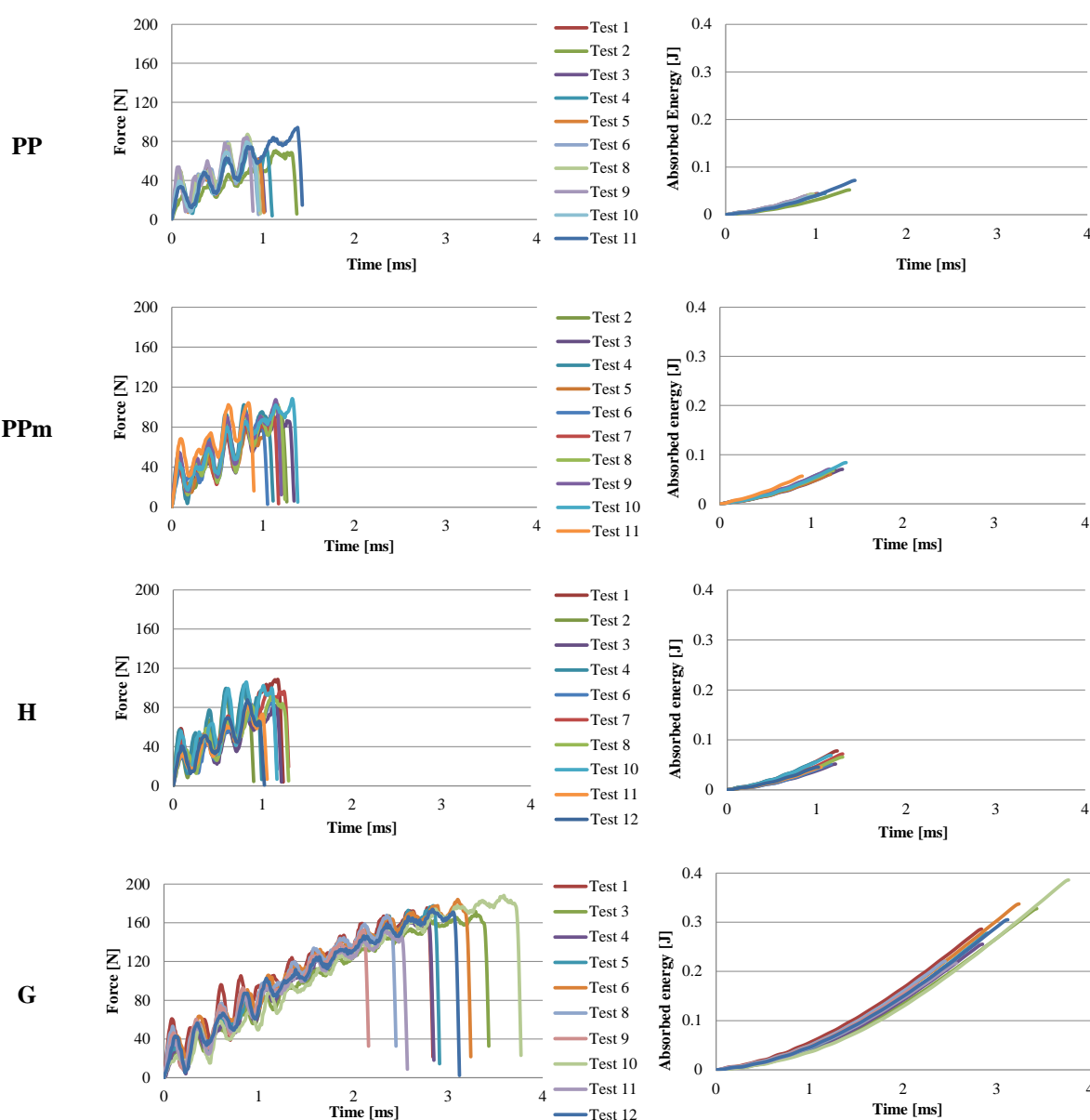
For the material PPm (Fig. 5b, the force-time curves have large oscillations especially in the first part of the destruction process, the oscillations being of 30-60 N, which means a mixed structure of amorphous and crystalline volumes. The breaking time for the most of the specimens is up to 1×10^{-3} s except for test eleven, for which the specimen broke at $t = 0.9 \times 10^{-3}$ s. On absorbed energy-time zones, two zones can be distinguished: the first up to 0.07 J which has a very large curvature followed by a linear zone except for test 11, the result falling in a very narrow band of 0.025 J. The very short time to failure shows the more fragile nature of PP. The addition of Kritilen in PP does not introduce noticeable changes in the form of force-time curves, but in the case of PPm several specimens "crowd" the breaking to higher values of moments (considered for $F=0$). If one compares the values of some parameters from the Charpy test for PP and PPm, it is observed that PPm has slightly higher values, both for F_{max} and for the energy absorbed on impact (Table 5). The time to failure ($F=0$) is approximately the same for PP and PPm (0.85...1.4 ms). It turns out that the addition of this agent Kritilen PP940 has improved the behavior of PP on impact, even if its concentration is only 1%, and it also improved the shape quality of the samples when they were extracted from the mold. One may compare the curves in Fig. 5a (for the neat polypropylene) to those in Fig. 5b (for PP+1% kritilen).

The behavior of material H in the Charpy test is similar to that of the PPm material (Fig. 6), but the time to failure (considered at $F=0$) is close, the specimens having the time to failure from 0.9×10^{-3} s to 1.29×10^{-3} s. The oscillations of the force-time curve show the presence of two polymeric structures, one more tenacious and the other weaker. The oscillations of the force-time curve show that in the breaking section the material is composed of an alternating succession of more resistant micro-volumes and weaker materials from a mechanical point of view, but also amorphous and crystalline micro-volumes of the two constituent polymers (PP and PA6, see Fig. 5f).

Material G (Fig. 7b) has much smaller amplitude of force oscillations. The oscillations start with values between 30-60 N, after which the amplitude of the oscillations does not exceed ~ 20 N. The maximum values of the force are concentrated between 150-180 N, which reflects that the specimens are more similar in terms of response to the request, that is, the quality of the injection process is more controllable for this material. The energy-time curves are very close and very similar. The scattering band of the curves is narrower up to 0.5 J (up to 1 ms) and then on the linear area it is slightly more scattered. The value of the moment of completed failure ($F = 0$) is in the range of $t = 2.16 \times 10^{-3}$ s to $t = 3.77 \times 10^{-3}$ s. If G is compared with the other materials (Table 5), it is observed that the maximum value of time to failure has the value of $t = 3.77 \times 10^{-3}$ s, the highest of all materials of the

second family. If the materials are ordered in descending order of the greatest value of time to failure ($F=0$), this is G, PA6m, PA6, PP and very close to each other, PPM and H. For F_{max} the highest value is for PA6, followed by that for PA6m.

The SEM images (Fig. 6) shows that the introduction of PA6 in higher concentration changed the morphology of the blend. Material H has a PP matrix with PA6 droplets and pores of the order of a few microns. The droplets located right on the breaking zone are very deformed, elongated and the matrix breaks as a more brittle polymer, with linear micro-flows, probably as a result of a lower crystallinity of PP. Material G has the inverted phases, as it resulted from the EDX analysis. The PP droplets are larger and do not have cohesion on the whole surface with the matrix, which seems to be a homogeneous blend of PA6 and EPDM. But the most important feature, the energy absorbed during impact, has the highest value for PA6m (0.305...0.389 J).



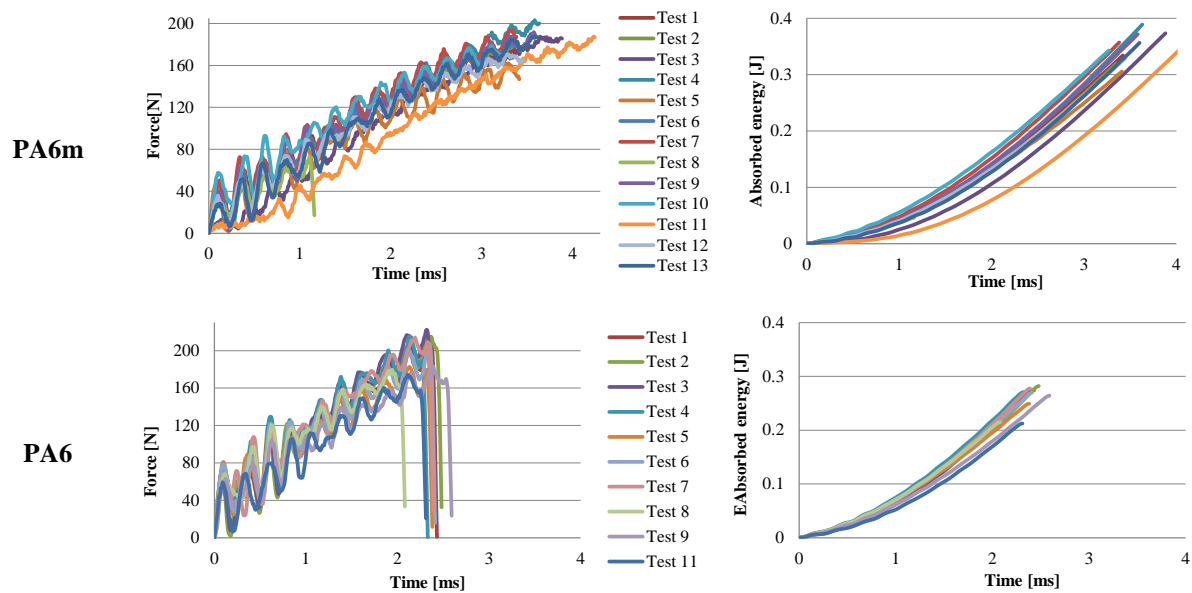
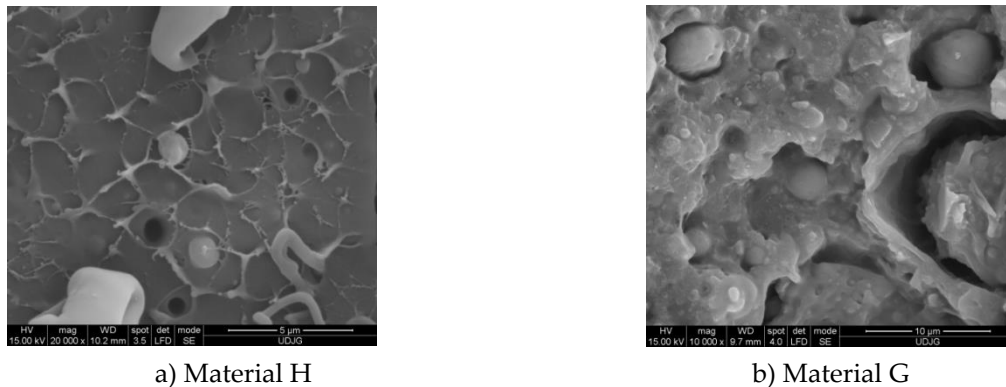


Figure 5. Curves for force and absorbed energy in time, for the tested materials



a) Material H

b) Material G

Fig. 6. Fracture morphology at break, after the impact test

The addition of EPDM in PA6m has a force-time diagram similar to that of simple polyamide, but the failure occurs after a slightly longer time interval. At $t=2.59 \times 10^{-3}$ s, for PA6, all the specimens were already broken, whereas for PA6m the damage of the specimens (with incomplete failure), is achieved between $t=3.34 \times 10^{-3}$ s and $t=3.59 \times 10^{-3}$ s. In other words, the addition of EPDM increases the time to failure (even partially, in the case of PA6m material). The evolution over time of the destructive energy has similar forms only that most of the PA6m specimens break partially after storing an energy between 0.305 J and 0.389 J, while PA6 reaches only 0.279 J at the complete failure of the specimens.

The energy at break plot for PA6m is characterized by two zones: a curved line in which the energy increases after a curve up to 0.15 J, after which the evolution of the energy stored in the test tube is linear. Comparing the four materials (PPm, H, G and PA6m), the value of the maximum force was obtained for PA6m. The material for which the following maximum force value was obtained is G, with 170.7 N, only 6.46% lower than the PA6m material. PPm has the maximum force about half of G, and for H the lowest value was obtained, in other words, H is the weakest material in terms of the maximum force required for damage.

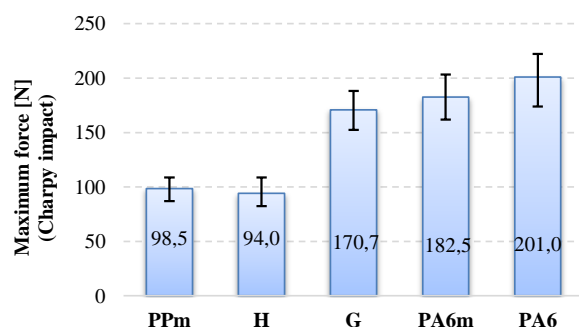


Fig. 7. Average values of the maximum impact force Charpy for the second family of blends

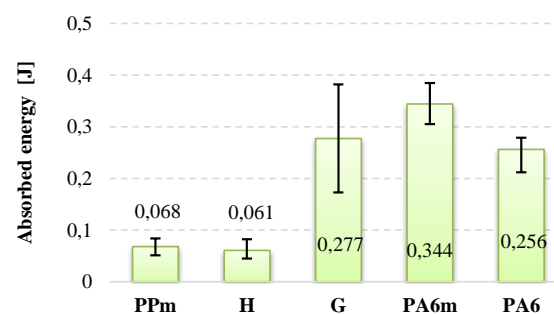


Fig. 8. Average values of the absorbed energy for the second family of blends

Regarding the energy at break (also named absorbed energy till break) (Fig. 8), it is noticed that the best results were obtained for PA6m, both for the average value of the energy at break (0.344 J) and for the spreading interval, which is below 0.084 J. PPm and H materials have about five times less energy at break than PA6m material. It is clear that in applications with shock resistance materials, PPm and H are not recommended, instead the PA6m (PA6 + EPDM) coat gave better results than for PA6. Material G should not be removed from the recommendations for shock applications with speeds up to 1 m/s, but the scattering of the results is higher and the average value of the energy at break is very close to that of the simple polymer PA6. The choice between these two materials, G and PA6 is made by analyzing other criteria necessary for the design, such as water absorption, dimensional stability, processability and price.

Aspects of impact-breaking mechanisms at this low speed (0.97 m/s) are shown in SEM image (Fig. 9). PPm and H materials have a brittle fracture appearance, while G and PA6m materials have fracture surfaces typical of ductile fracture. All tested PA6m samples showed the same form of failure while maintaining a link between the test fragments (without complete failure) (Fig. 9d).

Studying these images, it is not possible to specify whether the failure advanced only from the notch or occurred in the impact area of the impactor, also. The aspects of breaking material H are similar to PPm. Material G has a different appearance from the materials discussed above: the breaking surface is much rougher and it is likely that the tear was initiated first near the notch but then under the impactor. The very uneven area is very likely to have yielded more abruptly than the material under the notch and under the impactor, some dispersed droplets are partially detached from the matrix, but others, usually smaller, are trapped in the matrix. The most interesting SEM images were obtained for PA6m (Fig. 9d). An area parallel to the breaking surface of the crack is observed in which the material has a pronounced plastic yield at an angle of approximately 45° to the breaking surface. The thickness of this layer is about 200 microns and was not observed in the other materials that contained EPDM (H and G). Stopping the crack progress is observed in Figs. 22a and b. The addition of EPDM to PA6 led to the propagation of a failure without fibrillation but with strong local flows on a band near the failure surface.

Analysing the plots for maximum value of von Mises stress, during a time interval at 3×10^{-2} s, the materials could be in two behavioral groups

- materials with brittle fracture (H and PPm),
- materials with ductile fracture (G and PA6m).

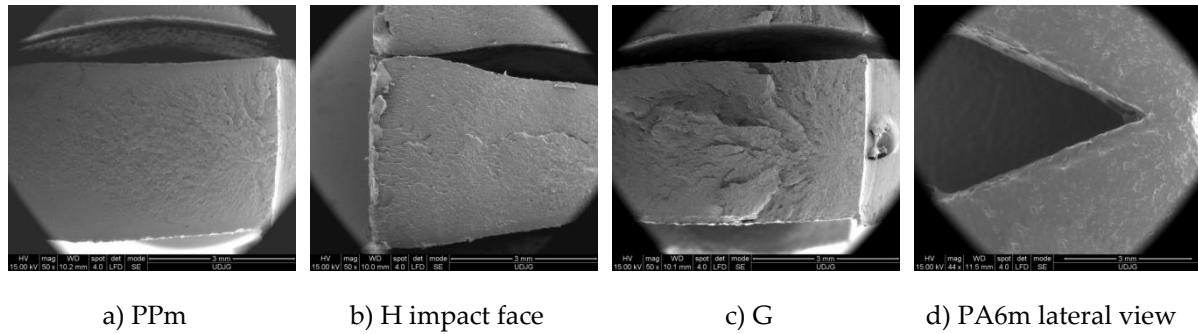


Fig. 9. Typical aspects of the surfaces obtained after sample breaking

The fracture of the model is uniform on the sample width and it advances uniformly in the section. The actual fracture of G and (even PPM somehow) has a core with brittle aspect and ductile aspect around. This could be explained by the fact that material model does not take into account the influence of strain rate and non-homogeneity of amorphous and crystalline micro-volumes.

For materials G and PA6m, the results are very good, in the sense that PA6m exceeds PA6, and G also exceeds the energy at break on impact of polyamide.

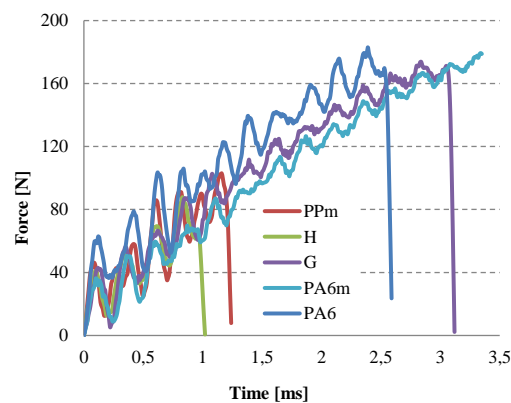


Fig. 10. Typical curves force-time for the tested materials

Table 5. Characteristics obtained from Charpy tests, for the second family of blends

Characteristic	PPm	H	G	PA6m	PA6
Absorbed energy at break [J]	0.068	0.061	0.277	0.334	0.256
Maximum force [N]	98.54	94.05	170.70	182.52	200.96
Impact resistance [kJ/m ²]					
average	2.26	2.017	9.23	11.47	8.52
range	1.7...2.8	1.5...2.733	5.76...12.73	10.16...12.96	7.0...9.3

The impact strength of the specimen was calculated with the formula

$$R_{\text{impact}} = \frac{\Delta E}{A_0} \left[\text{J/m}^2 \right] \quad (1)$$

where ΔE is the energy absorbed up to $F=0$ and $A_0 = b(h_{\text{specimen}} - h_{\text{notch}})$ is the transversal minimum section area (at the tip of the notch), b being the width of the specimen and h_{specimen} being the specimen height and h_{notch} being the depth of the notch.

5. Analysis of Simulations for Each Material

Some images were obtained by considering a half of the transparent specimen (at time $t=0$ s) (the specimen is not divided into two entities, and the section is right in the plane of symmetry of the notch). This virtual sectioning facilitates the observation of the development of the failure and the change of the distribution of equivalent stresses. A qualitative and quantitative analysis of stress concentrators and how they evolve at any given time as the failure propagates, can be performed.

Material PPM. At the moment closest to the impact ($t=5.0 \times 10^{-4}$ s), two stress concentrators are observed on the specimen, one just under the impactor, the other at the tip of the notch, both presenting a “butterfly” distribution; the higher values of the equivalent stress are recorded under the impactor, in the middle of the notch tip, $\sigma_{ech\ max}=13.59$ MPa, below half the stress at break.

In the following moments, the two stress zones increase in area and value, thus, at time $t=1.0 \times 10^{-3}$ s, $\sigma_{ech}=18.2$ MPa. At $t=1.5 \times 10^{-3}$ s, the crack has not yet been created, but the equivalent stress has increased to $\sigma_{ech}=23.9$ MPa, under the impactor. At $t=2.0 \times 10^{-3}$ s, the equivalent stress increased to 29.6 MPa under the impactor and 23.03 MPa at the tip of the notch. The specimen is increasingly stressed at time $t=2.5 \times 10^{-3}$ s (Fig. 11a) and the initiation of the crack may be seen in the middle of the tip width of the notch, the crack being already developed on a length of less than 1 mm, the equivalent stress reaching 31.8 MPa. From simulation, until the moment $t=2.5 \times 10^{-3}$ s, the critical value of EPS was not reached, $EPS_{(PPm)critical}=0.09$, and therefore, the crack was not initiated.

Stress concentrators are created at the edges of the theoretical impact line due to the fact that large deformations appear as an edge effect at the ends of the impact line (Fig. 12).

At time $t=3.0 \times 10^{-3}$ s (Fig. 11b), the crack is already initiated and it is observed that it propagates on the height of the specimen, causing an uneven band of maximum stresses of 33 MPa. The opening of the crack and the continuation of the impact caused on the opposite surface a band of equivalent stress almost as big, which still does not yet cause the cracking because the impactor causes compression. The middle volume of the specimen between this first crack and the compressed side is almost non-tensioned (in blue and dark blue colors), with values of 3-7 MPa.

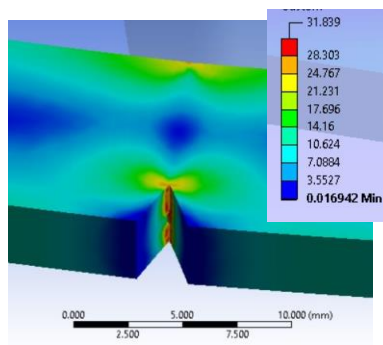
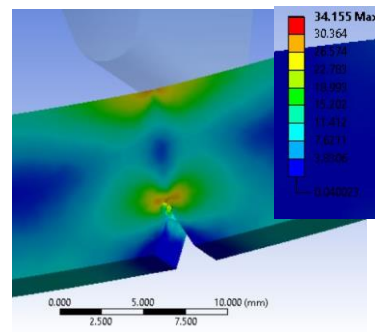
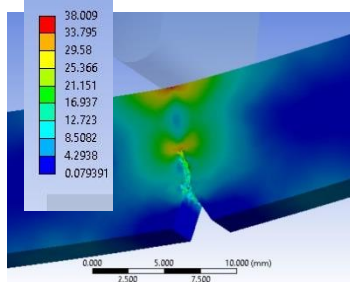
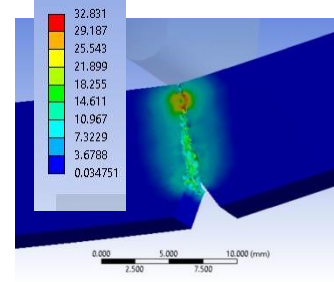
a) Crack initiation, $t=2.5 \times 10^{-3}$ sb) Crack development on the entire width, $t=3 \times 10^{-3}$ sc) propagation of the first crack, $t=3.5 \times 10^{-3}$ sd) Second crack initiation (under the impactor)
 $t=4.5 \times 10^{-3}$ s

Fig. 11. Selection of important moments in simulation for material PPM

At $t=3.5 \times 10^{-3}$ s (Fig. 11c), the crack is already propagated over almost half the distance between the tip of the notch and the impacted surface. Next, the highest equivalent stress is observed under the impactor $\sigma_{ech}=38$ MPa.

At time $t=4.0 \times 10^{-3}$ s, the initiation and propagation of the second crack is observed from the impacted part of the specimen to its center. The maximum equivalent stress is visible only at the tip of one of the cracks, at that one initiated from the tip of the notch. On the height of the specimen, the still undetached area appears to be 2 mm. At this moment, the material left between the two cracks has only a small area, with low stresses of 7 MPa.

At time $t=4.5 \times 10^{-3}$ s (Fig. 11d), the sample has two broken areas, the one propagated from the notch, but also a smaller one under the impactor. A maximum equivalent stress of 32 MPa is observed, in a narrow ribbon remained between the tips of the two cracks. Although at the beginning, the impact had symmetrical characteristics as compared to the initial plane passing through the tip of the notch, it is observed that, later, the stress distribution within the material becomes slightly asymmetric. This phenomenon can occur due to the automatic discretization of the model, although a fine mesh was used, but also to the elasto-plastic behavior of the material. The failure has a zig-zag character, which is also visible on the SEM images (Fig. 9a) and on a macrophoto (Fig. 21a).

At time $t=5.0 \times 10^{-3}$ s, the still unbroken material has a size of less 1 mm, this decreasing at time $t=5.5 \times 10^{-3}$ s, leading to the growth of the two cracks, the crack starting from the tip of the notch being longer in length than that started from the impacted surface; linkages (small bridges) between the two fragments of the specimen distributed unevenly across the width of the specimen can be observed. At moment $t=6.0 \times 10^{-3}$ s, the specimen fragments are already separated. If high equivalent

stresses occur at later times, they are due to the pushing of the fragments into each other until the impactor separates them.

At $t=6.0 \times 10^{-3}$ s, the maximum equivalent stress moved to the tip of the crack started under the impactor and has a value of 33 MPa. The moment $t=6.5 \times 10^{-3}$ s is characterized by $\sigma_{ech\ max}$ lower than the previous one, meaning that the failure process (also described by stress distributions) alternates with a process of relaxation of the material (σ_{ech} decreases), which is specific to plastics. At $t=7.0 \times 10^{-3}$ s, $\sigma_{ech}= 33.29$ MPa, that may be seen in the virtual cross section of the specimen, which means that there are still small areas unbroken (unseparated), local bridges between the two already detached fragments of the specimen. At time $t=7.5 \times 10^{-3}$ s, only the crack under the impactor, may be stressed due to compression, due to the opening of the specimen. Starting from $t=7.5 \times 10^{-3}$ s till $t=1.0 \times 10^{-2}$ s, the equivalent stress drops to 20 MPa. These stress values, without reaching the stress at break, are due to the collision of the two fragments of the specimen.

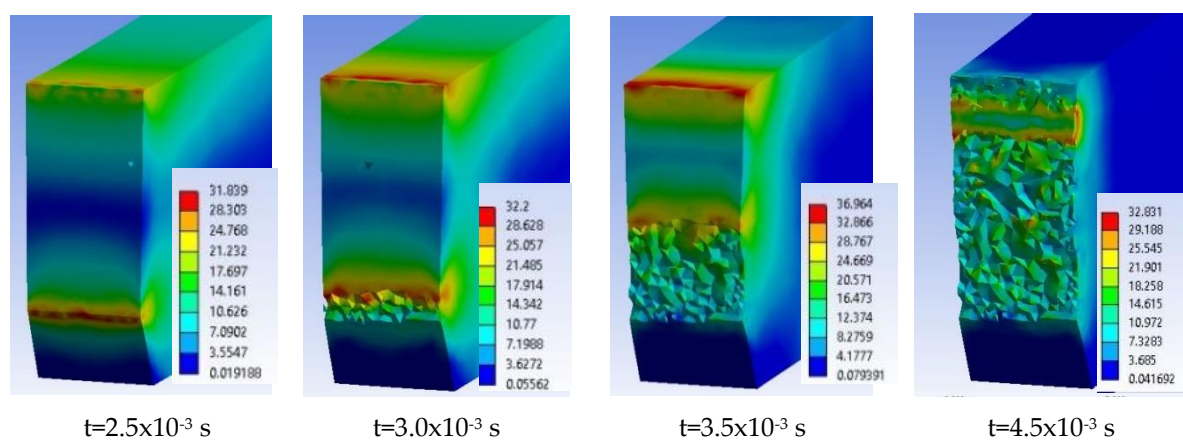


Fig. 12. Successive moments from the impact of the test specimen made of PPM material

The smooth surfaces that appear from the moment $t=7.5 \times 10^{-3}$ s, indicate the areas where the upper crack is closed due to the rapid movement of the fragmented gates of the specimen.

The conclusion drawn from the above comment is that the impact does not generate high stress in all the volume of the impacted specimen, but determines volumes of stress concentrators where the crack starts.

Figure 12 shows the breaking surface for the material PPM, its appearance being similar to that obtained in the simulation, but the crack under the impactor is less developed on actual specimen and a superficial crushing destruction is observed which could not be highlighted by modeling. The cracking occurred on a short length and from the impactor.

Figure 13 presents a selection of moments during the impact simulation for material H, von Mises stress distribution being observed in lateral view, the appearance and development of the crack at the tip of the notch and then of the crack under the impactor. Due to the color scale, the areas with maximum von Mises stress values (red on each image) are well highlighted. The end of the simulation for material H is at the moment $t=5.0 \times 10^{-3}$ s.

In the details in Fig. 14, particularities of the breaking process can be noticed: crack initiated at $t=2.0 \times 10^{-3}$ s (a), at time $t=2.5 \times 10^{-3}$ s, the two cracks advances, less of 1/3 of the specimen height being unbroken (b) and a virtual cross section reveals the asymmetric stress distribution at the cracks' tips (c). The failure propagates from the notch (first) and then from under the impactor. There is an area destroyed by crushing (compression), just below the impactor, as seen in SEM images. The

distribution of equivalent stresses at the tip of the cracks is typical of visco-plastic materials. The perfectly smooth surface visible in Fig. 14a is virtually resulted by sectioning with the imaginary plane. It is observed how the crack advances from one moment to another and the area where the last strip of material is lasting ($t=3.25 \times 10^{-3}$ s) before the total fragmentation of the specimen.

If a qualitative comparison is made with SEM images of the H material, they are close enough in appearance. In Fig. 15, one may notice that the material H has a fragile failure and the initiation of the crack is made first from the tip of the notch, but there is a second crack, initiated from under the impactor, which joins the first at almost 1/4 of the height of the specimen. The actual appearance of the broken surface (Fig. 15) resembles the appearance of the failure at the end of the simulation.

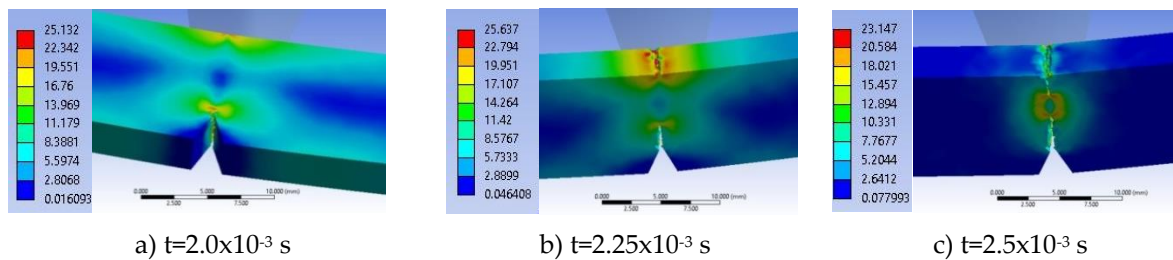


Fig. 13. Selection of important moments in simulation for material H (equivalent stresses, MPa)

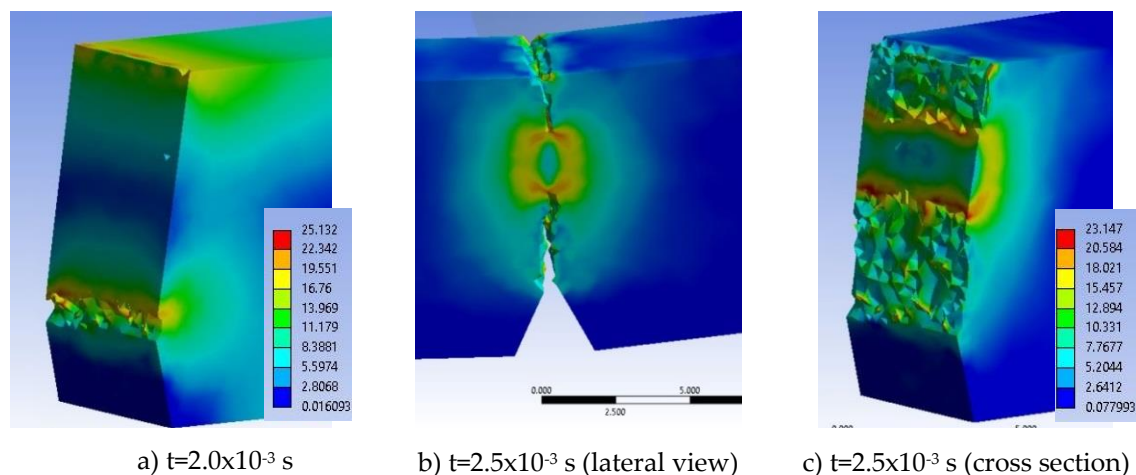


Fig. 14. Appearance of failure in the plane containing the notch tip and the impactor axis, for material H

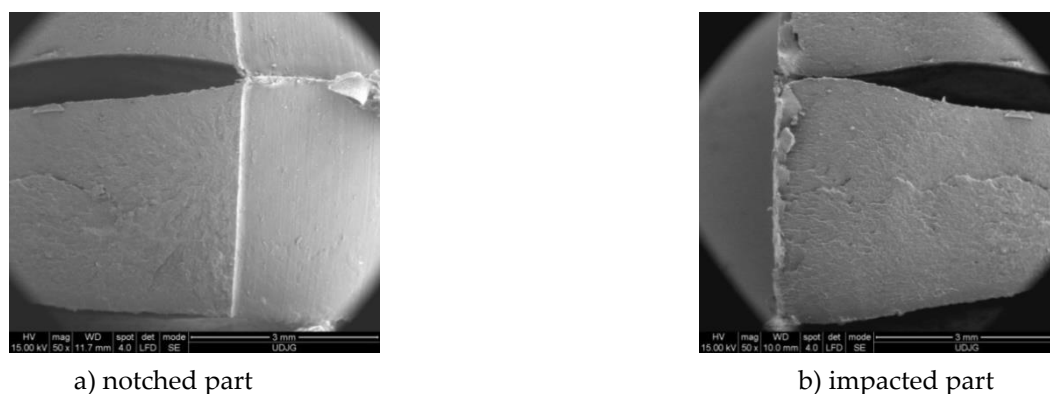


Fig. 15. The failure surface of a Charpy specimen, made of material H

From experimental data, material G is the second material, in a ranking based on energy at break. For this reason, the simulation of impact failure is important when compared to the material with the best results, PA6m. Figure 16 shows the evolution of the crack generated from the tip of the notch. Figure 16a presents the initiation of the crack at the notch tip, the zig-zag development of the

crack from the notch tip (Fig. 16 b, c and d), the generation of the second crack under the impactor, starting from both edges of the specimen (Fig. 16e) and a moment when a small material bridge is remained between the two fragments (Fig. 16f), until the complete separation of the fragments of the specimen (see moments in Fig. 17). Comparing the images in the simulation from one moment to the next allows for establishing the start points of the cracks and how they develop.

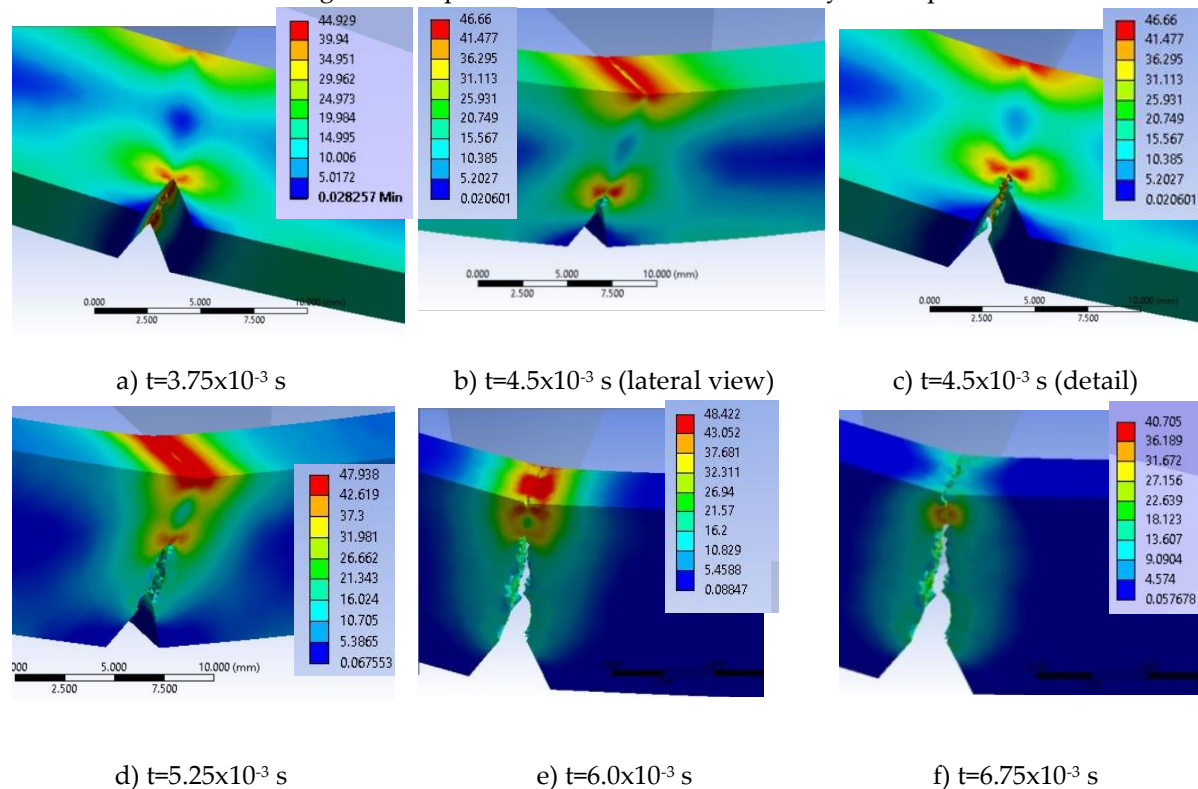


Fig. 16. The evolution of the crack generated from the top of the notch, before the initiation of the crack under the impactor, for material G

For example, for material G, in Fig. 16a, the impactor has created on the impact surface a field of equivalent stresses of high values, close to the stress at break and deformed the specimen so as to force the development of the crack from the notch tip (b), but also the initiation of lateral two cracks on the width of the specimen under the impactor, this crack having a slower propagation speed, in the middle of the specimen maintaining a high stress field (Fig.16e). Lateral views of the samples in Fig. 17 presents the crack just before complete separation of the fragments. The impactor pushes the specimen, making the fragments to change their positions from horizontal to oblique ones and it is observed that the union of the two cracks suddenly diminished the stress field in the area, strong stress concentrators being in the material ribbon (bridge) left unbroken (a and b). At $t=1.5 \times 10^{-2}$ s, the resulted fragments are completely separated (Fig. 17c).

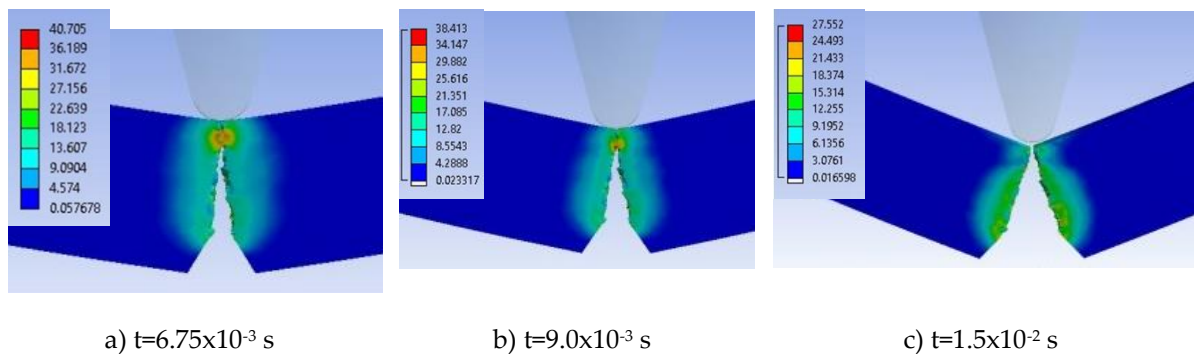


Fig. 17. Initiation and evolution of the crack under the impactor, until the separation of the broken fragments for material G

Simultaneous development of stress concentrators is noticed, one around the notch tip and the other under the impactor, but the failure criterion ($EPS=0.156$) is reached for the first time at the tip of the notch, at time $t=3.75 \times 10^{-3}$ s, the zone of high von Mises stress (with red color) remaining at the tip of the crack, advancing as it grows, but there is also an area of the same values under the impactor, as the impactor pushes the specimen.

The opening of the crack and the change of the angle between the still undetached fragments of the specimen concentrate more the area with high stress.

Images from Figures 16 and 17 are taken from different angles, for pointing out important moments in the failure process. This is one of the advantages of simulation that destruction mechanisms can be studied and viewed from angles favorable to their explanation.

At the beginning of the impact ($t=7.5 \times 10^{-4}$ s), it is observed the formation of two zones of stress concentration on the width of the specimen, along the tip of the notch and under the impactor, but the crack is not yet initiated. For material G, the failure occurs between moments $t=3 \times 10^{-3}$ s and $t=3.75 \times 10^{-3}$ s, and the crack begins in the middle of the notch tip width. At time $t=4.5 \times 10^{-3}$ s, the crack is propagated over the entire width of the specimen and has already advanced by almost 1.5 mm (Fig. 16b). The crack advances towards the other surface of the specimen and the von Mises stress distribution has high values on the impacted surface as well (Fig. 16c and d).

At time $t=6 \times 10^{-3}$ s, the specimen is not yet completely broken, leaving a band of ~2 mm still uncracked. Another step in the crack development is shown in Fig. 16f, showing a moment of crack converging for material G.

Comparing the image in Fig. 18d with SEM image (Fig. 9c), one may noticed that:

- the aspect of failure is rough, both in the model and on the actual specimen, the actual uneven aspect of the specimen surface being probably caused by the inhomogeneity of the material;
- a very thin compressed strip is observed on the specimen side the impactor stroke.

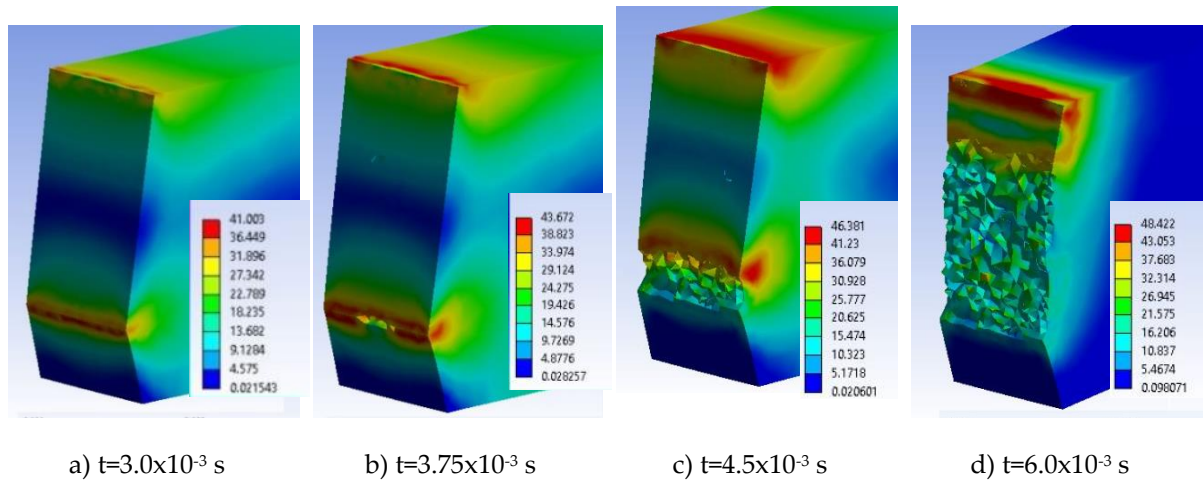


Fig. 18. The evolution of the crack generated from the tip of the notch, before the initiation of the crack under the impactor, for material G (stress scale in MPa)

In Figure 18, several successive images were chosen to show how the crack advances in the most ductile material (PA6m). High values of von Mises stress are visible in a narrow band around the notch tip and in an irregular one and less uniform in the zone slightly lateral from the symmetric plane of the sample and impactor (a). The crack was started from the tip of the notch, in the middle of its width at $t=3.75 \times 10^{-3}$ s (b). The high stress field advances as the crack develops, also keeping high values on the impacted side (Fig. 18 c and d, but also Fig. 19 a and b).

Changing the angle of observing the specimen failure, the development of the first crack and the initiation of the second one, under the impactor are visible at time $t=1.25 \times 10^{-2}$ s (Fig. 19c), there is a crack of much smaller depth than the one started from the tip of the notch. The images from the following moments show that the material left in common, between the two fragments decreases from time $t=1.125 \times 10^{-2}$ s (Fig. 19c) till $t=2.0 \times 10^{-2}$ s (Fig. 19e), leaving only a thin band that connects the two fragments. At the last moment of the simulation ($t=2.5 \times 10^{-2}$ s, Fig. 19f), there is a remaining common material band and a decrease of the equivalent stress values with only a high spot generated by bending the non-detached fragments.

From the sequence of moments in failure process in Fig. 19, it can be seen that:

- the specimen did not detach completely (both experimentally and in simulation),
- the running time is the longest for this material, as compared to the other modeled materials,
- for PA6m material, the EPS at break has the biggest value.

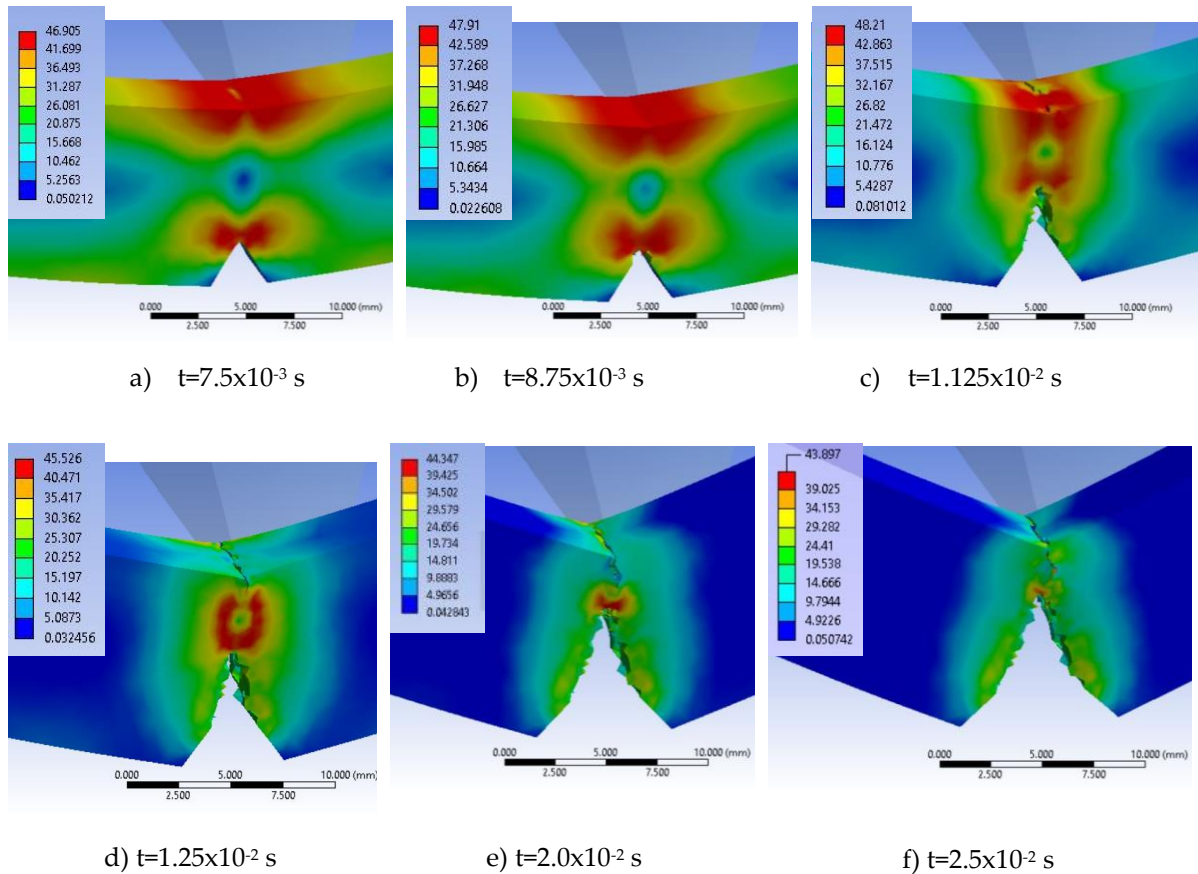


Fig. 19. Lateral view of the specimen made of PA6m, during impact, with von Mises stress distributions (scale is for equivalent stress, in MPa)

Analyzing the actual aspect after specimens had been tested (Fig. 21b), it was observed that there was a very narrow band of material that did not break, as noticed in the simulation. The PA6m material is more prone to local deformation, the area under the impactor was strongly deformed, observing the developing trapezoidal shape with the larger side under the impactor (Fig. 20).

A virtual cross section of the specimen reveal how the cracks are generated and the shape change of the specimen (Fig. 20). The crack initiates between $t=6.25 \dots 7.5 \times 10^{-3}$ s (a and b), being located in the middle of the notch tip. This advances quite quickly with larger stress concentration zones in front of the crack tip and on the impacted side (Fig. 20c). At this time $t=1.125 \times 10^{-2}$ s, a crack initiated in the area where the impactor strikes is visible.

The cracks advance intermittently (one is developing faster, the other is waiting to act and then the roles are changed).

The breaking process is continued in Figs. 22 it is observed that the maximum values of von Mises stresses remain between 47.8 MPa and 43.74 MPa, which means that at any time between $t=1.375 \times 10^{-2}$ s and $t=2.5 \times 10^{-2}$ s, the material is still breaking.

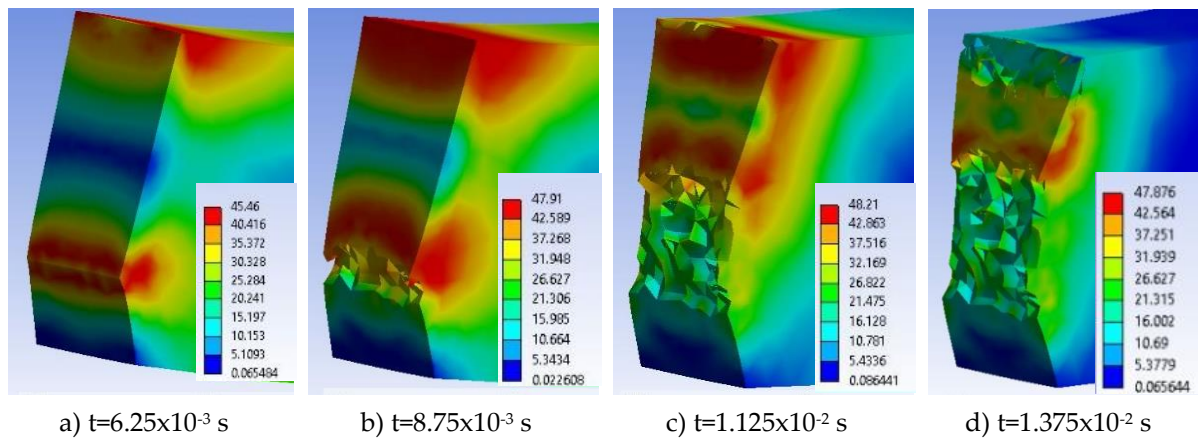


Fig. 20. Moments during impact for material PA6m



a) PPm (sample ends were cut for SEM investigation)

b) PA6m

Fig. 21. Breaking of specimens following Charpy tests, for material

Especially after crack(s) initiation, the aspect of stress distribution is not perfectly symmetric, the explanation being the more viscous-plastic character (larger plastic deformations and low slope in the plastic field). The propagation of the crack under the impactor, along the entire width of the specimen, relaxes this area, the stress concentrator arching between the two cracks.

Qualitative validation of the crack propagation mode in the PA6m material may be argued by comparing the actual shape of the cracks (Fig. 21b) with the simulated shape (Fig. 19f).

6. Conclusions from Comparing Simulation and Experimental Results

The review of available and recent impact modeling documentation in the Charpy test highlighted mesh pattern too coarse or too fine, disregard for friction in the vast majority of works, simplified modeling of the specimen material, with only a quarter or a half of the test system (specimen, impactor and supports) and simplifying hypotheses that may alter the virtual behavior of the specimen.

The originality of the proposed model consists in the following:

- finer discretization of notch area to highlight the mechanisms of failure and their development over time,
- this made it possible to differentiate the destruction mechanisms according to the material introduced in the simulation,
- in the simulations were introduced simplified curves (in 10 points) of the most representative curves real stress - real deformation for the materials of the mixture family,

- depending on the base polymer (PA6 or PP), the initiation and development of failure for the 4 materials were highlighted,
- the author used a less widely used destruction criterion, EPS,
- the validation of the model and the simulation results was done,
- qualitative: the shape of the broken surfaces by comparing to SEM images,
- quantitatively by comparing the impact duration: the duration of the destruction of the specimen is longer than the real one, explainable by the fact that the material model does not take into account the influence of the material deformation speed in the Charpy test, the model being introduced with a 0.016 m/s (1000 mm/min) (maximum strain rate for tensile tests). It is very likely that the appearance of the stress-strain curve will change for 1m/s in the sense of increasing the yield limit and decreasing the EPS.

Comparison between the stress distributions at the same time moments of the simulation, for different materials, is useful because the degree of damage of the specimen could be different (Table 6).

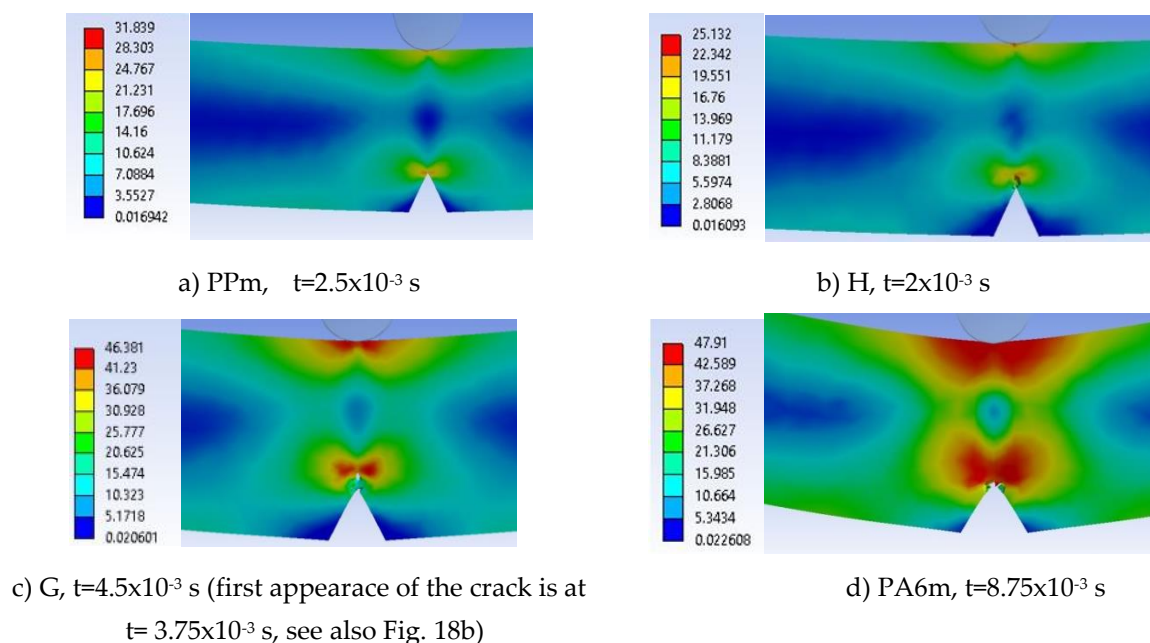


Fig. 22. Crack initiation times and their aspects, for each material and von Mises stress distribution (scale is in MPa)

Moments when the crack initiation is visible on the simulation are presented in Figure 22. For material H, the crack appears at time $t=2 \times 10^{-3}$ s, for PPm, the crack appeared at time $t=2.5 \times 10^{-3}$ s. Material G has the crack initiated at time $t=4.5 \times 10^{-3}$ s. The longest time recorded on the simulation for PA6m, $t=2.5 \times 10^{-2}$ s. From these images it is observed that the PPm and H materials are less deformable, the deformation of the notch shape being almost imperceptible. For more ductile materials, the V of the notch opens visibly and the crack shape differs for G and PA6m. For material G, the crack propagates of brittle type in the sense that it develops towards the impactor, while for material PA6m a strong deformation of the material without the crack advancing so rapidly, this is also visible on SEM images from the same angle.

FE simulation of Charpy tests for different polymeric materials with a material constitutive model deduced from tensile tests has produced results matching experimental data, validating the model constants for low impact velocity (1 m/s).

Table 6. Moments in fracture mechanism for each material simulation

Material	Time moment from the simulation				
	No crack initiation till	Crack initiation	Crack on side contacting the impactor	Fragmentation end (criterion stress value)	Visible detach of the fragment
G	3.75×10^{-3} s	4.5×10^{-3} s	6×10^{-3} s	6.75×10^{-3} s	1.5×10^{-2} s
		3.75×10^{-3} s	6×10^{-3} s	8.25×10^{-3} s	-
H	1.75×10^{-3} s	2×10^{-3} s	1.25×10^{-3} s	4×10^{-3} s	5×10^{-3} s
	1.75×10^{-3} s	2×10^{-3} s	1.5×10^{-3} s... 2×10^{-3} s	3.5×10^{-3} s	4×10^{-3} s
PPm	2.5×10^{-3} s	3×10^{-3} s	4×10^{-3} s	6.5×10^{-3} s	1×10^{-2} s
		3×10^{-3} s	4×10^{-3} s		
PA6m	large opening	8.75×10^{-3} s	1.2×10^{-2} s		no detaching
	of the notch	7.5×10^{-3} s	1.25×10^{-2} s		

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- in the simulations were introduced simplified curves (in 10 points) of the most representative curves real stress - real deformation for the materials of the mixture family,
- depending on the base polymer (PA6 or PP), the initiation and development of failure for the 4 materials were highlighted,
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The higher the value of EPS and the higher the yield point, the wider the distribution of high stresses (red) (in a larger volume).

Figure 24 presents the evolution of the maximum values of the von Mises stress for the four material models. PPm and H materials have better contoured graphs, while the shape of the curve for material G and PA6m indicates a more ductile behavior for these two materials. In general, the maximum values of von Mises stresses indicate the initiation of a crack and/or its continuation after a very short moment of relaxation of the stresses. The last maximum value can also indicate a strong, very punctual compression of the specimen fragments if they collide. Analyzing the images it is likely that the last maximum of material G is due to this compression contact. PPm and H materials have graphs of the maximum values of von Mises stresses with distinct peaks (three for PPm and two for H), indicating cracks (one from the notch and the other initiated from under the impactor)

and/or hits of the fragments with strong local compression. For G and PA6m materials, these curves reflect a much more ductile behavior.

Table 7. Analysis of important moments during impact

Material	Moment of impact	Moment of initiation of the first crack [s]	Moment of initiation of the second crack [s]	Moment of total detachment of fragments [s]	Total running time [s]
PPm	0	2.5×10^{-3}	$3.5 \dots 4.0 \times 10^{-3}$	7.0×10^{-3}	1.0×10^{-2}
H	0	1.75×10^{-3}	2.0×10^{-3}	4.0×10^{-3}	5.0×10^{-3}
G	0	3.75×10^{-3}	6.0×10^{-3}	$9 \dots 9.75 \times 10^{-3}$	1.5×10^{-2}
PA6m	0	7.5×10^{-3}	1.125×10^{-2}	does not fully detach	2.5×10^{-2}

If it is analyzed the time until the breaking of the Charpy specimen, it is observed that the breaking time increases from material H, PPm, G to PA6m, for which the breaking is not with the total detachment of specimen fragments ($t = 2.5 \times 10^{-2}$ s). In reality, the time of destruction of Charpy specimens is ranked in the same way as in simulations.

Figure 25 shows the evolution of the impactor velocity during the impact and the values of residual velocities are in the same order as the EPS values. For the material constitutive models introduced in the simulation, the lowest value of EPS produced the smallest reduction of the impactor velocity; as the residual velocity enters the formula of the energy absorbed by the test specimen, it results that the material with the highest EPS (PA6m) absorbed the greatest energy. The conclusion would be that the residual speed is proportional to the EPS value (Table 8).

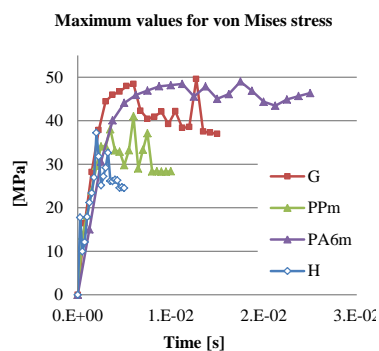


Fig. 23. Evolution of the maximum values of von Mises stress during the simulation, for each material

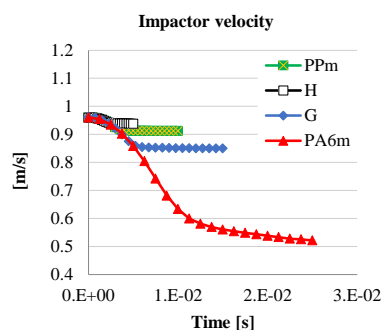


Fig. 24. Evolution of the impactor velocity during impact

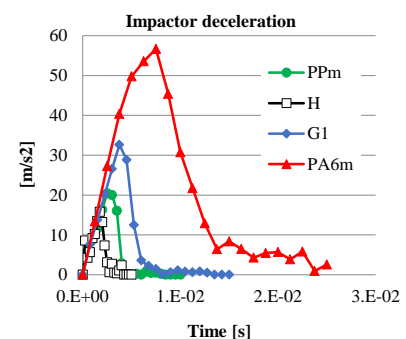
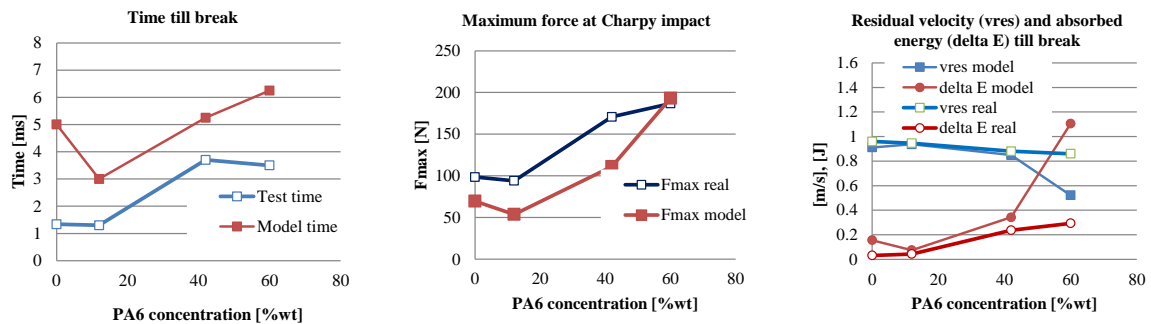


Fig. 25. Evolution of impactor acceleration during impact.

Small differences in energy at break and residual velocity were obtained between the model and actual material parameters for materials PPm, H and G (Fig. 26c). The best concordance for these two parameters was obtained for material H, followed by G and PPm.

Table 8. Impact characteristics

The parameter	PPm	H	G	PA6m
EPS	0.09	0.036	0.156	0.308
Maximum von Mises stress during impact [MPa]	41.1	37.2	48.4	48.9



a) time till break (first time F=0)

b) maximum force

c) Residual impactor velocity and absorbed energy at final moment (delta E - energy absorbed by the specimen on impact)

Fig. 26. Comparison between simulation and experimental data

The biggest difference between the model and the actual test, taking into account these parameters, was obtained for PA6m, the material with better Charpy impact characteristics. From this analysis, it results that the constitutive model of multilinear material introduced in the simulation of the Charpy test gave results closer to reality for the more fragile materials. For the most ductile material, with a high yield value, the model had a much higher impact energy absorption than the real one, which would mean that the introduction of the multilinear model obtained at a test rate of 1000 mm/min (0.016 m/s) from tensile tests, does not satisfactorily simulate the behavior of the specimen at impact with speed $v=0.96$ m/s. Works in the field [20] [24], [36] [47], highlighted that even in the field of low impact velocities (1...10 m/s), polymers are sensitive to the rate of stress and implicitly of deformation rate, usually in the sense of increasing the stress at break and decreasing the deformation at break.

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All authors have read and agreed to the published version of the manuscript.

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Conflicts of Interest: “The authors declare no conflict of interest.”

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