EXPERIMENTAL AND NUMERICAL STUDY OF THE INTERACTION OF NON-NEWTONIAN FLUID IN KETCHUP PACKAGING

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ABSTRACT

Fluid–structure interaction involving Newtonian and non-Newtonian fluids, such as water and solutions; multiphase mixtures, suspensions/emulsions, lubricants, paints/pigments, slurries, industrial polysaccharides, biological fluids; and food sauces; has a wide range of applications in several sectors. Since this kind of fluid does not obey the Newtonian relationship between the shear stress and shear rate, it is important to investigate the influence of the non-Newtonian effects in the design of structures under fluid–structure interaction loads.

Taking this into consideration, this research work aims to understand the influence of fluid dynamics of ketchup on a package. For this purpose, several experimental tests and simulations were performed, compared, and analyzed.

The first phase of this work consisted in studies of the container's geometry, thickness, and material properties, to better characterize it, for using this data in the simulation. The second phase was to analyze preliminary studies of numerical models, such as Co-Simulation fluid-structure, Smoothed Particle Hydrodynamics, and Coupled Eulerian-Lagrangian, to understand which model better qualifies for this research. The last phase corresponded to the tests and simulations with compression loads applied to empty ketchup containers and with fluids inside (i.e., ketchup and water).

From the obtained results, it was possible to verify that Smoothed Particle Hydrodynamics and Coupled Eulerian Lagrangian would be the better models, so these were selected to simulate the package at compression with fluids. The compression test results were as expected since the compression of the empty bottles had a greater deformation and the force was lower than the containers with the different fluids. This is due to the internal pressure generated by the fluids that oppose the deformation of the package since the compression equipment must apply higher force for the same displacement. In the numerical simulation, with the first study (structural simulation without the fluid), it was possible to validate the material model, as well meshes and the boundary conditions, such as velocity/displacement and interactions, because the obtained force/displacement curve was similar to the experimental one, just like the container behaviour. The curve force/displacement obtained with simulation with the fluids was fairly close to the experimental ones.

This research work shows that it is possible to have a good correlation between the experimental results and simulation with non-Newtonian fluids inside their packages, however, it is also possible to improve and optimize the main results of this work, by making, for example, some changes in the design and materials of the package. Thus, more research work will be developed to fill existing gaps.

1 INTRODUCTION

Fluid-structure interaction involving Newtonian and non-Newtonian fluids, such as water and solutions; multiphase mixtures, suspensions/emulsions, lubricants, paints/pigments, slurries, industrial polysaccharides, biological fluids; and food sauces; has a wide range of applications in several sectors. Since this kind of fluid does not obey the Newtonian relationship between the shear stress and shear

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rate, it is important to investigate the influence of the non-Newtonian effects in the design of structures under fluid-structure interaction loads [1, 2].

In recent years, several models have been developed and used to optimize the different packages of Non-Newtonian fluids due to performance goals. In general, fluid problems involve several challenges, such violent free-surface fluid flows, significant/abrupt hydrodynamic loads and considerable structural deformations. These challenges have more impact in case of deformable elastic structures, such as packages, so, accurate and efficient modelling of FSI problems is very important in product development engineering (e.g. fluid container). Numerical simulation is a potential method that could help to develop more efficient plastic packages for non-Newtonian fluids, however, due to the elaborated simulation process and computational costs, fluid-structure interaction is a complex problem in Engineering, with applications in several sectors requiring from the engineers a wide range of multidisciplinary knowledge to achieve a optimised design. However, it is necessary to point out that some critical problems remain in the design of these devices due to neglecting the fluid-structure interaction phenomena [3, 4].

Normally to simulate fluids numerically are used Smoothed Particle Hydrodynamics (SPH), and Coupled Eulerian-Lagrangian (CEL). SPH is gaining attention to be a robust method in the field of computational fluid dynamics being used to study several debris flow problems, on the other hand at a reasonable computational cost, CEL method can be used to evaluate large deformation behaviour while accurately capturing fluid-structure interactions [5, 6]. However, there are also research studies that use Co-Simulation models that combine fluid models with structural models, which can be simulated simultaneously and with an interaction between them [7, 8].

Taking this into consideration, this research work aims to understand the influence of the fluid dynamics of ketchup on a package and validate the numerical model that better represent this mechanical behaviour. So, several experimental tests and numerical simulations were performed, compared, and analysed.

2 METHODOLOGY

2.1 Materials

Commercial specimens of Guloso tomato ketchup package (bottle made with polyethylene terephthalate - PET, and lid made with Polyethylene - PE), Guloso tomato ketchup (Non-Newtonian), and water (Newtonian fluid) were used for this study. Table 1 displays the water and ketchup properties (ketchup properties at a shear rate of 50 mm/min. and 67,5 mm velocity and distance between walls respectively) and Figure 1 shows the packaging under study and its geometric properties.

Table 1: Fluid materials properties [9]

Materials	Density (kg/m^3)	Viscosity (Pa.s)	Propagation of sound (m/s)
Water	1000	0,01	1483,00
Ketchup	1190	10000	1526,40

2.2 Methods

The first phase of this work consisted of studies of the container's geometry, thickness, and material properties, to better characterise it, for using this data in the numerical simulation. The second phase was to analyse preliminary studies of numerical models, using the commercial software Abaqus, such as, Smoothed Particle Hydrodynamics, and Coupled Eulerian-Lagrangian, to understand which model better qualifies for this research [10, 11, 12] The last phase corresponded to the experimental tests and numerical simulations with compression loads applied to empty ketchup containers and with fluids inside (i.e., ketchup and water).

2.2.1 Geometry study

The geometry study consists of evaluating the container under study, firstly it was necessary obtaining all the main dimensions (Figure 1) to create the CAD using the commercial software SolidWorks.

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Following it was studying the thickness of the packaging. The thickness variation it was measured of three packages was measured using a tip micrometer evaluating the four study areas (Figure 2).

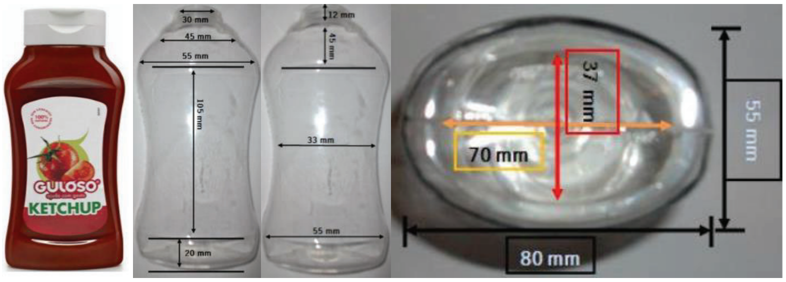

Figure 1: Guloso tomato ketchup bottles and dimensions

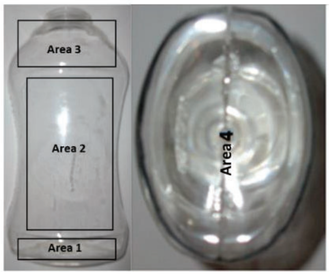

Figure 2: Representation of the packages thickness study zones

2.2.2 Experimental Tests

2.2.2.1 Material Characterization

From the ketchup package, several samples from different zones were characterised to evaluate physical, and mechanical properties using several techniques (Figure 3). To obtain a good numerical approximation to the experimental study research case. The density of the ten PET samples (25x10mm) was calculated using Method A of ASTM D 792.

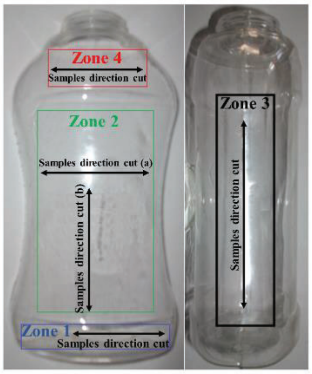

Figure 3: Representation of the study zones and direction of the tensile samples

To determine the tensile properties, the specimens were characterised based on ISO 527-2. A universal testing machine (Shimadzu AGX-50kN) with pneumatic clamps and a 1 kN load cell was used. The five samples (ISO 527-2 sample type - 5A) for each zone (Figure 3) were tested under tensile mode at a speed of 1 mm/min for the Young Modulus, and 50 mm/min for the Yield Stress (Figure 4). All experiments were carried out at room temperature (≈23 °C) and 50% HR.

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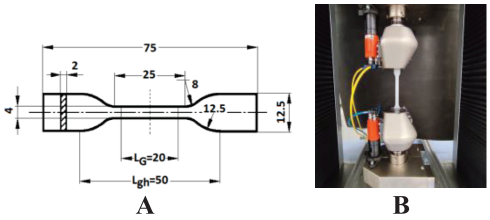

Figure 4: Material experimental characterization. A – ISO 527-2 sample type for cutting (dimension in mm). B – sample in Shimadzu testing machine

2.2.2.2 Package Tests

To determine the compressive properties of the package, the specimens were characterised based on ASTM D 695. A universal testing machine (Shimadzu AGX-50kN) with circular plates and a 50 kN load cell were used. The five samples per each condition (i.e. empty, with ketchup, and with water) were tested under compressive mode at a speed of 50 mm/min and with a maximum displacement of 33.5mm (20% of the total height of the package). All experiments were carried out at room temperature (≈23 °C) and at 50% HR. To make it easier to compare the results between experimental tests and numerical simulation, a GoPro 4 camera was used.

2.2.3 Numerical Simulations

Firstly, a generic cylindrical object was created to verify the results correlation of the different numerical methods (CEL, SPH, and Co-Simulation) for the fluid-structure interaction problem calculation for the compression test. However, the Co-Simulation method presented a low precision for this study case, in consequence, this method was not used in package simulation.
For the structural simulation, the model preparation follows the scheme represented in Figure 5. The structural simulation aims to evaluate and validate the numerical model of the package, mesh, and boundary condition of the compression test.

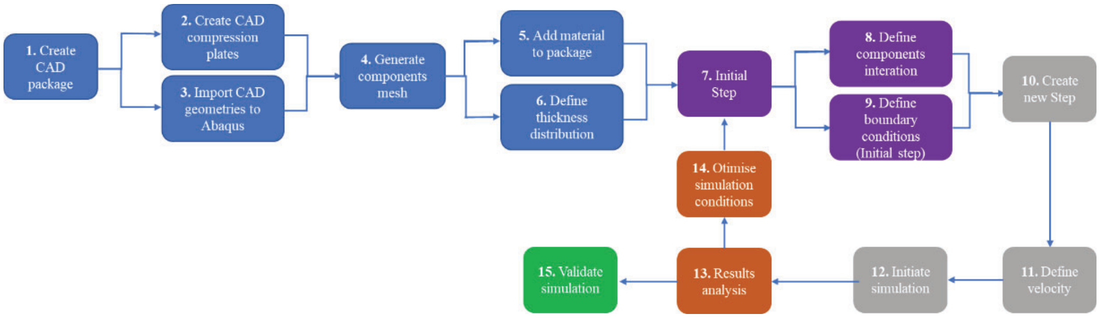

Figure 5: Structural simulation model preparation

Table 2: Boundary conditions and mesh conditions for structural simulation

Mesh		Boundary Conditions
Type	S4R	• Contact condition between plates and package and package itself;
Element see	1,5	• Encastre lower plate. And apply velocity of 0,0008 m/s to higher plate.
Number of elements	11918	

2.2.3.1 Coupled Eulerian-Lagrangian

The CEL model couples two calculation methods, the Lagrangian method with the Eulerian method. The Langrangian method is used in numerical simulation to solve fully structural problems, that is, it is the calculation method used for calculating components with a Lagrangian mesh. The Eulerian method is most used in numerical simulation to solve problems with fluids, as fluids normally have a higher mesh distortion than structures, that is, fluids deform more easily, and the Langrangian mesh cannot follow these deformations, while the Eulerian mesh gives a good answer to this problem [13, 14, 15].

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For the CEL simulation, the model preparation follows the scheme represented in Figure 6.

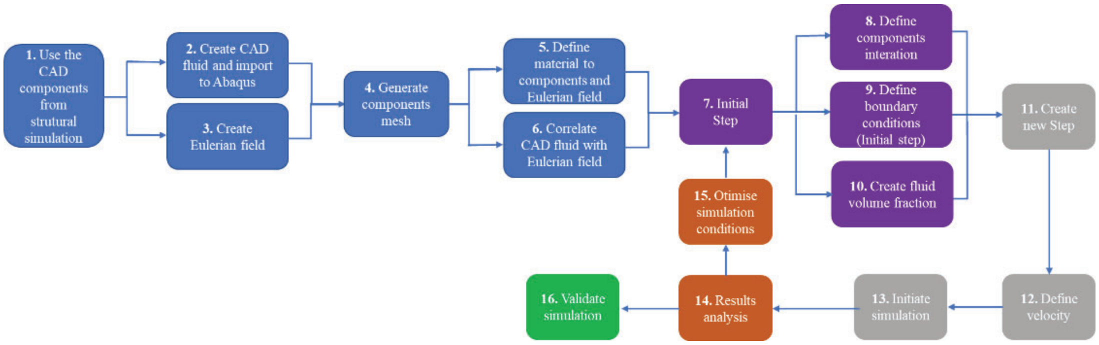

Figure 6: CEL simulation model preparation

Table 3: Boundary conditions and mesh conditions for CEL simulation (keeping the structural boundary and mesh conditions)

Mesh		Boundary Conditions
Type	EC3D8R	• Contact condition between fluid and package (internal part);
Element see	3,5	• Define the volume fraction of Eulerian field
Number of elements	8316	

2.2.3.2 Smoothed Particle Hydrodynamics

The SPH model is a simulation model in which the mesh of a component under study is converted into particles, normally more used for fluids, as these are subject to greater mesh distortion, but this model can also be used in problem analysis with solids that, when subjected to some type of load, become completely fragmented, such as the impact of hail (where the water is in a solid state in the shape of a ball) [16, 17, 18]. Therefore, the mesh, when converted into particles, allows it to have greater deformation.

For the SPH simulation, the model preparation follows the scheme represented in Figure 7.

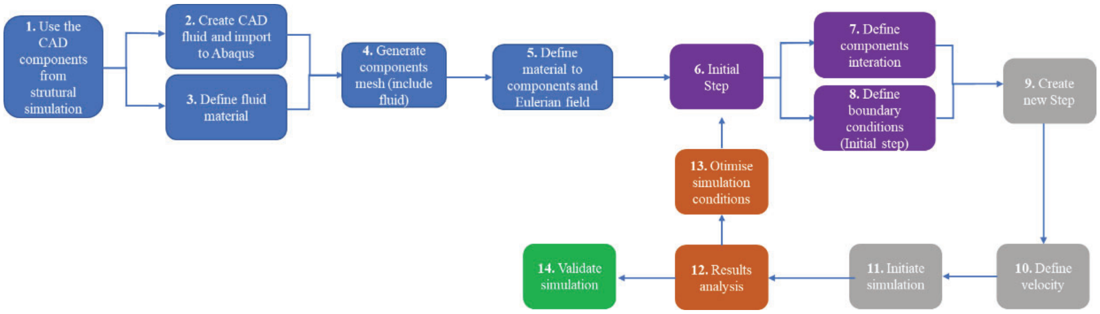

Figure 7: SPH simulation model preparation

Table 4: Boundary conditions and mesh conditions for SPH simulation (keeping the structural boundary and mesh conditions)

Mesh Fluid		Boundary Conditions
Type	C3D4	• Contact condition between fluid and package (internal part);
Element see	5	• Convert all the nodes mesh into particles.
Number of elements	16254	

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3 RESULTS

3.1 Experimental Tests

3.1.1 Geometry study and Material characterization

The geometry thickness study and data test results of the material corresponding to material density and tensile properties are summarised in Table 5. The presented values represent the average results and correspondent standard deviations.

Table 5: Results of geometry study and material properties

Properties			
Density (kg/m^3)	2120 ± 10,00		
Thickness (mm)		Young Modulus (MPa)	at 1 mm/min.
Area 1	0,33 ± 0,08	Zone 1	1053,10 ± 134,74
Area 2	0,32 ± 0,11	Zone 2a	1051,29 ± 137,61
Area 3	0,25 ± 0,01	Zone 2b	1567,46 ± 112,61
Area 4	0,53 ± 0,04	Zone 3	1794,12 ± 191,93
		Zone 4	1235,47 ± 154,68
Yield Stress (MPa)	at 50 mm/min.	Roture Stress (MPa)	at 50 mm/min.
Zone 1	51,85 ± 7,50	Zone 1	47,79 ± 5,61
Zone 2a	42,37 ± 6,23	Zone 2a	44,58 ± 9,66
Zone 2b	65,87 ± 4,63	Zone 2b	63,44 ± 15,38
Zone 3	61,12 ± 7,02	Zone 3	89,58 ± 12,85
Zone 4	43,01 ± 4,31	Zone 4	39,91 ± 3,44
Yield Strain (%)	at 50 mm/min.	Roture Strain (%)	at 50 mm/min.
Zone 1	5,92 ± 0,57	Zone 1	122,00 ± 65,63
Zone 2a	6,47 ± 0,23	Zone 2a	159,35 ± 55,95
Zone 2b	6,00 ± 0,43	Zone 2b	109,94 ± 44,82
Zone 3	6,28 ± 0,49	Zone 3	111,60 ± 45,23
Zone 4	7,23 ± 0,84	Zone 4	115,40 ± 15,54

3.1.2 Package Tests

Data test results of the package corresponding to the compression test are presented in Figure 8 and Figure 9. The Table 6 presented the values represent the average results and correspondent standard deviations.

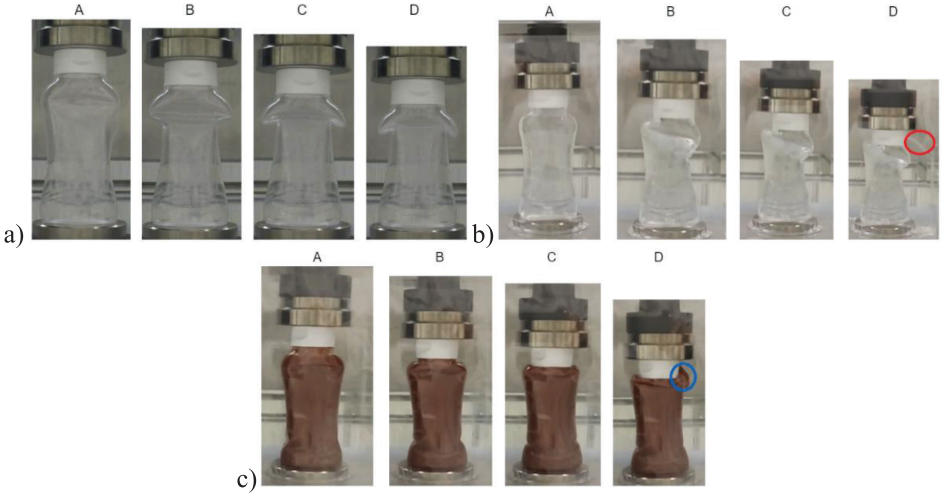

Figure 8: Evolution of the compression test with a) empty package. b) package with water and c) package with ketchup

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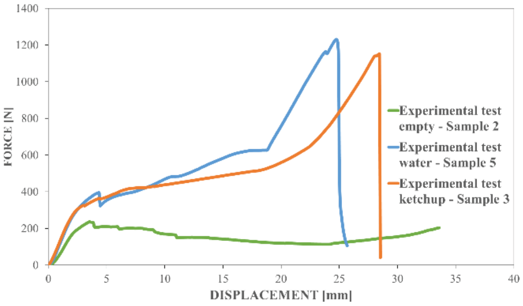

Figure 9: Experimental results representative curve of one the package sample. Package empty and filled with fluid (water and ketchup)

Table 6: Experimental results of the package empty and filled with fluid (water and ketchup)

Package	Displacement (mm)	Max. Force (N)
Empty	4,19 ± 0,67	248,49 ± 9,35
With Water	22,92 ± 7,66	983,69 ± 290,99
With Ketchup	26,06 ± 1,50	1075,68 ± 110,61

3.2 Numerical Simulation

3.2.1 Coupled Eulerian-Lagrangian

The CEL results of the numerical simulation of the package with water and ketchup corresponding to the compression test are presented Figure 10, Figure 11 and Table 7.

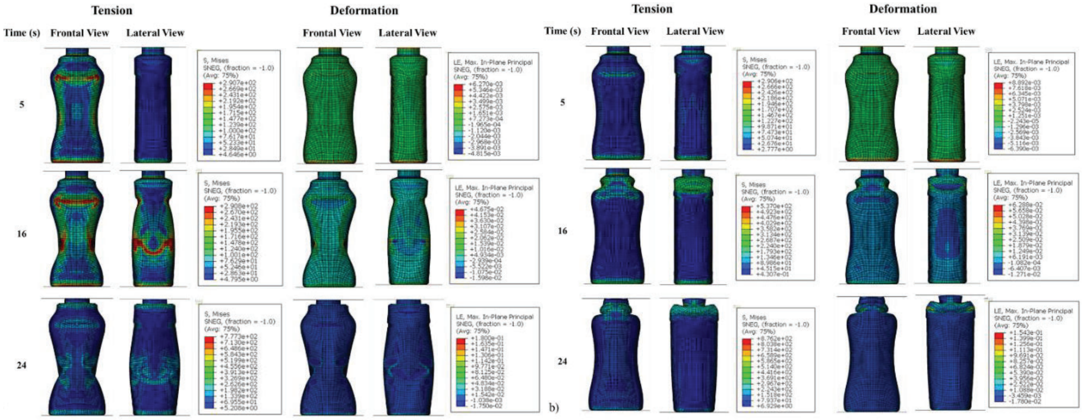

Figure 10: Tension and deformation results of CEL simulation over time: a) Package with water and b) with ketchup

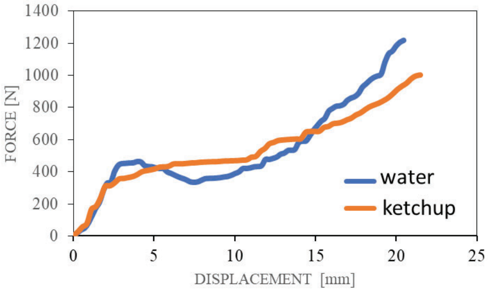

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Figure 11: Representative curves for package filled with water and ketchup of CEL model simulation

Table 7: CEL simulation - Compressive properties of the packages

Package	Displacement (mm)	Max. Force(N)
With Water	20,45	1217,66
With Ketchup	21,50	1003,25

3.2.2 Smoothed Particle Hydrodynamics

The SPH results of the numerical simulation of the package with water and ketchup corresponding to the compression test are presented Figure 12, Figure 13 and Table 8.

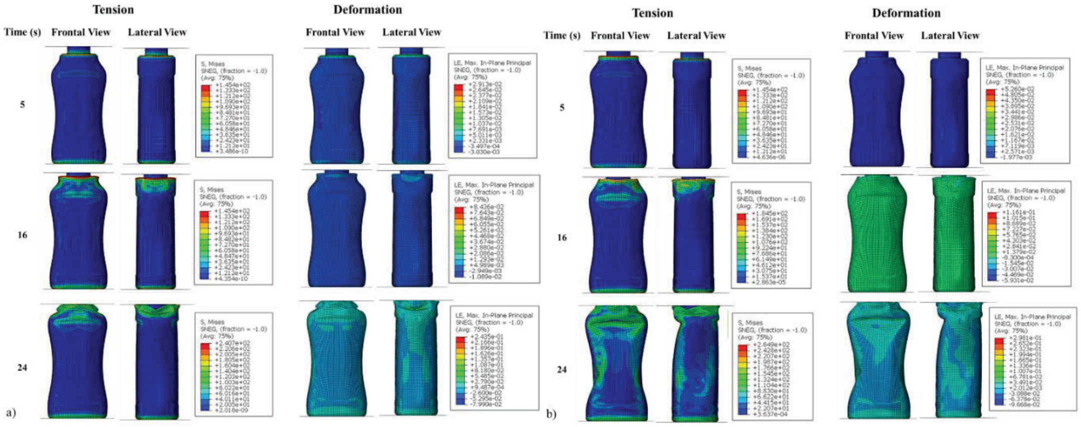

Figure 12: Tension and deformation results of SPH simulation over time: a) Package with water and b) with ketchup

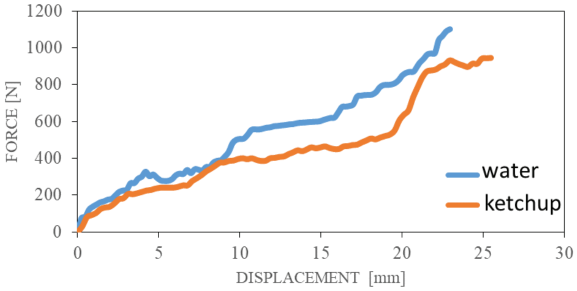

Figure 13: Representative curves for package filled with water and ketchup of SPH model simulation

Table 8: SPH simulation - Compressive properties of the packages

Package	Displacement (mm)	Max. Force (N)
With Water	22,92	1100,75
With Ketchup	25,44	944,42

4 DISCUSSION

It was verified that the variation in thickness in each zone of the ketchup package was not significant, having generally an uniform thickness, therefore, in the numerical simulation only the average value of the thickness of each area was considered. The tensile properties of the lower part of the package is similar to the value obtained from the horizontal centre of the package, this is due to these areas of the specimens having been removed horizontally. In the upper package area, the specimens were also removed horizontally, however there is a certain difference between these results and the previous ones, as in this area the specimens contained a curvature, which led to a different modulus. In the lateral areas and vertical centre of the package, the specimens were removed vertically, and therefore it was possible to verify a greater difference between these results and the specimens that were taken horizontally. There is also a variation in Young's modulus values on the diverse study zones, this was due to the fact that the specimens taken in some study areas had a slightly different geometry, as they contained curvature. It is possible to verify the results have a greater rupture deformation, that means, in the experimental compressive test the empty package should have a higher deformation before have a total rupture. However, with the package filled of fluid, the fluid inside must generate internal pressure which could lead to higher deformation of the material.

On the compression tests made with the empty packages it was possible to verify that the mechanical response of the packages tries to counteract the movement that is imposed. At point A (Figure 8 a)) the package begins to deform for the first time and therefore its geometry starts changing. From point C (Figure 8 a)) the package becomes more stable again, so the force necessary to make the upper plate move increases until the end of the test, represented by point D (Figure 8 a)). Similar to the experimental test with empty packages, it is possible to verify that the samples with water the force increases with the increase in the displacement of the upper plate up to point A (Figure 8 b)), where the package starts to deform, and from that moment on there is a drop in the force generated, however, there is an immediate stability of the force that is maintained until point B (Figure 8 b)), this happens because the reaction forces of the package are compensated by the forces of reaction that the water also makes to try to counteract the movement of the plate. Then, as in previous tests, the force increases again, as the package becomes stable again and its reaction forces intensify again and therefore the force generated by the machine increases to a maximum represented by point D (Figure 8 b)), where in this moment there are leakages from the packages. From the experimental results it was observed that the force generated by the machine is greater than the force generated in an empty package, this is due to the fact that water is an incompressible material and as such, it increases resistance of the system to compression solicitations. As in previous tests, in this with packages with ketchup, it was also possible to verify that in the evolution of the force/displacement curve presented initially there is an increase in force with the increase in displacement up to point A (Figure 8 c)). This break is due to the moment the packages begin to deform, but just like in tests with the packages with water, it stabilises immediately due to the reaction forces exerted by the ketchup. The force from point B (Figure 8 c)) becomes more pronounced, as the packages are stable and the reaction forces of the packages and fluid act with greater intensity, increasing the force generated by the equipment up to the maximum point C (Figure 8 c)). Finally, an abrupt drop in strength occurred, due to the release of air from inside the packages, but in this case the ketchup was not immediately at that moment, as the viscosity of the ketchup is substantially higher than that of water, which causes it to flow more slowly. Just like the tests with water, in these the tests with ketchup, the leakages occurred through the crack in the lid or if it burst.

From the CEL numerical model simulations with water and ketchup, it was possible to verify that the behaviour of the force/displacement is similar (Figure 11), observing that in the package with water the maximum force is higher in relation to the package with ketchup. It was also found that the increase in force is more pronounced in the case with water than in the one with ketchup, as the viscosity of water is significantly lower than that of ketchup, which leads to a faster response to counteract the movement imposed in relation to ketchup, which due to the superior viscosity value, the response to counteract the movement is slower, which means that the increase in force is not as pronounced as in the case with water. From the SPH numerical model with water and ketchup, it was possible to verify that the behaviour of the force/displacement is similar (Figure 13), and it was also possible to observe that in the package with water the maximum force is higher in relation to the case with ketchup. In comparison to the evolution of the curve, there is no more pronounced increase in the case with water than in the ketchup case. By comparing the numerical models SPH and CEL, it was possible to verify they have a good correlation with the experimental tests, as can be verify in Figure 14 and Figure 15. Regarding the displacement of the experimental tests it is equal and +2% higher with the one obtained with SPH

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method, for the water and ketchup respectively, and +11% and 17% higher than the CEL method, for the water and ketchup respectively, meanwhile, the forces in the experimental tests are -12% lower and 12% higher than the SPH method, for the water and ketchup respectively, and -24% lower and +7% higher than the CEL method, for the water and ketchup respectively. From the obtained results, it was possible to verify that Smoothed Particle Hydrodynamics and Coupled Eulerian-Lagrangian were the better models, so these were selected to simulate the package at compression with fluids. Based on the Figure 14 and Figure 15, the Coupled Eulerian-Lagrangian model match the initial stage of the mechanical behaviour, due the characteristic of fluid modelling that was considering a solid volume, therefor, the mechanical response of internal pressure occur simultaneous with the experimental test, however due this characteristic and since the fluids were considered an incompressible material, during the compression simulation, the mechanical response occur earlier when compared with the experimental test.

In the case of the Smoothed Particle Hydrodynamics, in initial stage that behaviour occurs later than experimental test, because the proporties of fluid modelling that has considered a particle volume and the particles have spaces between them, that leads to a delay to generate internal pressure. However due to this characteristic and since the fluids were considered an incompressible material, during the compression simulation, this model has a similar mechanical behaviour when compared to the experimental test.

The compression test results were as expected since the compression of the empty bottles had a greater deformation and the force was lower than the containers with the different fluids. This is due to the internal pressure generated by the fluids that oppose the deformation of the package since the compression equipment must apply higher force for the same displacement. In the numerical simulation, with the first study (structural simulation without the fluid), it was possible to validate the material model, as well as meshes and the boundary conditions, such as velocity/displacement and interactions, because the obtained force/displacement curve was similar to the experimental one, just like the container behaviour. The curve force/displacement obtained with simulation with the fluids was fairly close to the experimental ones.

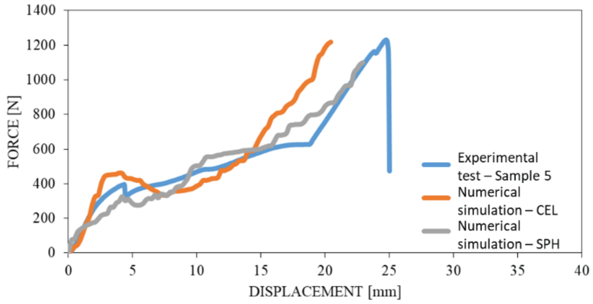

Figure 14: Experimental and Numerical results curves for package filled with water

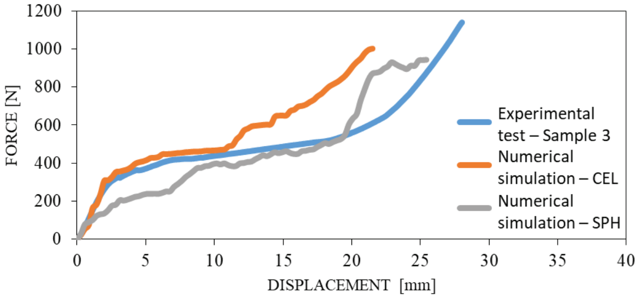

Figure 15: Experimental and Numerical results curves for package filled with ketchup

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5 CONCLUSIONS

In the search to understand the influence of the fluid dynamics of a ketchup on a package, tests, numerical simulations and analyses were performed.
The following conclusions can be drawn from the investigation:
•Through the results obtained numerically and experimentally that the reaction force generated by packages with water inside them was greater than the force of packages with ketchup, due to the lower viscosity of the water and the for the water as be a incompressible fluid when compared with the ketchup that as a compressible fluid and had a higher viscosity, which allows a faster response to the imposed load, and therefore the effort exerted by the equipment has to be greater for the same displacement.
•The behaviour of the packages when subjected to compression, the experimental results are closer to the simulation results in the case of the water.
• The results showed that the overall mechanical response of the package is similar to the numerical simulations made by SPH and CEL methods.
• The obtained maximum values from SPH method are closer to those obtained experimentally.
• The obtained force/displacement curves from CEL method are closer to those obtained experimentally.
So, this research work shows that it is possible to have a good correlation between the experimental results and simulation with non-Newtonian fluids inside their packages. However, the main results of this work can be further improved and optimised, considering the possibility of fluid leakage from the package, something that will impact the internal pressure.

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