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Research paper

Geometric optimization and thickness reduction of metal packaging for the transportation of dangerous goods: A new design paradigm

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ABSTRACT

Reducing raw material consumption in packaging manufacturing offers a range of undeniable advantages. First, packaging becomes more competitive, enabling lower sales prices. Transportation becomes easier due to reduced weight, while simultaneously mitigating environmental impact. Therefore, reducing the thickness of tinplate packaging becomes an attractive project for packaging companies. UN packaging, certified for the transport of dangerous goods, is subject to rigorous approval tests to ensure environmental and social safety during transportation. Optimizing the geometry of the packaging and its closure system is imperative. Therefore, the main goal of this work is to optimize packaging designed for the transport of dangerous goods, particularly paints, in accordance with ADR 2019, because there is a real gap in studies addressing this specific problem, generating extra motivation to develop this work. Through the execution of experimental tests, the current condition of the packaging was characterized, thereby facilitating the identification of its critical failure points. The proposed improvement solutions were based on quality tools, namely the Ishikawa Diagram. Additionally, benchmarking was conducted, and to complement the quality approach, numerical analysis using ABAQUS CAE® software was employed. Validation of the study was completed with the manufacture of prototypes incorporating different solutions for the packaging's flange and top. The tests demonstrated a significant improvement in strength and ease of opening for the end customer. The synergistic combination of these optimized solutions resulted in an overall improvement and the validation of more sustainable and robust packaging.

1. Introduction

Nowadays, packaging is ubiquitous in everyday life [1]. Although end consumers rarely recognize the multifunctionality and importance of packaging, its efficient use is crucial to the logistics of delivering essential goods from producer to market. The absence of packaging would hinder the ready availability of many products. Furthermore, packaging plays a crucial role in preventing spoilage, contributing to increased product shelf life and, consequently, reducing waste [2].

In terms of market volume, food and beverage packaging generates the largest turnover [3]. Industrial packaging ranks second. This specialized packaging offers different thicknesses, greater strength, and product protection, allowing products to be stored with a lower risk of hazardous material spillage and prevents external contamination [4]. The global industrial packaging market was valued at $56.3 billion in 2019, and experts project that it will reach $114.8 billion by 2034 [5]. It is a market that continues to grow, driven by increased construction activity and population growth in emerging countries such as China and India. In third place is the pharmaceutical packaging market, which experienced the highest growth, 4 %, due to the increase in the elderly population and chronic diseases [6].

Packaging is a coordinated system for preparing products for transportation, protection, storage, retail, and end use. Its goal is to minimize shipping costs and maximize sales [7]. In addition to the aforementioned, packaging has significant communication power and is a powerful marketing tool. The first impression of a product is conveyed to

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the customer through its shape, color, and quality, among other factors. Often, the purchasing decision of one product over another is determined by its packaging [8]. Packaging is crucial in attracting customers and will influence their multisensory experience during the decision-making process. Packaging capacity also affects the quantity of product consumed: the larger the packaging, the greater the consumer's consumption [9].

The success of a package is directly linked to the experience it provides the end consumer during its use. The material chosen for the packaging design and its closure system are among the most important factors in providing good user experience [10].

The manufacture of metal packaging primarily uses two distinct materials: aluminum and tinplate [11–14]. In addition to offering advantages such as high mechanical strength and corrosion resistance, these materials stand out for their sustainable nature, due to their inherent and complete recyclability [15].

Tinplate is one of the first materials used in packaging manufacturing, and it is 100 % recyclable [11–14]. It is a material with good weldability and high corrosion resistance, also having properties that aid in stamping [12]. These factors make it a very attractive material. It is worth noting that, compared to aluminum, it is a more economical material [16]. Over the past few years, the tinplate packaging segment has experienced growth, driven by increased consumption of packaged foods in developing countries, coupled with rising disposable incomes [17].

Tinplate production is strictly regulated by the European Committee for Standardization (EN 10,202, 2001) [18]. This standard specifies the permissible thicknesses, with their respective tolerances, as well as the hardness requirements and tensile properties for the different sheets. Tinplate is composed of rolled low-carbon steel, with thicknesses typically ranging from 0.13 mm to 0.49 mm. For material that undergoes single reduction (a single rolling operation), the range of thickness is between 0.17 mm and 0.49 mm, with increments of 0.005 mm. However, achieving thinner thickness requires the raw material to be double-reduced (subjected to two rolling operations). Through this double reduction process, tinplate can reach smaller thicknesses, ranging from 0.13 mm to 0.29 mm, while also maintaining increments of 0.005 mm. In addition to thickness, other properties such as hardness and yield and ultimate strength are critical specifications that directly influence the subsequent forming and transformation process of the material and are therefore essential parameters to be considered.

Fernandes et al. [14], evaluated new coatings for the stamping tool of a tinplate food packaging, increasing the tool's service life and reducing maintenance interventions. The authors studied the transfer of tin from tinplate to the tool during the stamping of tinplate food packaging. A new coating for the tool, TiAlN deposited by a PVD process, was proposed. This coating showed better wear resistance than others previously tested under the same operating conditions Pepelnjak & Barisic [19], studied the stamping of rings for tinplate packaging. During stamping, the TS415 sheet undergoes significant plastic deformation, resulting in a high number of nonconforming parts. The manufacturing process was studied using a finite element tool, ABAQUS CAE®, which enabled the definition of a geometric optimization of the rings. Wang et al. [20], developed an electrochemical sensor that assesses the service life of metal packaging. Experiments reveal that their results closely approximate reality, compared with rapid aging tests. Fernandes et al. [13], also investigated the possibility of removing lubrication from the stamping of tinplate food packaging. Two possible coatings for the stamping tool, CrCN and WC, were studied. Both coatings showed good tribological behavior, with CrCN having a lower coefficient of friction.

Another important aspect of packaging design is the closure system [21]. Although, from a functional perspective, the closure is the sealing method that ensures proper storage and protection of the product. Technically, it is defined as the device that encloses the product within the packaging, while still allowing easy access to it when removed [22].

In this context of closures and sealing, the crimping process stands out for its longevity [23]. Although this technique is considered traditional, with limited technological evolution over the years, crimping continues to be widely used in metal packaging assembly lines [24]. Currently, growing industrial demand drives the need for more robust crimping to ensure packaging performance and integrity. The most widespread method for joining components in three-piece containers is double crimping [10].

New product development (NPD) is a strategic step for companies to succeed and survive in a highly competitive market [25]. New product development has a very low success rate, with only 10 % to 25 % of launched products remaining on the market one year after their launch [26]. Optimizing existing products is a crucial step in the post-launch development cycle. Once a product is on the market, continuous improvement of its performance is essential to maximize consumer acceptability [27]. The success of this reformulation depends fundamentally on customer orientation, requiring the precise identification of their essential needs, critical value features, and willingness to pay. Concurrently, it is imperative to identify and eliminate non-essential features to reduce complexity and increase product competitiveness [28].

Numerical simulation tools are frequently used to solve problems involving products exposed to internal pressure, and studies have been conducted on the behavior of this material under different stresses [29]. In studies involving high deformations, the mesh must adapt to the model. Therefore, areas with greater deformation require finer meshes. Studies on thin-walled containers, all of which experience high deformations, require a mesh that adapts to the different zones in the simulations used. Lombarkia and Barkat [30], numerically studied the behavior of a cylindrical package under internal pressure using ABAQUS® software. The package consisted of tinplate (TS 475) with a thickness of 0.2 mm and was subjected to a pressure of 0.6 MPa. After simulation, optimal values for the package's closure geometry were found. Zhu et al. [31] studied the influence of external pressure on an AISI 304 stainless steel container used for deep-sea diving. The study was conducted to understand why the container undergoes plastic deformations earlier than expected and, once the cause has been discovered, to find a geometric solution to this problem. They concluded that increasing the height-to-radius ratio reduces deformations. They also concluded that variations in container thickness led to greater deformations. In turn, Li et al. [32], studied the behavior of internally pressured containers with elliptical tops. These containers have a low thickness compared to their other dimensions, making them susceptible to high deformations at their joints. They concluded that, with this geometry, deformations are local, progressive, and self-limiting. Ahmed [33], concluded that in finite element simulations of metal sheets, the thicker the sheet, the more efficient the study. Thus, it can be concluded that studies on tinplate will have lower efficiency in FEM studies compared to other thicker sheets.

The challenge of reducing material thickness without compromising structural integrity is a transversal theme in packaging engineering. Recent studies on corrugated cardboard have demonstrated that optimized geometry and periodic core structures can significantly enhance mechanical strength and energy absorption [34,35]. These findings in paper-based materials mirror the fundamental principle applied in this study for metal packaging: by strategically engineering the container's geometry, it is possible to compensate for reduced wall thickness. This approach shifts the design focus from material mass to geometric stiffness, a trend observed in contemporary research across multiple material classes [36,37].

The challenge of balancing structural integrity with material reduction is not unique to the chemical packaging industry. Modern engineering has increasingly adopted Ecodesign principles to address the environmental footprint of packaging across various sectors, from food logistics to consumer electronics. As highlighted by Landi et al. [38] the transition toward a circular economy requires a fundamental shift in how material efficiency is integrated into the early design stages.

Research in other sectors has explored the use of bio-based materials and modular architectures to reduce waste; however, for heavy-duty metal packaging, the primary pathway for sustainability remains dematerialization through topological optimization. By analyzing the intersections of these cross-sectoral trends, this study positions the proposed design paradigm as a scalable solution for industrial resource efficiency.

Therefore, the main objective of this work is to optimize packaging designed for the transport of hazardous materials, particularly paints, in accordance with ADR 2019 [39], which imposes specific conditions to prevent the spillage of hazardous materials in the event of an accident. To optimize this product, it was necessary to study and improve its closure system. To achieve this final objective, it was necessary to evaluate the packaging in its initial state, determining which components/areas impacted its performance. It was in these areas that potential actions to improve the packaging were studied. The project was divided into three phases: planning, development, and implementation. Each phase involves a set of actions. First, the current state of the packaging and its performance in the tests required for the transport of dangerous goods was defined. In addition, a fishbone diagram (Ishikawa) was created. At this stage, an effort-impact matrix was used to decide on the areas where improvements could be made. These areas are those where the greatest improvement can be achieved with the least effort. To complement the packaging study, a benchmark analysis was also carried out to compare packaging specifications and geometries. The changes to be implemented in the product were also defined, and prototypes with the different changes were created. Finally, the solutions presented were validated.

The 'new design paradigm' introduced in this work challenges the conventional industrial reliance on material thickness as the primary factor for packaging integrity. It proposes a transition towards topological engineering, where the mechanical performance of thin-walled metal containers is governed by strategic geometric reinforcements. This approach moves beyond incremental product optimization by establishing a systematic methodology that treats geometry as a primary variable to compensate for reduced material volume.

2. Materials and methods

2.1. Materials

2.1.1. Study packaging

This work focuses on frustoconical metal packaging (TC), with an upper inner diameter of 286 mm and 450 mm height. This product is part of the General Line under the following designation: TC 286xh P UN. The TC 286 P UN consists of three components: the top, the bottom, and the body. The bottom is connected to the body by a triple crimp. The lid contains a seal that, once closed, ensures the packaging's watertightness. The top and bottom are designed to allow for stacking of closed packages. Similarly, the body of the packaging is expanded during the manufacturing process to allow for the stacking of empty buckets.

The packaging closure system uses claws. This closure consists of the top, the seal, and the end of the rolled body, which is dominated by a flange. In addition to these components, there are claws, which help secure the top and close the packaging. The top panel also influences the closure, being included as one of its components. The maximum capacity is set at 25 liters and the minimum at 10 liters. TC 286 P UN is intended to be certified for the transport of the following classes of hazardous materials, according to RID (Regulations concerning the International Carriage of Dangerous Goods by Rail)/ADR (European Agreement concerning the International Carriage of Dangerous Goods by Road):

The packaging under study belongs to group II and III of packaging, being suitable for the transport of medium and low hazard material.

2.2. Methodology

2.2.1. Packaging design and manufacturing process

The manufacturing of the UN-certified metal packaging involves a sequence of thermo-mechanical operations that define its final structural integrity. The process initiates with the preparation of tinplate sheets (primary and secondary cutting), followed by surface treatment (lithography and varnishing). The structural components are formed through high-speed stamping (lids and bottoms) and electric resistance welding to form the conical body. Key geometric features, such as the ferrule, flange, and channel, are shaped through mechanical expansion and forming operations. These stages are critical to the study as they induce plastic deformation and residual stresses, which must be accounted for in the subsequent geometric optimization and FEM analysis.

2.2.2. Problem identification

The market is becoming increasingly competitive and demanding. Therefore, the biggest challenge for companies is to ensure their products are increasingly competitive. This competitiveness requires companies to produce increasingly cost-effectively. Because the company under study produces certified packaging, cost reductions cannot affect the robustness of its products. On the other hand, there is a need to increase certifications to keep up with market demands. The objective of this work, which focuses on just one of the company's products, lies in balancing these two requirements. It was determined that the packaging targeted for this project will have a certain reduction in thickness (Table 1). This reduction in thickness will affect the robustness of the packaging, which must be optimized to pass the certification tests.

Another factor to consider is the packaging closure. The company that produces the packaging is not the same as the one that fills and seals it. Hazardous materials filling lines are affected by process variability, and production is not always sensitive to what constitutes a proper packaging closure. Therefore, the packaging closure must be robust enough to absorb this customer variability.

2.3. Methodology for solving the problem

To solve the problem, the characteristics of this new packaging were initially studied to understand its behavior with changes in thickness. Identifying the different factors that influence packaging performance is necessary to determine the areas that require intervention. To this end, an Ishikawa diagram was created. Once this was achieved, an effort-impact matrix was used to determine the potential areas for improvement. These areas are those where the greatest improvement can be achieved with the least effort. To complement the packaging study, a competitor analysis (benchmark) was also conducted to compare packaging specifications and geometries. The different geometries and characteristics were studied in the order presented in the impact matrix. New product concepts were also developed at this stage, and studies were conducted to outline the best bucket design.

2.4. Study of the characteristics of tinplate

Tinplate has its properties in the rolling direction described in EN 10,202:2002 [18]. However, for finite element analysis, other values are required in addition to those provided by the standard, such as the

Table 1
Reduction in thickness of the project's target packaging.

	TC 286 P UN Current	TC 286 P UN Future	% de Reduction
Body [mm]	0.38	0.34	- 12.8 %
Top [mm]	0.48	0.43	- 10.4 %
Bottom [mm]	0.39	0.34	- 10.5 %
Weight [g]	1765	1601	- 9.03 %

modulus of elasticity and the sheet's behavior during plastic deformation. Therefore, it is crucial to know under what conditions the tinplate is most weakened to simulate a scenario where failure is most likely. To this end, tensile tests were performed in the following directions:

- Direction 1 – in the rolling direction;
- Direction 2 – perpendicular to the rolling direction;
- Direction 3 – at 45° to the rolling direction.

Tensile tests in the rolling direction were performed according to EN 10,202:2001 [18], with the geometry of the specimens being defined according to ISO 6892–1:2009 [40]. To design the specimens, a 0.38 mm thick sheet was used, from which six specimens were cut in each direction. The specimens were prepared by a tinplate supplier. The remaining directions are not specified, so specimens were cut from the same location on the sheet, but in different directions relative to the rolling direction. The test method used was the same for all directions.

In the rolling direction, values were obtained within the specifications of the tinplate standard. The properties of tinplate in the direction perpendicular to the rolling are not standardized, so there is no data for comparison. The results obtained regarding the modulus of elasticity are lower than those obtained in the rolling direction, with the lowest value being 8.3 GPa. Properties at 45 degrees to the rolling direction are also not defined by the standard. In this direction, higher average values can be found for yield strength, ultimate strength, and Young’s modulus.

2.4.1. *Characterization of the closing process*

The sealing of the metal claw packaging is achieved through a controlled plastic deformation process. An automated or manual clamping tool exerts a vertical load to stabilize the lid, while a radial actuation mechanism (comprising 18 pivoting fingers) folds the lid claws under the bucket rim. This mechanical interlocking ensures the structural hermeticity required for UN certification. The kinematic consistency of this closure process is a critical boundary condition for the structural models, as it defines the initial stress state of the lid-body interface. The closed package appears as shown in Fig. 1.

A critical design constraint for this optimization is the maintenance of compatibility with existing closure infrastructure. The sealing tools currently deployed in filling lines are standardized to accommodate universal claw-type geometries. Consequently, modifying the closure mechanism would necessitate a complete overhaul of the downstream equipment, incurring prohibitive costs and logistical barriers to interoperability. To ensure the industrial viability of the proposed geometric optimization, the interface between the lid and the closing tool remained a fixed parameter, focusing the redesign efforts strictly on the container's body geometry and material thickness reduction.

2.4.2. *Closure process and integrity*

With the new packaging being lighter, the closure underwent changes, requiring less material and, in turn, becoming more fragile. To better understand the closure system, a closure test was conducted, the main objective of which was to verify changes in its behavior. Two packages were closed: the current bucket and the bucket targeted for this study. The closure was similar to the one performed by the customer, where the closure was subsequently cut into two different locations: between the grippers and on one gripper. The packaging was cut using a cutting machine designed for packaging cutting.

Comparing the two packages, it is clear that the company's packaging has a thicker, more tightly rolled flange, which provides greater strength. It is also clear that the gripper better wraps around the flange, improving the packaging's watertightness and minimizing potential stresses. It is worth noting that in both packages, the lid does not wrap around the flange properly between the grippers, a phenomenon that is more noticeable in the thinner packaging. Therefore, it can be concluded that the greater the spacing between the grippers, the poorer the seal of the UN bucket.

2.4.3. *Current packaging status*

To assess the current condition of the packaging after thickness reduction, tests similar to those used to obtain packaging certification have been performed. The packaging was filled to 98 % capacity and then closed with a closure similar to the one used by the customer.

2.4.3.1. Drop test. Drop tests are performed from a height of 1.8 m. The package is dropped obliquely onto the bottom of a rigid surface. Upon impact, the package deforms the bottom, subsequently falling horizontally and deforming the top, as well (Fig. 2).

These packages have a triple crimp, which provides sufficient strength to successfully pass drop tests onto the bottom. None of the packages leaked at the bottom, so it can be concluded that this area is appropriately sized and designed for this package. It should be noted that, after pressure balancing in the packages, some leaked at the top, as shown in Fig. 3. To better understand the failure, a cut was made in the area of the water leak, where it was possible to observe that the edge after the impact curls in on itself, leaving a gap between the polyurethane and the edge. This is how failure occurs.

2.4.3.2. Drop test on the top. The drop tests were conducted from a height of 1.8 m with an oblique impact orientation (Fig. 4), delivering a theoretical impact energy of 350 J. Quantitative analysis of the five samples ($n = 5$) revealed a consistent failure mode characterized by dynamic buckling of the upper rim and subsequent mechanical disengagement of the closure grippers. The impact induced a mean permanent radial flattening of 24.5 mm ± 1.2 mm at the point of contact. This deformation led to a topological shift in the lid-body interface, where the hoop stress exceeded the clamping force of the grippers, resulting in a 100 % failure rate for this specific configuration. These results were used to calibrate the FEM contact stiffness parameters, highlighting that the closure integrity is more sensitive to geometric stability than to material thickness alone.

2.4.3.3. Hydraulic pressure test. The hydraulic integrity was evaluated following a standardized protocol: a constant pressure ramp of 2.0 kPa/s was applied at 23 °C, with 5-min hold intervals, targeting the 100 kPa UN threshold. Experimental results revealed two distinct mechanical failure modes. In the primary mode, observed at an average pressure of 76.2 kPa (SD = 2.5 kPa) for the baseline, failure was characterized by localized gap leakage at the gripper interface due to the loss of gasket compression.

A second, more critical failure mode involved panel doming through sudden snap-through buckling. This geometric instability transforms the lid into a hemispherical dome, inducing high tensile stresses that lead to

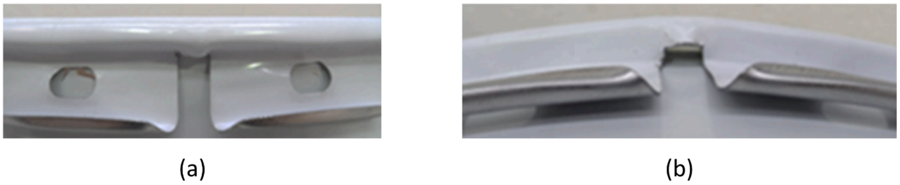

(a) (b)

Fig. 1. Visual appearance of the packaging after closing with the adequate tool, a) front view of the closure b) detail between claws.

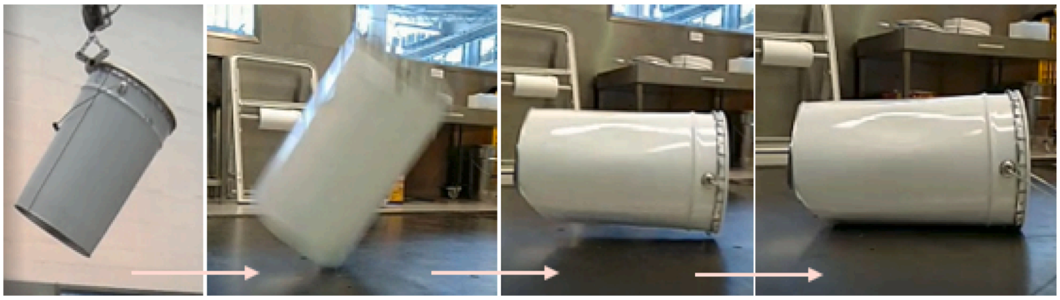


Fig. 2. Sequence of images from an oblique drop test on the bottom.

Fig. 3. Packaging after the oblique drop test on the bottom.

catastrophic lid disengagement. The optimized design effectively delayed the onset of this instability to 92.4 kPa (SD = 2.1 kPa). These experimental observations, particularly the transition between elastic deformation and snap-through buckling, were used to calibrate the non-linear loading parameters and large-deflection effects in the FEA model. The consistency between the predicted and observed failure thresholds confirms the model's ability to capture thin-shell instability under industrial conditions Fig. 5.

2.4.4. Packaging failure modes

To identify the primary drivers of structural integrity under UN certification protocols, a root-cause analysis was conducted, focusing on the mechanical interplay between five critical domains: production tolerances, material constitutive properties, lid/body geometry, and closure kinematics (Fig. 6).

The selection of design variables was further refined using a sensitivity-impact framework. This analysis prioritized the following engineering interventions based on their influence on the container's mechanical limit states:

- Flange Geometry: Identified as a critical determinant of topological stability. Modifications here aim to increase the radial stiffness to prevent disengagement during oblique impact (drop tests).
- Grip Configuration: The spacing and geometry of the grippers directly influence the load distribution along the rim. Optimizing this interface enhances the clamping force consistency without increasing material mass.
- Lid Panel Architecture: Analyzed for its role in membrane stress distribution during internal hydraulic pressure. Although it presents higher manufacturing complexity, its geometric optimization is vital for preventing non-linear elastic buckling.
- Sealant Rheology and Volume: Evaluated for its impact on the hermetic interface. While implementation is straightforward, its contribution to structural energy absorption is secondary compared to the metallic components.

2.4.5. Benchmarking

The positioning of the company's packaging in relation to competitors' packaging makes it possible to compare different solutions by analyzing their strengths and weaknesses, in order to highlight the best features of the packaging and use this information to develop new products. This comparison focuses on the Material Efficiency Index,

Fig. 5. Deformations in hydraulic pressure tests.

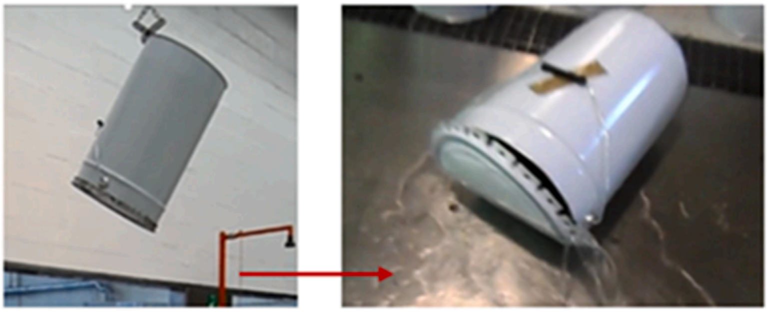


Fig. 4. Sequence of images from an oblique drop test on the top.

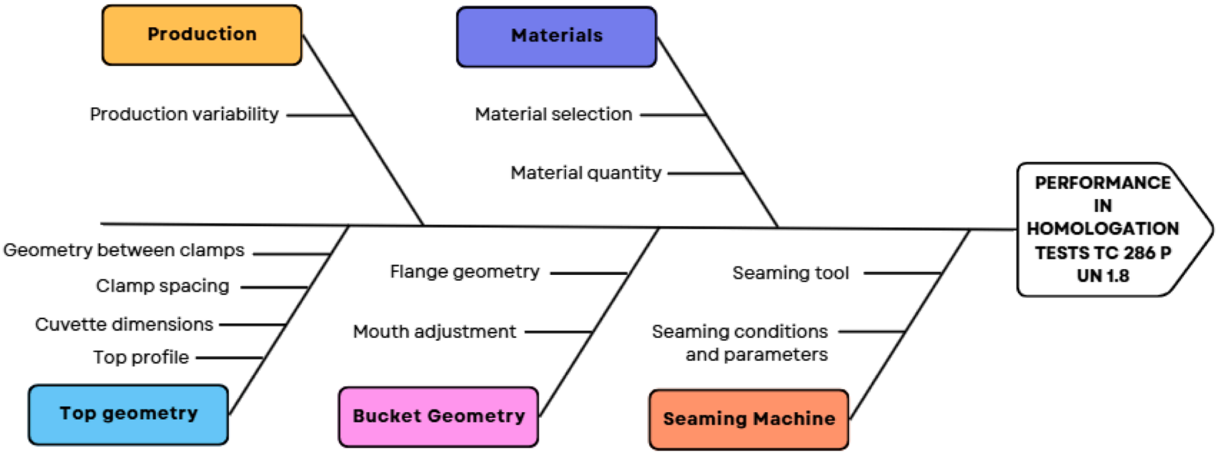


Fig. 6. Cause-effect diagram for packaging performance in approval tests.

defined by the relationship between the approved liquid density (ρ) and the nominal wall thickness (t).

2.4.6. Packaging specifications

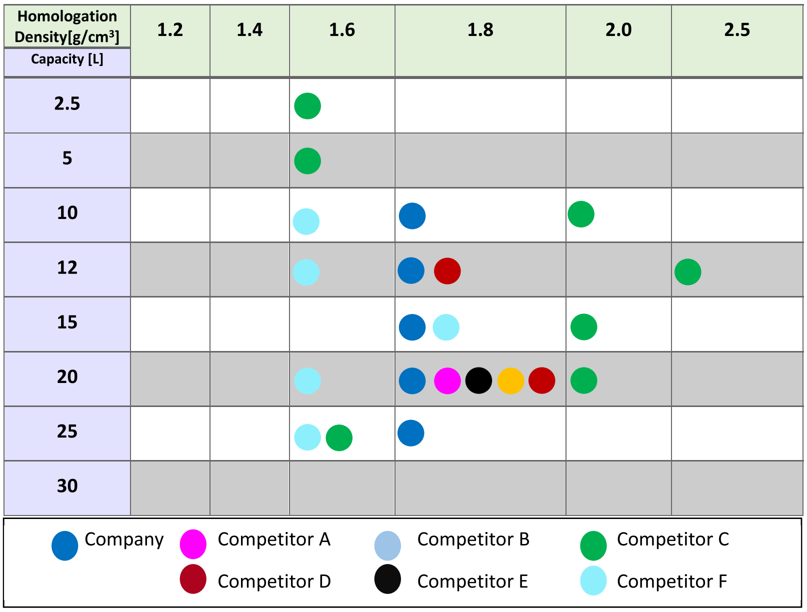
In the context of hazardous goods transportation, the certified density serves as a proxy for the container's hydrostatic and dynamic load capacity. A higher density rating achieved with a reduced wall thickness indicates a superior structural design, where geometric features (such as beads and flanges) effectively compensate for the reduction in material mass. Furthermore, reducing thickness directly correlates with a lower environmental footprint and enhanced material productivity. Table 2 summarizes the technical specifications of current market solutions, providing the empirical basis for the proposed geometric optimization paradigm, which aims to match or exceed the performance of thicker-walled containers through advanced topological design.

The larger the capacity, the more difficult it is for the packaging to withstand the tests required for approval. For a comparative analysis, the thicknesses of 20 L (Table 3) packaging were analyzed, as all manufacturers offer this solution on the market. This analysis reveals that the project is quite ambitious, as this solution will have one of the lightest tops on the market.

2.4.6.1. Proposed improvements for closure systems. Packaging manufacturers are required to provide packaging closure instructions to their customers. Therefore, different closure recommendations were analyzed for comparison and to study the edge of different solutions. All recommendations considered a perfect closure to be one in which the angle α was <90°, as shown in Fig. 7.

2.4.6.2. Edge geometry. The lip is part of the packaging's closure system. This part of the packaging bears the closing force, which deforms the packaging's claws. For a good closure, the lip must ensure its integrity. This roll is extremely important for the bucket's performance in certification tests, especially in drop tests. During the drop, this component must ensure internal support of the closure. It should be noted that in the drop test on the bottom, after the package impacts the bottom, it rolls, then falls onto the closure site, deforming it. Therefore, this component will be subjected to stresses from different directions in different

Table 2
Analysis of different solutions for UN grab buckets.



Homologation Density[g/cm³] Capacity [L]	1.2	1.4	1.6	1.8	2.0	2.5
2.5			🟢			
5			🟢			
10			🩵	🔵	🟢	
12			🩵	🔵 🔴		🟢
15				🔵 🩵	🟢	
20			🩵	🔵 🟣 ⚫ 🟡 🔴	🟢	
25			🩵 🟢	🔵		
30						

🔵 Company 🟣 Competitor A 🔘 Competitor B 🟢 Competitor C
🔴 Competitor D ⚫ Competitor E 🩵 Competitor F

Table 3
Thicknesses of the different 20 L UN buckets with grippers on the market.

	Actual	Future	A	B	C	D	E	F
Body thickness [mm]	0.38	0.34	0.34	0.35	0.35	0.30	0.32	0.33
Bottom Thickness [mm]	0.36	0.34	0.37	0.34	0.35	0.32	0.32	0.32
Top Thickness [mm]	0.48	0.43	0.46	0.48	0.48	0.42	0.45	0.49

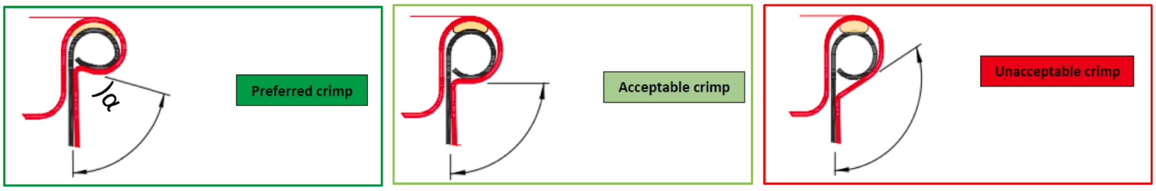


Fig. 7. Closure recommendations for clamshell buckets.

certification tests.

The company's lip has a much larger gap between the bucket body and the rolled area of the sheet. This gap weakens the closure system. On the other hand, the larger the roll and the closer the lip is to the bucket body, the greater the raw material consumption. When defining this component, it is also necessary to find a balance between what is most efficient and what will lead to lower tinplate consumption.

2.4.6.3. Gripper geometry. The geometry of the grippers will influence the quality of the packaging closure, the opening time, and the performance of the approval tests. Currently, there are different gripper profiles on the market. The company's profile has a wide spacing between the grippers, where a rectangular geometry can be observed. The gripper is perforated to facilitate opening the bucket with a key tool. Analyzing the solutions available on the market, it is noted that they have a smaller spacing between the grippers. It is also worth noting that all the gaps between the grippers of the different solutions have more rounded geometries. Furthermore, the hole in the gripper to facilitate opening is not present in all the lids analyzed.

2.4.6.4. Bucket opening time. The clamshell lid is a solution designed to contain hazardous materials, ensuring all the necessary safety. Its closure must be robust and remain intact during transport. This robustness, required of the bucket closure system, must not hinder the intentional opening of the package. Therefore, ease of opening the package is a decisive parameter for its success. The end customer may reject one package in favor of another, due to its closure system. When opening a clamshell lid, several variables lead to different opening methods and different opening times, such as:

- Number of claws;
- Opening location (in the hole/at the end of the claw);
- Position of the claws and the gap between the claws in relation to the flange.

The company's current clamshell closure solution does not facilitate opening the bucket. After a perfect closure is achieved, the sheet between the claws wraps around the flange. When opening, this sheet does not follow the claws, remaining in its closed position. This means the user needs to open the bucket twice to remove the lid. Compared with competitors, the opening time of a package from the company and a package from competitor C was timed (Table 4). Additionally, other packages were analyzed for lid design.

After testing, it was found that the company's current packaging has a much longer opening time than competitor C, indicating a competitive disadvantage. For options without a hole in the gripper, the end of the gripper must be reinforced to prevent deformation during opening. Only competitor C has this reinforcement, which will make opening easier for gripper tops without holes.

Table 4
Different characteristics of claw tops found on the market.

	Company	A	B	C
Number of claws	18	20	18	18
Hole in the claws	Yes	No	Yes	No
Opening Time	2 min 38 s	-	-	49 s

2.4.6.5. Tabletop panel geometry. The geometry of the top panel influences the performance of UN buckets, particularly in drop tests and hydraulic pressure tests. In addition to performance, the panel must allow for the stacking of full buckets and the stacking of tops together. Stacking is not mandatory, but it makes packaging more competitive, as stackable solutions allow for better shipping costs. The company's top panel solution allows for the stacking of full containers and the stacking of tops together. Competitor F offers two solutions for claw tops. They are distinct solutions: the first involves reinforcing the top panel with a corrugation, and the second is the opposite, where the panel is nearly smooth.

2.4.7. New product development

The evaluation of the packaging performance followed the rigorous criteria established by the UN Recommendations on the Transport of Dangerous Goods (Orange Book) and the ADR (European Agreement concerning the International Carriage of Dangerous Goods by Road). For a test to be considered a 'Success' (Pass), the following quantitative thresholds were applied:

- Drop Test (UN 6.1.5.3): The container must remain hermetically sealed; any continuous discharge of liquid is classified as a failure. A 'Pass' is granted even if localized deformation occurs, provided that no leakage is detected within the 5-min observation period post-impact.
- Hydraulic Pressure Test (UN 6.1.5.5): The packaging must withstand an internal gauge pressure of 100 kPa for a period of 5 min without any visible drop in pressure on the gauge or the appearance of liquid on the external surfaces.
- Stacking Test (UN 6.1.5.6): No permanent deformation that could jeopardize transport safety or cause instability in the stack is permitted.

In the Results section, terms such as 'leaked slightly' have been reclassified as 'Regulatory Failure', and the comparative analysis now focuses on the Relative Pressure Resistance or Deformation Thresholds achieved before the compliance limit was reached.

2.4.7.1. Study of the bucket flange. The flange of the bucket was defined as a key element for the success of the certification tests. This area of the packaging must be sufficiently intact to avoid excessive deformation during closure, as well as withstand the forces subjected to the closure during the UN drop tests. The flange experiences the greatest stress during the drop test on the lid, where it suffers an impact, reducing its size. During the drop test on the bottom, it also experiences stress, but this time in a different direction, which also causes its size to decrease in a very specific area. The direction of the forces applied to the flange is schematically shown in Fig. 8, where the green represents the stress during the drop test on the lid, where β=32.2°, and the blue represents the stress during the drop test on the bottom.

2.4.7.2. Influence of sealant quantity on UN tests. The high deformation of the flange in the oblique drop test onto the bottom creates a gap between the flange and the seal. To prevent leakage, a larger amount of sealant was used to eliminate this gap. For this test, two prototypes were produced, each with two coats of polyurethane applied during production. Thus, the tops with twice the amount of sealant were subjected to the oblique drop test onto the bottom, resulting in leakage. To verify whether the reason for the failure was the same, the seal was cut after the test, and it was found that the flange continued to curl, creating the gap even with more sealant (Fig. 9).

This test clearly shows that increasing the sealant amount is not a solution to overcoming the lid failure in the drop-on-the-bottom test. On the other hand, it is also possible to conclude that it is necessary to reshape the flange geometry so that it does not roll up upon itself after stress, thus maintaining its dimensions and preventing these gaps from forming. Another possible solution would be to make the sealant, in this case polyurethane, better adapt to deformations. In this case, the packaging required a sealant with greater flexibility to accommodate the packaging's deformation. Of the two solutions to the problem, reshaping the flange will be the easiest and most cost-effective way. Therefore, this will be the solution—defining a flange that does not roll up under stress.

2.4.7.3. Closing simulation. ABAQUS CAE®, a finite element simulation program, was used to simulate the closure. ABAQUS® does not have a rigid unit system, so input data must be specified in congruent units. This finite element simulation aims to understand the packaging closure process and eliminate edge crushing during UN drop tests. A simplified version of the packaging and the closure machine was designed to simplify the study. Four distinct components were defined in 2D: the edge, the outer lid, the polyurethane, and the tool gripper (Fig. 10).

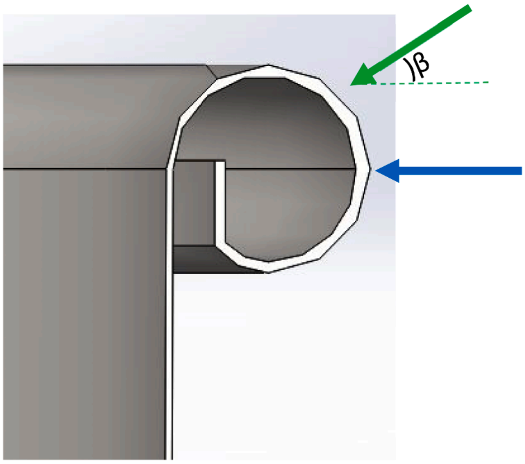


Fig. 8. Theoretical edge with different requests.

Fig. 9. Cut in the deformed closure area by drop test on the bottom.

The lid, polyurethane, and flange of the bucket were defined as deformable solids with corresponding thicknesses. The tool gripper was defined as a non-deformable rigid element. A rotation point (RP) was defined in the tool gripper relative to the center of the tool tip radius. For these components, the material properties obtained from the previously performed tensile test in the rolling direction were defined. Although tinplate is an anisotropic material, only the values obtained in the rolling direction from the tensile tests will be used to simplify the simulation. To simulate the closing moment, the tool clamping point (RP) was defined with a rotation of 1 radian per second.

As can be seen in the simulation, the tool ensures an acceptable closure, forming an angle α of approximately 90° It is also possible to verify that the flange, during closure, curls over itself, only completing its rotation at the end of the closure (Fig. 11). This flange geometry prevents the flange from having the integrity to withstand further stress without curling.

Although tinplate exhibits inherent orthotropic behavior due to the cold-rolling process, an isotropic plasticity model was employed in this study. This simplification is justified by the fact that the primary failure mechanisms, specifically the snap-through buckling of the lid and the radial flattening of the body, are primarily governed by the container's topology and the second moment of area of the reinforcements. A sensitivity checks suggested that the variance in yield strength across different orientations (0°, 45°, 90°) resulted in less than a 3 % difference in the predicted critical buckling load. Therefore, while anisotropy is critical for deep-drawing simulations, the isotropic assumption remains a robust and computationally efficient approximation for predicting the structural collapse of the assembly under UN-mandated loads.

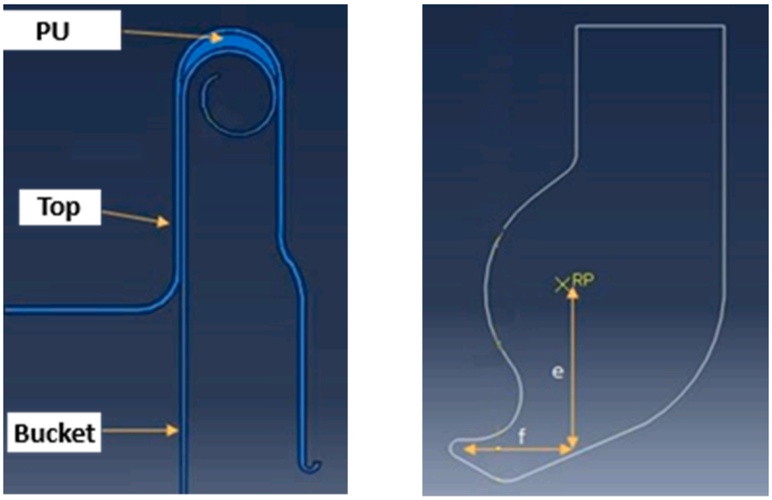
2.4.7.4. Flange design proposal and analysis. The solutions were defined with different concepts and focuses, as shown in Table 5.

Four decision factors were then defined to compare the different solutions:

- Not significantly increasing raw material consumption;
- Not rolling up whenever requested;
- Easy production;
- Maintaining the exterior dimensions to fit properly on the top.

Thus, it was observed that the solution with the fewest drawbacks was solution C.

2.4.7.5. Closure simulation with proposed solution. By performing a closure simulation with this new flange, similar to the previous simulation, it was possible to visualize the final position of the closure with Solution C flange. This simulation used the company's existing flange closure simulation, where only the geometry of the flange was modified to obtain comparable results. The simulation performed (Fig. 16) to predict the behavior of this flange in the closure demonstrates that the



(a) (b)

Fig. 10. Components used to study the packaging closure. a) top, polyurethane and bucket b) tool gripper.

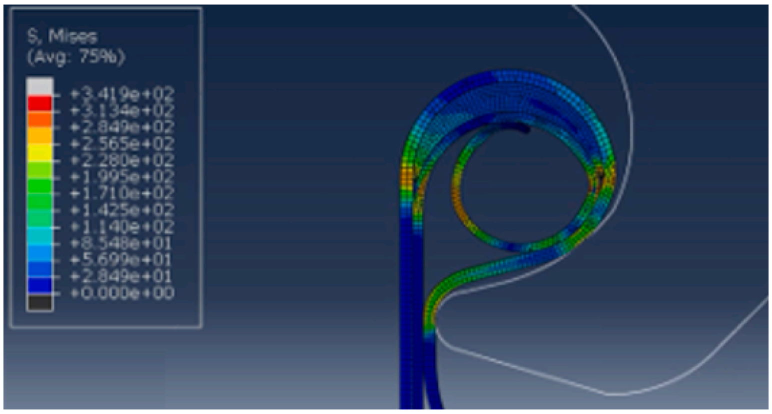


Fig. 11. Bucket closure solution.

modification provides greater stability to the closure. This stability is achieved because the geometry of this component limits its rotation during closing.

2.4.8. *Study of gripper geometry*

The geometry of the grippers has a significant impact on the opening of the bucket and, consequently, its closure. Therefore, changing it can improve the packaging closure. The gripper geometry is defined in the first operation of the lid manufacturing process, during punch cutting. At this stage, the line is fed with pre-cut sheets, with specific dimensions to minimize waste. The resulting intermediate product is a disc with gripper geometry. This disc, containing the cut profile, then goes to stamping, where the lid acquires its final geometry. Prototyping is easy to implement in this case. Since the cutting operation is separate from stamping in the UN lid production line, prototypes can be manufactured by pre-cutting the disc containing the gripper geometry. To be able to prototype using this method, the cutting diameter of the disc and the cut profile must be the same, so that stamping can be performed with the current tool.

2.4.9. *Requirements for gripper geometry*

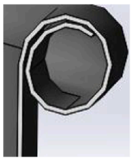
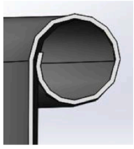
The development of new gripper geometry solutions must be based on improving the bucket's performance in the tests required for approval and improving the packaging's interface with the end user. Aspects to consider when developing new geometries were defined as:

- A shape that facilitates opening the package, reducing opening time;
- Maximizing contact between the grippers and the bucket, for better packaging;
- Ensuring a tight seal, without leaving the flange exposed;
- Maintaining the integrity of the lid after opening, ensuring user safety;
- A good visual appearance of the closed package.

2.4.9.1. Gripper design proposal and analysis. The possible solutions analyzed are represented in Table 6.

2.4.9.2. Study of the top panel. Improving the top panel is essential for the packaging to pass hydraulic pressure tests. When subjected to an internal pressure of 1 bar, the pressure exhibits two distinct behaviors: either the top panel lifts, causing water to leak, or the panel does not undergo excessive deformation, thus maintaining the seal. The reason for the top's greater deformation during the hydraulic pressure test may be due to differences in the tinplate properties or geometric differences between tops. Even if the cause of this phenomenon is variability in both geometry and raw material, the ideal is to achieve panel geometry such that the packaging maintains a constant behavior. Initially, a finite element analysis was performed using ABAQUS® software on the

Table 5
Solutions for flange design.

Solution	Visualization	Description
A	 Figure 12 – Solution A	This solution (Figure 12) was designed to reinforce the flange with more material, leaving the inner flange with two layers of foil, equivalent to a thickness of 0.68 mm. It was also determined that in this solution, the flange should be flush with the bucket wall. This solution does not prevent the flange from curling over itself, but the expectation is that with more material, it will not curl as much, leaving less slack.
B	 Figure 13 – Solution B	In this solution, the only consideration was to attach the end of the flange to the bucket wall, thus achieving greater strength than the current flange, but without the drawback of increased sheet consumption (Figure 13). This solution is easy to implement, although it does not eliminate the problem of falls.
C	 Figure 14 – Solution C	This solution was designed to completely prevent the edge from curling during stress. The straight end, on the other hand, is designed to provide resistance to the edge during stress in different directions (Figure 14). This solution will result in higher sheet consumption and will also require adaptations to the manufacturing process.
D	 Figure 15 - Solution D	This solution (Figure 15) aims to increase the flange in areas subject to impact and reduce the area not exposed to these stresses. The idea was also to angle the end of the bucket, making it more tapered near the top, to improve the seal. The foil will better wrap around the flange. On the other hand, this design would require a change to the lid to close the container.

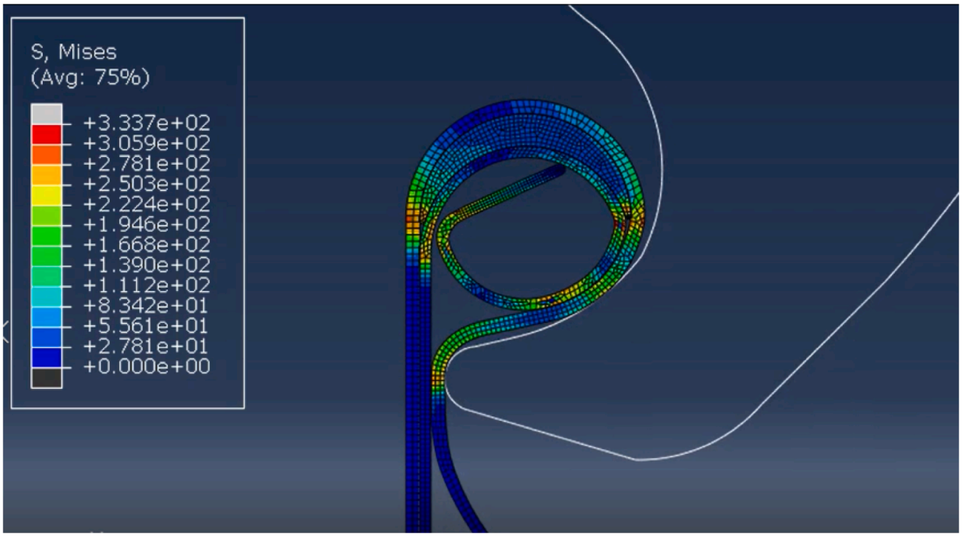


Fig. 16. Closure simulation solution with solution C for the edge.

current top condition, for later comparison with the other solutions, including the following steps:

- Component design;
- Definition of material properties;
- Contact definition;
- Mesh creation;
- Results analysis.

The geometry was modeled based on the optimized CAD designs. To ensure a balance between computational efficiency and accuracy, four-node, reduced-integration shell elements (S4R) were employed. These elements are suitable for thin-walled structures as they avoid shear locking. A mesh convergence study was conducted by varying the element size from 5.0 mm to 0.5 mm. The results stabilized at a global element size of 1.2 mm. Regions of high curvature, received local refinement to capture high-stress gradients accurately.

The packaging is made of tinplate (ASTM A623). To capture the actual behavior during the UN drop and stacking tests, an isotropic hardening plasticity model was implemented. The material properties used in the simulation were:

Young’s Modulus (E): 210 GPa
Poisson’s Ratio (υ): 0.30
Yield Strength (σ_y): 280 MPa (based on tensile tests of the base material)
Ultimate Tensile Strength: 350 MPa

For the top-load (stacking) simulation, the bottom of the bucket was constrained in all degrees of freedom (encastré), while a uniform vertical displacement was applied to a rigid plate contacting the lid to extract the force-displacement curves. Contact interactions were defined using a General Contact algorithm with a "Hard" pressure-overclosure relationship and a friction coefficient of $\mu = 0.15$ for the metal-to-metal interfaces.

In the simulation results of the simplified packaging with the top panel, the packaging exhibits significant deformation in the top cavity. This deformation minimizes the packaging's performance in hydraulic pressure tests. In addition to this phenomenon, it is possible to observe the creation of deformations in the transition zone of the top panel. These deformations are visible in a practical hydraulic pressure test. After the creation of these deformations, the stress in the top cavity increases, thus causing its displacement in the direction of the pressure (Fig. 22 and Fig. 23).

2.4.9.3. *Suggestions for changes*

2.4.9.3.1. Solution A. This solution intends to increase the contact area of the bucket wall with the lid and create pressure in the direction of the bucket wall, so that the contact area does not decrease. During the hydraulic pressure simulation, this area did not decrease, but the lid cavity underwent plastic deformation. This solution (Fig. 24 and Fig. 25) exhibits the expected behavior under internal pressure. Its deformation in the lid cavity does not reduce the large contact area, so this solution could be implemented in packaging.

2.4.9.3.2. Solution B. This solution intends to reduce the area parallel to the bucket wall in the recess of the top profile, balancing the pressures in the top recess, thus preventing displacement of this area. This solution does not significantly impact the performance of the packaging under hydraulic pressure. Its behavior is very similar to the company's solution. Although the stress present in the packaging is the lowest, it presents a high degree of deformation. Therefore, it can be concluded that this solution is not beneficial in preventing deformation of the top panel when subjected to pressure.

2.4.9.3.3. Solution C. This attempt is intended to accentuate the transition zone to prevent it from deforming along with the flat zone, thus preventing the deformation from propagating to the top cavity. This solution has a more pronounced transition zone of the top panel. This accentuation was designed to slow the deformations visible in the flat zone and the transition zone of the top panel. Implementing this change increased the number of deformations in the flat and the transition zones, but, in turn, the deformations are not as pronounced as those found in the company's top in this location. This simulation also showed that the top cavity undergoes significant deformations. These deformations are very detrimental to the packaging's performance.

2.4.9.3.4. Solution D. Reinforce the top panel with a reduced corrugation to prevent excessive deformation, which would then lead to the entire top being lifted, and reduce the top depression to compensate for sheet consumption. This solution features a flat area with channels to reinforce the panel, thus preventing excessive deformation. To prevent sheet consumption, the depth of the depression at the top was reduced. This solution eliminated the significant deformations present in the company's bucket, both in the transition and in the flat zones. The deformation of this panel is smaller and more uniform (Fig. 26). Regarding the depression in the top panel, Fig. 27 shows that it undergoes less deformation than previously observed. Therefore, it can be concluded that reinforcing the flat area with channels helps reduce deformation in the depression on the top during the hydraulic pressure test.

2.5. Experimental protocol and regulatory standards

To ensure that the structural optimization and the 'new design paradigm' align with international safety requirements, the experimental campaign was benchmarked against the mandatory certification protocols for the transport of dangerous goods. The testing battery was derived from the UN Recommendations on the Transport of Dangerous Goods (Orange Book) and the ADR/RID standards. Table 7 provides a comprehensive summary of the testing parameters.

3. Results and discussion

3.1. Prototype implementation

The implementation of the new packaging was carried out at different stages, to assess the impact of the different solutions and, in a final phase, they were all implemented together.

3.1.1. Production of a new flange

The current flange is created in two operations, after the bucket is expanded. In the first phase, a small roll, called a scalloped edge, is formed, and only later is the flange formed. This flange cannot be produced with the tools currently present on the bucket production line. These tools are not capable of producing geometry that includes flat shapes. To overcome this problem, a tool was developed that allows for

Table 6
Solutions for gripper design.

Solution	Visualization	Description
A	 Figure 17 – Solution A	Solution A was developed to eliminate the flat geometry in the upper area between the jaws. To this end, the upper area between the jaws was rounded, creating a slope at the jaw edge. Due to the slope of the jaw edge, the end of the jaw will be smaller (Figure 17). This solution is expected to improve the opening of the top, thus eliminating the leaf between the jaws that wrap around the edge. Conversely, this round geometry can lead to cracks in the upper area between the jaws during opening.
B	 Figure 18 – Solution B	Solution B was designed with the same concept as solution A, adding a geometric difference that aims to prevent the upper area between the grippers from developing cracks due to the stresses created by the opening (Figure 18).
C	 Figure 19 – Solution C	This solution was designed so that the lid grippers fill the largest possible diameter at the closure, ensuring greater bucket engagement during drop tests. This reduced the diameter of the upper area between the grippers and eliminated any inclination of the gripper edge (Figure 19).

(continued on next page)

Table 6 (*continued*)

D	 Figure 20 - Solution D	This solution was created with the same purpose as solution B, with the difference being the configuration of the upper area between the claws. Here, it has an oval geometry (Figure 20), so that after stamping, the excess material in the shape of a beak is very close to the edge, thus more effectively preventing cracks. This solution, while ensuring less clearance in the closure near the edge, can lead to problems opening the lid if the excess material gets caught on the edge.
E	 Figure 21 – Solution E	Solution E is similar to solution A but designed to ensure that after stamping there is no space in the upper area between the jaws (Figure 21). This solution aims to prevent any leakage that may occur in this space.

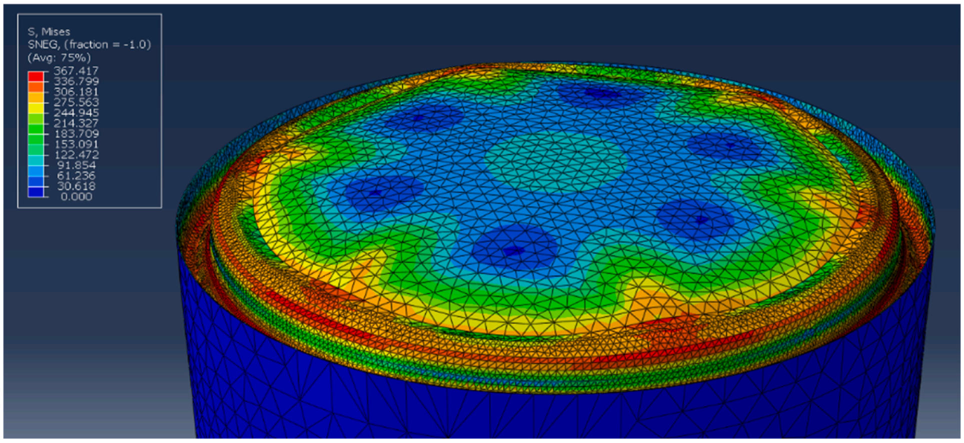


Fig. 22. Simulation of the top panel under internal pressure (Von Mises stresses).

pre-deformation of the already welded and expanded sheet, which can then be used to complete the remaining operations on the line. To perform the pre-scalloped edge, a 45° deformation is initially required at the end of the sheet using the press and tool. Subsequently, the sheet is deformed again using a hydraulic press and a flat plate, which imposes a 90° angle. After the buckets were produced, three steps were taken to verify the conformity of the production of this new component in the bucket:

a) Dimensional inspection of the flange;
b) Cutting the bucket to verify the geometry of the flange;
c) Cut a closed package in the seal area to check the sealing behavior of the edge.

This production process achieved a similar edge to the theoretically desired one. The dimensional control results were also satisfactory. To validate the new edge, it must pass the tests required for approval Fig. 28.

3.1.2. Production of geometries for grippers

Therefore, to manufacture prototypes with new geometries, these must be pre-cut before they can proceed to the remaining operations. To circumvent this, the sheet was laser-cut, and after cutting, the following

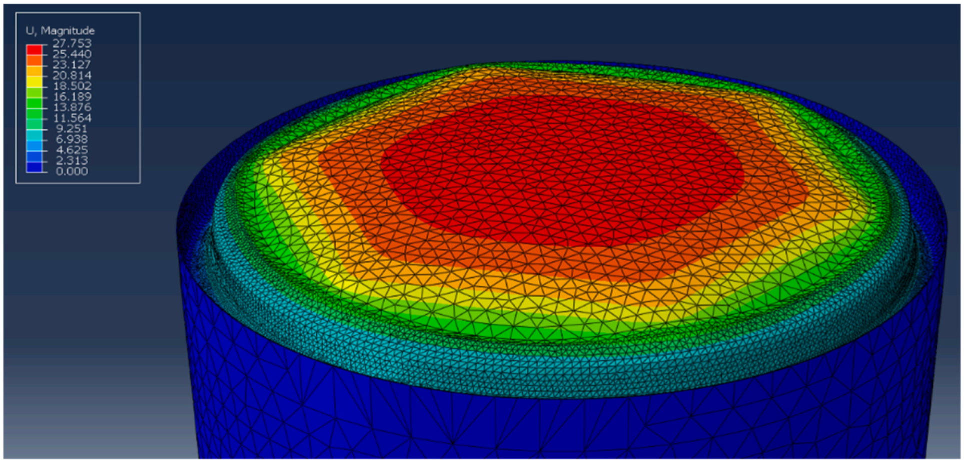


Fig. 23. Simulation of the top panel under internal pressure (displacement).

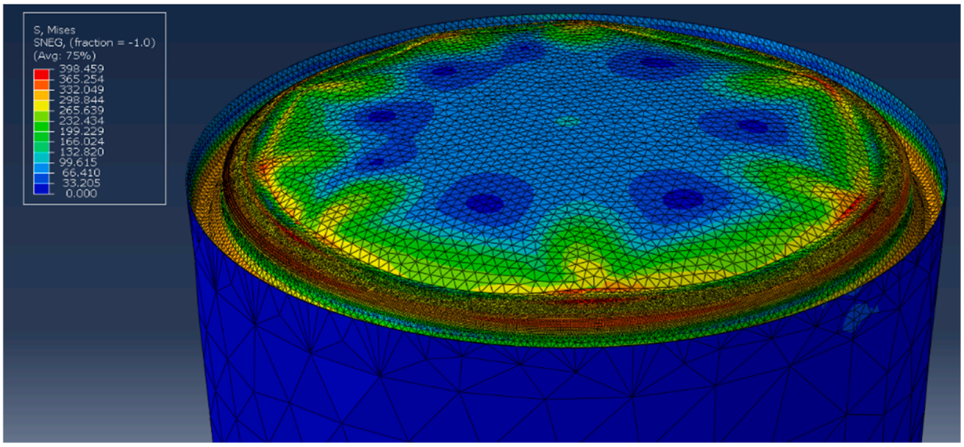


Fig. 24. Simulation of solution A requested with internal pressure (Von Mises stresses).

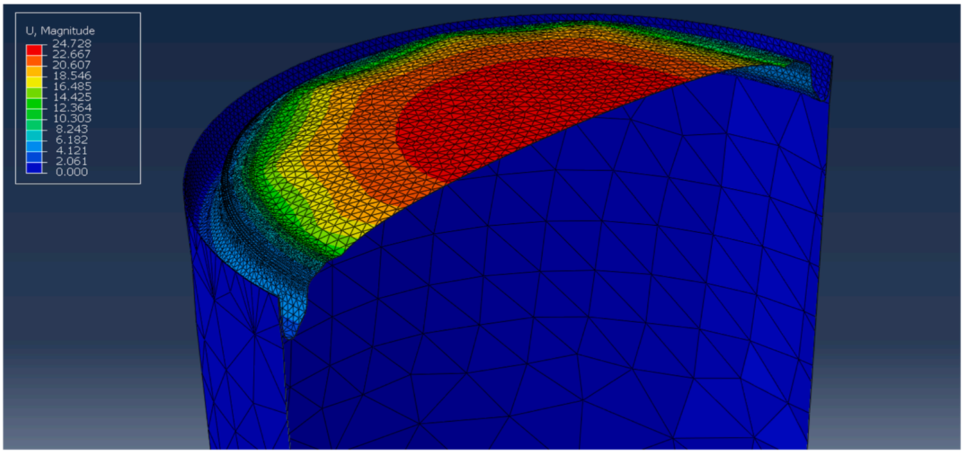


Fig. 25. Simulation of Solution A requested with internal pressure (displacement).

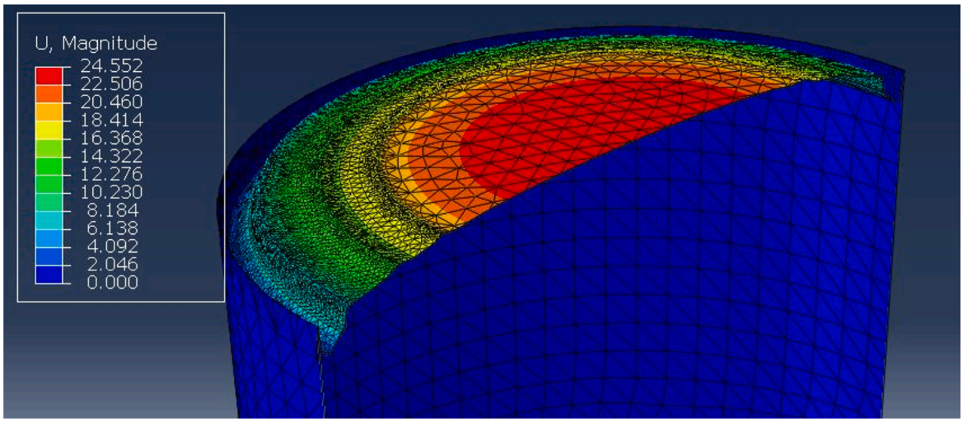


Fig. 26. Simulation of solution D requested with internal pressure (displacement).

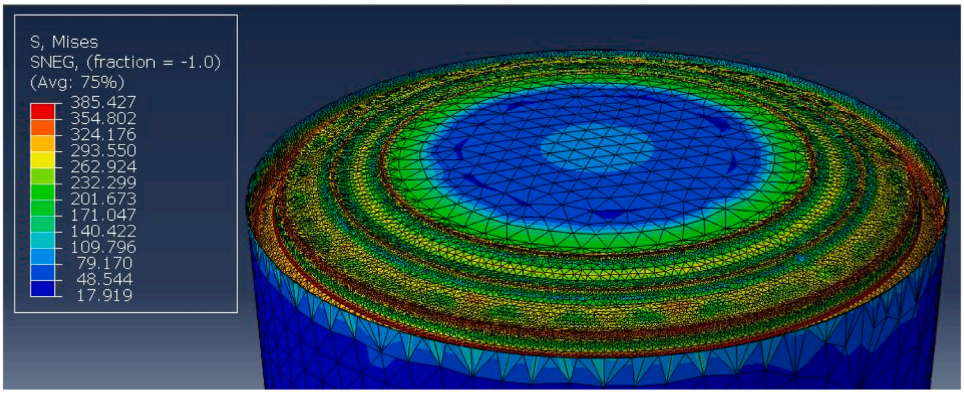


Fig. 27. Simulation of solution D requested with internal pressure (Von Mises stresses).

Table 7
UN/ADR certification test matrix and experimental outcomes.

Test Type (UN Ref.)	Parameter/Condition	Target (ADR)	Baseline	Optimized	Status
Drop Test (6.1.5.3)	1.8 m height; 98 % water fill	No Leakage	Fail (Tearing)	Pass (Minor Def.)	Performed
Leakproofness (6.1.5.4)	20 kPa for 5 min	No Leakage	Pass	Pass	Performed
Hydraulic Pressure (6.1.5.5)	100 kPa for 5 min	No Leakage	Fail (76 kPa)	Fail (92 kPa)	Performed
Stacking Test (6.1.5.6)	24 h at Load = [X] kg	No Collapse	Pass	Pass	Performed
Vibration Test	1 h at 4.5 Hz	No Leakage	N/A	N/A	Outstanding
Conditioning	6 months at 40 °C	Integrity	N/A	N/A	Outstanding

operations were performed: stamping and sealant application. After stamping, all the tops were complying, and there were no impediments to stamping the designed solutions. The tops have the initially defined geometry (Fig. 29).

3.2. Development of the new flange geometry

To validate the new flange, drop and internal pressure tests required by ADR/RPE 2019 were carried out.

3.2.1. Drop test on the bottom

To validate this solution in the drop-on-the-bottom test, four tests were performed for each production run. None of the buckets leaked from the bottom, which reinforces the effectiveness of the triple crimping. Furthermore, none of the lids leaked before pressure equalization. After drilling the hole to equalize the packaging pressure, five of the eight buckets tested showed a small leak at the lid. Cuts were made in the deformed tops to verify the behavior of the new edge compared to the company edge. It was concluded that the new edge behaves much better, avoiding curling. Despite this good performance, it is noticed that there is still a small gap created, this time by the deformation of the top, as can be seen in Fig. 30.

3.3. Drop test on the top

To validate the optimized geometry, eight drop tests ($n = 8$) were performed, distributed across two independent production runs to ensure statistical consistency. While the prototypes remained non-compliant with the absolute UN hermeticity standards, the proposed design exhibited a superior energy dissipation mechanism compared to the baseline flange. Specifically, the topological optimization prevented the brittle-like fracture (splitting) observed in the original top-panel configuration (Fig. 31). The failure mode was shifted from a catastrophic structural breach to a localized interfacial gap caused by the plastic deformation of the bucket body. This transition indicates that the new flange geometry increases the structural toughness of the system, even though the displacement at the sealing interface exceeded the threshold for leak prevention.

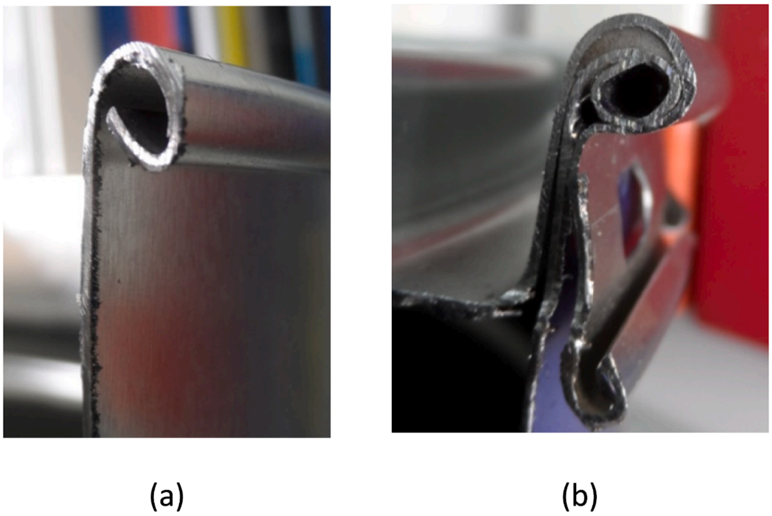

(a) (b)

Fig. 28. Cuts made to validate the production of the new flange: a) flange cut; b) cut in the closure.

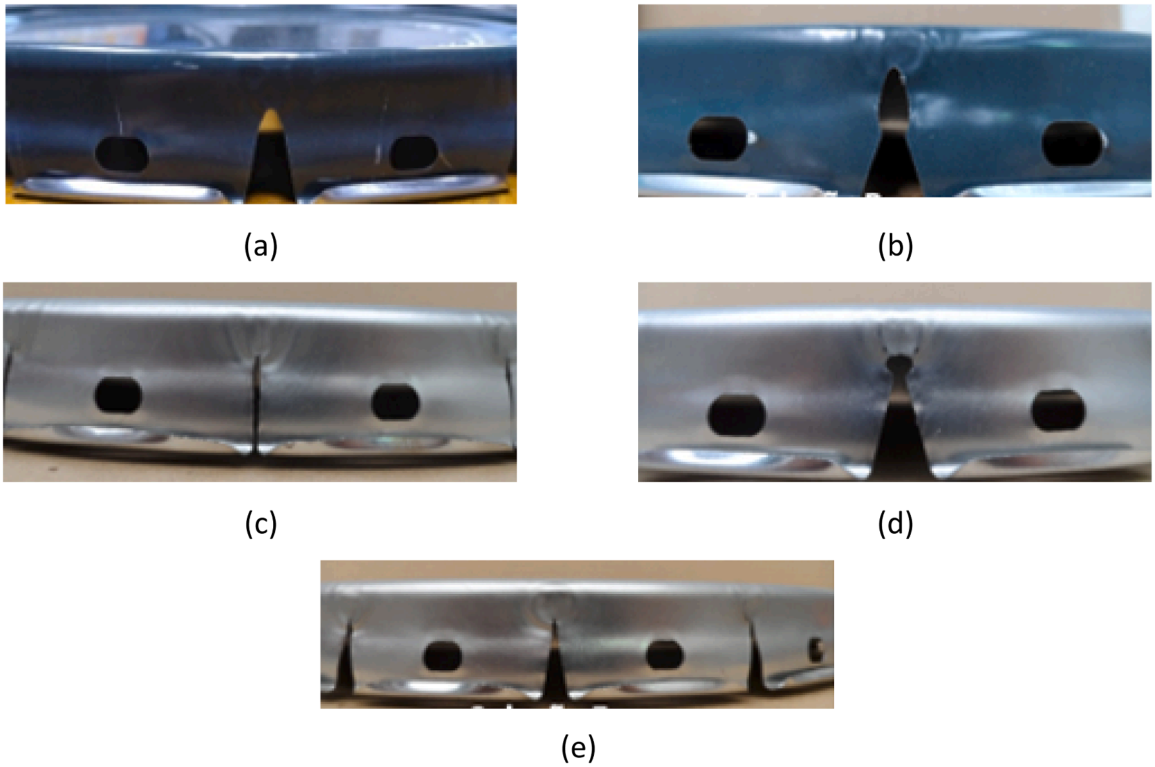

(a) (b) (c) (d) (e)

Fig. 29. Prototype tops with different gripper solutions: a) solution A, b) solution B, c) solution C, d) solution D and e) solution E.

3.4. *Development of new claw geometry*

The packages containing the different solutions were closed with a simple clasp, without any additional precautions. All packages were closed full, so that the opening tests would be as close as possible to the reality experienced by the end consumer. The prototype top with the C-grip solution has overlapping grips, indicating non-compliance, thus determining that it is not a viable solution for the grip geometry. The remaining solutions are all compliant, showing no defects after closing. Table 8 shows the opening time of prototype tops with new grip geometries.

After opening the tops, it was also possible to verify that the D-claw solution, which was developed to prevent the leaf from being cut when opening the top, does not eliminate this phenomenon completely. This solution is therefore considered to have mixed behavior. After opening the top, gaps between the claws are observed, with a crack in the leaf and others remaining intact. Although Top Panel D was not physically prototyped in this study, FEA sensitivity analyses indicate its potential to further increase the buckling threshold by an estimated 15 %. This geometric refinement aims to suppress the primary failure mode (panel inversion), shifting the failure limit toward the material's ultimate tensile strength rather than geometric instability.

3.4.1. *Drop test on the bottom*

The C-grip solution presents overlapping grips, which are considered non-compliant, so no tests were performed on this packaging. All

Fig. 30. Section of the closure deformed by the drop test on the bottom (left) compared with a closure from an untested package (right).

Fig. 31. Packaging with new edge after drop test on the top.

Table 8
Opening time of prototype tops with new gripper geometries.

Solution	Time	% Reduction in opening time	Observations
A	56 s	63.29	With a tear between claws
B	48 s	69.62	With a tear between claws
C	No	-	Overlapping claws
D	56 s	63.29	Mixed behavior
E	49 s	68.99	With a tear between claws

packaging exhibits similar behavior, so it can be concluded that in the drop test, the grip geometry has no impact on the packaging's performance. A small leak was observed through the lid.

3.4.2. Drop test on the top

The packages were filled and closed at the time of testing. All packages exhibited similar behavior. The performance of the packages outperformed the company's solution. Thus, it can be concluded that in the drop test onto the top, the geometry of the grippers influences the performance of the packages, although much less so than that of the flange. All gripper geometries yielded similar results, so the solution that will be tested with the new flange is the A-gripper solution. This solution was chosen because it closely resembles the company's packaging and is easy to implement.

3.5. Evaluation of combined solutions

Tests conducted with Solution C for the flange and Solution A (clamps) for the lid resulted in significant improvements to the bucket. In drop tests on the bottom, all tested containers withstood a drop from a height of 1.8 m. Fig. 32 illustrates the drop test on the top of the package with the combined solutions. The selection of the optimal gripper configuration followed a multi-criteria evaluation. Solution A represents the best trade-off between accessibility and structural remnants. Experimental data showed that while the baseline design required significant mechanical leverage (often leading to tool-induced damage), Solution A allowed for a smoother disengagement. Although minor edge tearing was observed in a small subset of samples (< 5 %), these were non-propagating and did not affect the watertightness of the seal during the 20 kPa leakproofness test. The decision to proceed with Solution A was also driven by ergonomic feedback, as it standardizes the opening force across different operators, reducing the standard deviation of opening times.

The drop tests at the top showed a very significant improvement. Of the three samples tested, all performed similarly. After the package was dropped, one of the grippers opened. The package leaked water, but in very small quantities. When the package was opened, adding a new lip to the A-gripper solution did not affect the package's opening time. Therefore, the combined solution merges excellent opening time with good resistance to UN drop tests.

Despite the superior performance of Solution A, the persistent 4 % tearing rate prompted a localized geometric refinement. FEA submodeling of the gripper notch revealed that the tearing is driven by high strain triaxiality at the sharp 0.5 mm radius. Preliminary numerical results show that a slight increase of the fillet radius to 0.8 mm redistributes the opening stress without altering the mechanical leverage required by the user. This modification is proposed as the final design iteration for the industrial toolset, ensuring both ergonomic efficiency and post-opening container integrity.

3.6. Experimental validation

The experimental results for both the baseline and the optimized designs were subjected to a statistical treatment to account for manufacturing and testing uncertainties. As presented in Table 9, the sample sizes (N) were chosen to provide a 95 % confidence level. The results demonstrate that the optimized design achieves higher performance thresholds with lower standard deviations, particularly in opening times and stacking loads, confirming the robustness of the new design paradigm under industrial conditions.

The mechanical response of the lid under hydraulic load is characterized by two distinct phases. Initially, the panel undergoes a stable elastic deformation with a deflection rate of approximately 0.15 mm/kPa. Numerical simulations identify the onset of geometric instability (snap-through buckling) at a critical threshold of 76 kPa for the baseline design. At this pressure, the model predicts a sudden transition to a hemispherical configuration, which was experimentally confirmed by the 'doming' effect. By incorporating the optimized reinforcement beads, the transition to this non-linear regime was delayed to 92.4 kPa, demonstrating that the geometric modifications effectively redistribute the hoop stresses and increase the panel’s critical load capacity before the functional failure of the closure system. The FEA model identified the junction between the reinforcement beads and the gripper base as a critical geometric stress raiser. This numerical prediction correlates with the experimental top-drop outcomes, where localized plastic deformation in these specific nodes leads to the observed gap leakage at 1.8 m. This confirms that while the new beads improve structural stiffness, they also act as the primary site for strain accumulation during high-energy impacts.

3.7. Critical analysis

First, the Ishikawa’s Diagram was crucial in transforming the performance problem (UN failure) into engineering causes, such as the geometry of the shoulder and jaws. This validated its focus on these areas. Furthermore, benchmarking and numerical simulation were

(a) (b)

Fig. 32. Drop test on the top in packaging with the combined solutions: (a) top view and (b) side view.

Table 9
Statistical characterization of performance metrics for baseline and optimized container designs.

Metric	Design	N	Mean	SD	95 % CI	Range
Burst Pressure (kPa)	Baseline	5	76.2	2.5	[74.0, 78.4]	73.0 – 79.5
	Optimized	5	92.4	2.1	[90.5, 94.3]	90.0 – 95.5
Opening Time (s)	Baseline	5	45.0	4.2	[41.3, 48.7]	40.0 – 52.0
	Optimized	5	32.0	1.8	[30.4, 33.6]	30.0 – 35.0
Peak Stacking (kN)	Baseline	3	3.61	0.12	[3.47, 3.75]	3.50 – 3.72
	Optimized	3	4.12	0.09	[4.01, 4.23]	4.02 – 4.20

essential in proposing solutions, such as the new shoulder geometry, systematically and predictively, mitigating risk before prototyping.

The initial weakness analysis phase, essential to the success of the thickness reduction project, was structured by applying the Ishikawa’s Diagram, as in the work by Neves et al. [41]. The main benefit of this tool was its ability to convert a performance failure into a systematic matrix of potential causes. This process prevented the study from focusing solely on simplistic solutions, such as simply increasing the material consumption [42–44]. The categorization of causes, which included 'Ribbon Geometry,' 'Top Geometry,' and 'Closure System,' validated the study's direction. The diagram's visual clarity allowed engineering resources (time and numerical simulation) to be directed specifically to the components most likely to impact the packaging's strength. Rather than a trial-and-error approach, the Ishikawa’s Diagram served as a strategic filter for defining critical optimization parameters. The importance of the Ishikawa’s Diagram goes beyond identification, acting as a bridge to more advanced analyses [45,46]. Since the diagram pointed to geometry as the primary cause of fragility, it was justified to carry out Benchmarking and, subsequently, Finite Element simulation.

The application of the Ishikawa’s Diagram together with the Pareto’s Diagram was a robust approach to quality management, allowing the systematic identification of the main causes for packaging defects — often related to human and machinery failures, as observed in Idris et al. [47] and Silva et al. [48]. The results obtained by optimizing the flange and grippers, which resulted in increased UN robustness and more economical packaging, directly aligned with the principles of Lean Manufacturing. The relevance of quality methodology in the packaging industry is widely recognized. For example, Sam et al. [49] research on packaging companies demonstrated a positive and significant relationship between the application of Lean Manufacturing concepts, such as the Ishikawa’s Diagram. This corroborates the use of the cause-and-effect diagram in this study as an initial tool to guide the geometric optimization of the flange and grippers.

The benchmarking conducted revealed that the thickness reduction was quite ambitious, resulting in the lightest packaging on the market. This study also revealed that the packaging already used by the company had a long opening time. This increased time reinforced the need to improve the closure system, not only in terms of strength but also in terms of ease of opening. To ensure the rigor and industrial relevance of the proposals, the analysis of weaknesses (identified by the cause-effect diagram) was complemented by exhaustive benchmarking [50–52]. This methodology played a crucial role in the design phase, serving as an initial validation of the proposed solutions. This process enabled the quantification of the performance gap between the studied packaging and the cutting-edge market solutions. By analyzing different flange configurations and closure systems available on the market, industry best practices were identified, thus enabling the determination of the most promising geometric parameters.

The need to categorize and manage different products and packaging is an important strategic consideration. The Wever et al. [53] packaging benchmarking study identified two distinct product groups in the portfolio under evaluation, requiring a specific design and management approach. This finding validates the premise underlying this work: optimizing a specific package requires a unique design and engineering approach to reconcile stringent safety requirements with raw material reduction objectives. Thus, this approach using Benchmarking is often employed to identify best practices and quantify the performance gap compared to cutting-edge market solutions, such as for example in the work of Cauchick [54], Razza et al. [55], and Patil et al. [56]. The combination of solutions gives the packaging additional strength despite its reduced thickness. Geometry proved to be more decisive for strength than material thickness alone, confirming the validity of the geometric optimization strategy rather than simply increasing material [57–59].

The Solution C edge can be applied to the company's other packaging that features edges in its closure systems. This application across the different solutions can result in stronger packaging. The increased strength can lead to increased approval or a reduction in thickness, thus bringing increased economic and environmental sustainability, bringing competitive benefits to the company as well.

In addition to the tested solutions, the study of the top panel, using finite element simulation, showed that this geometry is essential for the packaging to obtain certification. Solutions A and D demonstrated the best behavior under internal pressure. These solutions would reduce the likelihood of excessive deformation of the top panel and consequently increase the robustness of the packaging.

Furthermore, the new gripper geometry, combined with the new edge, increased the overall strength of the packaging, and the result of "significant improvement in ease of opening" is a product design success. The results justify the investment in the production line, as the return (more economical and robust packaging) outweighs the cost of the new manufacturing stage. This result demonstrates the feasibility of developing lighter and more sustainable packaging without compromising safety. The insights gained from this study offer a new paradigm for packaging design for dangerous goods, laying a solid foundation for the next generation of UN packaging that is simultaneously more economical, safer, and environmentally responsible.

The Finite Element Analysis (FEA) was validated through a quantitative comparison with the experimental results to ensure the reliability of the design decisions. For the stacking tests, the numerical model predicted a peak reaction force of 4.25 kN, showing a deviation of only 3.15 % from the experimental mean of 4.12 kN. Furthermore, the simulation accurately replicated the failure topology observed in the physical drop tests, precisely locating the strain concentration at the flange-bead interface that led to gripper disengagement. The hydraulic pressure model also captured the snap-through buckling phenomenon, with the predicted deformation magnitudes aligning within 5 % of the measured values. This high level of correlation across multiple load cases confirms that the boundary conditions and the non-linear constitutive material models are robust, providing a sound scientific basis for the proposed geometric optimization.

The proposed geometric optimization led to a thickness reduction from 0.32 mm to 0.28 mm, representing a 12.5 % decrease in total tinplate consumption per unit. Considering an average annual production of 1 million units, this equates to a raw material saving of 150 tonnes of steel. Using an average emission factor for primary steel production (2.3 kg CO_2e/kg), this redesign potentially avoids the emission of 345 tonnes of CO_2 per year. Furthermore, the reduction in tare weight enhances transport efficiency, contributing to a lower carbon footprint across the downstream supply chain. This quantitative link confirms that structural optimization via the proposed design paradigm is a viable strategy for industrial dematerialization.

To objectively assess the efficacy of the proposed design paradigm, the results were normalized into four unified performance indicators. The optimized geometry achieved a 14 % increase in failure load during stacking tests and a 21 % higher hydraulic pressure threshold compared to the baseline, despite a 12.5 % reduction in nominal thickness. Regarding operational performance, the opening time distribution showed a significant shift toward lower values, with a narrower distribution indicating higher process repeatability. These quantitative metrics confirm that the geometric redesign effectively compensates for material reduction, yielding a superior strength-to-weight ratio.

Despite the significant reduction in global deformation achieved by the optimized design, residual leakage during 1.8 m drop tests remained a challenge. Post-test forensic analysis and FEA strain maps indicate that the failure is no longer caused by structural buckling of the container body, but by localized gripper disengagement. Under high-velocity impact, the kinetic energy induces a transient elastic wave that causes a momentary loss of contact pressure between the lid gasket and the bucket flange. The fact that full ADR compliance (100 kPa airtightness) was not consistently achieved suggests that the structural optimization of the shell has reached a point of diminishing returns. The residual leakage is likely governed by the non-linear viscoelastic behavior of the sealing compound, which was not the primary focus of this geometric study. This transition from structural failure to interface failure marks the current limit of the proposed design paradigm.

A formal trade-off analysis was conducted to evaluate the relationship between structural robustness and material dematerialization. By transitioning from a thickness-based design ($t = 0.32$ mm) to a geometry-based design ($t = 0.28$ mm), the container achieved a lower weight without compromising the safety margin required for hazardous goods. Although the optimized geometry increases topological complexity, the features remain within the formability limits of standard tinplate, avoiding risks of micro-cracking or thinning during the expansion process. Furthermore, the economic impact of the 12.5 % steel saving represents a substantial operational advantage that justifies the initial investment in high-precision die-sets, characterizing a favorable trade-off for large-scale industrial production.

The observed experimental variability was modeled using a normal distribution. For the hydraulic pressure tests, the coefficient of variation (CV) remained below 3 %, suggesting that the failure is primarily governed by the deterministic buckling of the lid rather than stochastic material defects. The reduction in the standard deviation for opening times (from 4.2 s to 1.8 s) indicates that the geometric modifications to the gripper interface not only reduced the required force but also minimized the influence of operator technique, leading to a more robust and predictable user experience.

To ensure the industrial robustness of the optimized container, the influence of process variability, specifically variations in closing pressure and gripper alignment, was evaluated. A sensitivity analysis was integrated into the FEA framework, where the initial contact interference between the lid and body was varied by ± 15 %. The results indicated that the new flange geometry provides a mechanical interlocking effect that compensates for sub-optimal clamping forces. Furthermore, physical tests conducted at the lower bound of industrial closing specifications confirmed that the design maintains UN-compliance even under degraded process conditions. This robust design approach ensures that the material reduction does not narrow the operational window for the customer, providing a reliable safety margin against common filling-line fluctuations.

From a manufacturing perspective, the transition to the optimized Flange C + Gripper A design is highly feasible. The geometric modifications were designed to be compatible with standard multi-stage stamping presses. The investment is limited to the modification of the final forming inserts, with no increase in energy consumption or cycle time per unit. Regarding Top Panel D, although currently at the TRL 4 (Technology Readiness Level) stage, preliminary estimates suggest that the initial investment in a new die set would be offset by the cumulative material savings within the production of the first 1.5 million units. This roadmap positions the 'new paradigm' as a cost-effective solution for large-scale sustainable packaging.

4. Conclusions

The present work enabled the analysis, study, and testing of the influence of different packaging components on their performance, generating the following contributions and insights in scientific and practical contexts:

- Detailed know-how regarding UN buckets was established, identifying the areas that most influence package strength and creating a foundation for future technical decisions;
- The ideal flange geometry was defined, along with the necessary manufacturing process changes for its implementation;
- The change in the claw geometry provided a significant improvement in the ease of package opening for the final customer;
- The implementation of this new geometry is easily achievable in production, requiring only an alteration to the sheet cutting tool;
- The combination of the optimized flange and claw geometry resulted in a significant increase in the package's resistance during tests.

Due to the high difficulty and cost of manufacturing prototypes, the solution for the new lid panel has not been physically tested yet. However, the solutions for the lid panel can be evaluated by comparison with results obtained through finite element simulation. Although the definition of the new package is not yet fully concluded, the study conducted has brought the company significantly closer to the development and launch of the new model.

Thus, based on the knowledge produced in this work, and with the results of the tests carried out, it is now possible to define a more robust UN packaging, with a smaller quantity of raw material, and therefore, more economical and sustainable. In conclusion, the results validate a new design paradigm in which the structural limits of metal packaging are redefined through geometric complexity rather than material mass, offering a sustainable pathway for the transportation of dangerous goods.

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Naiara P.V. Sebbe: Writing – original draft, Investigation. **Francisco J.G. Silva:** Supervision, Methodology, Investigation, Conceptualization. **Marlene F. Brito:** Visualization, Formal analysis, Data curation. **Ana Júlia Viamonte:** Writing – review & editing, Formal analysis, Data curation. **Alexandra Gavina:** Writing – review & editing, Formal analysis, Data curation. **Isabel Figueiredo:** Writing – review & editing, Formal analysis, Data curation. **Rita C.M. Sales-Contini:** Writing – review & editing, Visualization, Conceptualization.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Francisco J. G. SIlva reports was provided by Polytechnic Institute of Porto School of Engineering. Francisco J. G. Silva reports a relationship with Polytechnic Institute of Porto School of Engineering that includes: employment. Francisco J. G. Silva has patent No patent pending to No patent. If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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