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Approach methodology for the sustainable design of packaging through computational tools: Case study: Water bottles

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ABSTRACT

This paper presents a methodological approach that enables reducing design times through parametric analysis and computerized tools. It also describes a case study using the proposed methodology. Technical-economic benefits are presented for the substitution of the bottle's material from PET to ABS over the bottle's life cycle. It was identified that the global carbon footprint of ABS is smaller (0.07 kg CO_2e) than that of PET (0.096 kg CO_2e) in the manufacture of water bottles. However, in water euritrification there is a negative ratio of 0.4 kg.

1. Introduction

Climate change and environmental pollution are two interrelated issues that are of major concern at the global level [1,2]. In response, the scientific community and industries have increased efforts to reduce the environmental impact of products and processes by developing more sustainable designs and researching alternative materials that lessen the products' environmental impact over their life cycle [3–6]. Plastic is one of the materials that is most widely used worldwide from a wide range of products, and which has a high environmental impact throughout its life cycle [3,4,7].

Global production of plastics (polymer resins and fibers) reached 381 million tons in 2015, 8 times more than in 1975 [3]. Ecosystems and oceans have been significantly affected by the accumulation of plastic products because plastics take a very long time to degrade at the end of their life cycle [3,4]. Of all products made of plastic, the most prominent and most consumed are bottles made of polyethylene terephthalate (PET) [4,7,8].

In general, PET bottles are used to store liquids, and their design features vary depending on the type of liquid to be used [7,8]. New developments in the sustainable design of PET bottles have focused on reducing the thickness of PET bottles [8,9]; however, the material has not been replaced, even though there are different materials available that offer similar properties and have a lower environmental and financial impact. Some of the factors that have prevented such substitution are technology, customer perceptions on sustainable products and the burdensome inter-disciplinary process of performing sustainable design with a green logistics [8–11]. Due to the above, this study presents a methodological approach that reduces design times and enables assessing the benefits of using a

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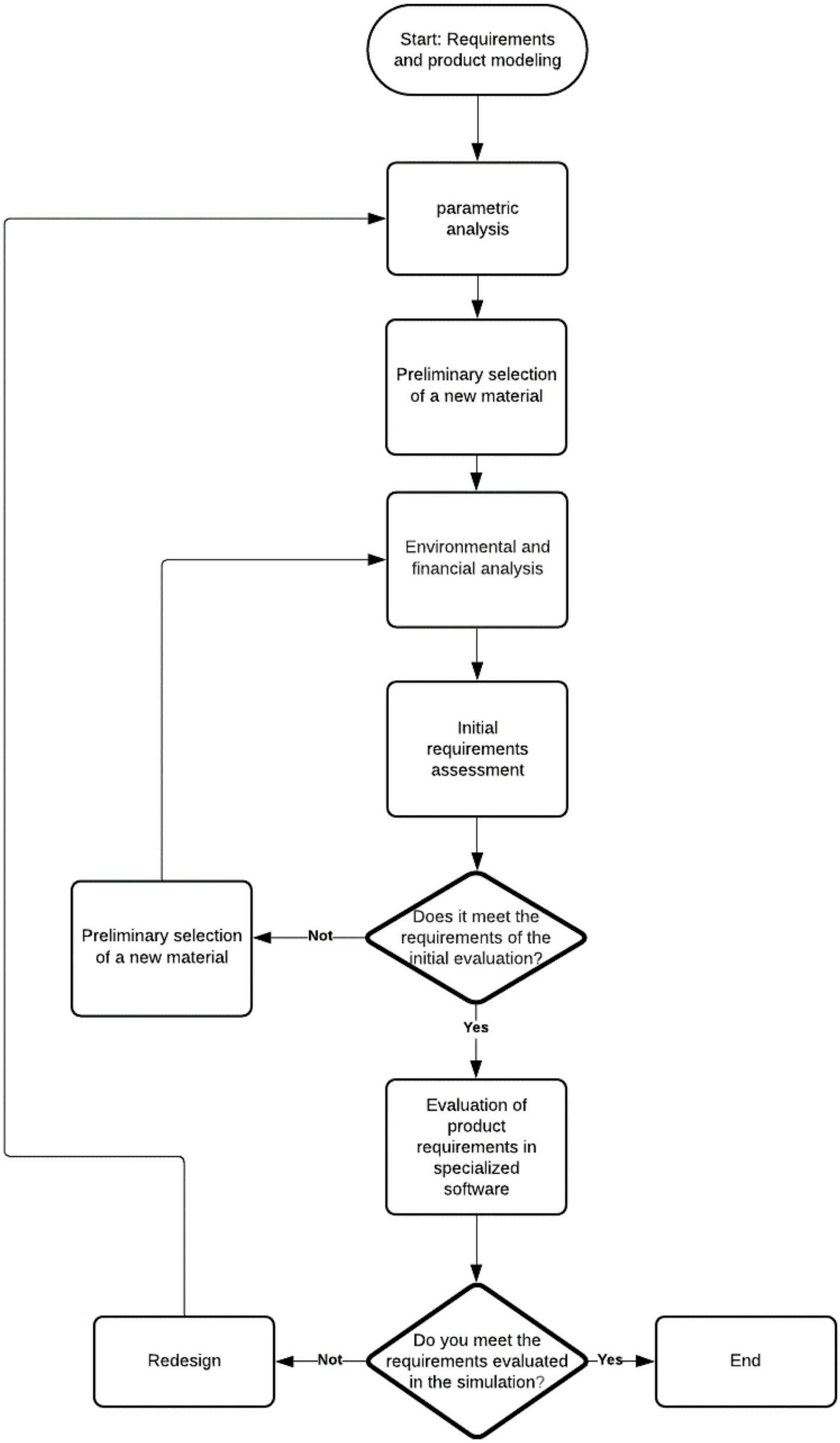

Fig. 1. Methodology for material selection and quick design.
Source: Prepared by authors.

substitute material for PET in water bottles.

2. Methodologies

In the following two sections, first, we explain the general methodology proposed for the study and the characteristics of the product to be studied. In the second section, we introduce and display relevant information for the analysis of the environmental impacts over the life cycle of the studied product.

2.1. General methodology

The design of packaging for the distribution of products is a subject little investigated at the logistics level [10–12]. Fig. 1 displays the new methodology developed in this study. The purpose of this study is to assess the substitution of the PET bottle material for ABS quickly and practically. The procedure requires as inputs the product requirements and a CAD model, as these provide information on functionality and design criteria.

This information is used initially to compare the properties of the currently used material to the proposed material through parametric analysis.

Afterward, the CLM methodology (Leiden University Institute of Environmental Sciences) [12] is applied to study the bottle's environmental and financial impact over its life cycle, in order to perform an initial assessment of the requirements to be fulfilled and to reduce the time and work required for the simulation. If the characteristics of the pre-selected material fulfill the initial requirements, its technical performance is assessed by means of specialized software. If it meets the final requirements, the process ends; otherwise, the product must be redesigned.

The EduPack software is used for the parametric analysis because it enables comparing the properties of the selected materials against other materials with similar properties. SolidWorks is used for 3D product modeling. The SolidWorks Sustainability application is used for the environmental and financial analysis of the product's life cycle. The latter is based on the assumption that the product is shipped by truck over a distance of 1600 Km. Lastly, an assessment is performed on whether the pre-selected material fulfills the design criteria through a finite element simulation implemented in SolidWorks, taking into consideration an impact on the bottle at 50 m/s. The requirements are displayed in the results section in order to follow the logical sequence of the proposed methodology, and so as not to repeat the same information.

For the analysis, the manufacturing region and the region of use were taken into account. The choice of manufacturing region determined the energy resources and technologies used in the material creation and cycle manufacturing stages of product life. The choice of the utilization region helped determine energy resources consumed during the product utilization phase and the destination of the product upon reaching the end of its useful life. The blows were also calculated environmental factors associated with product transport from its place of manufacture to its use. The choice of the manufacturing region determined the energy resources and technologies used in the material creation and cycle manufacturing stages of product life.

2.2. Environmental impact methodology (CML)

The CML methodology (Leiden University Institute of Environmental Sciences) has been used by numerous scientists worldwide to assess environmental impacts over a product's life cycle [12]. The following are the indicators used by this methodology [12]:

- Depletion of abiotic resources
- Acidification potential (AP)
- Eutrophication potential (EP)
- Global warming potential (GWP)
- Ozone layer depletion (ODP)
- Human toxicity potential (HTP)
- Terrestrial ecotoxicity potential (TETP)
- Marine sediment ecotoxicity
- Marine aquatic ecotoxicity
- Freshwater aquatic ecotoxicity (FAETP)
- Land competition

For practical effects, and because their results are the most significant for this study, only the following indicators will be used: the carbon footprint, total energy consumption, atmospheric acidification, and water eutrophication. The SolidWorks Sustainability application is used for financial analysis.

3. Results and discussions

3.1. Product requirements and modeling

Fig. 2 shows the 3D model and the dimensions of the bottle of the study. The dimensions are in centimeters. The initial material

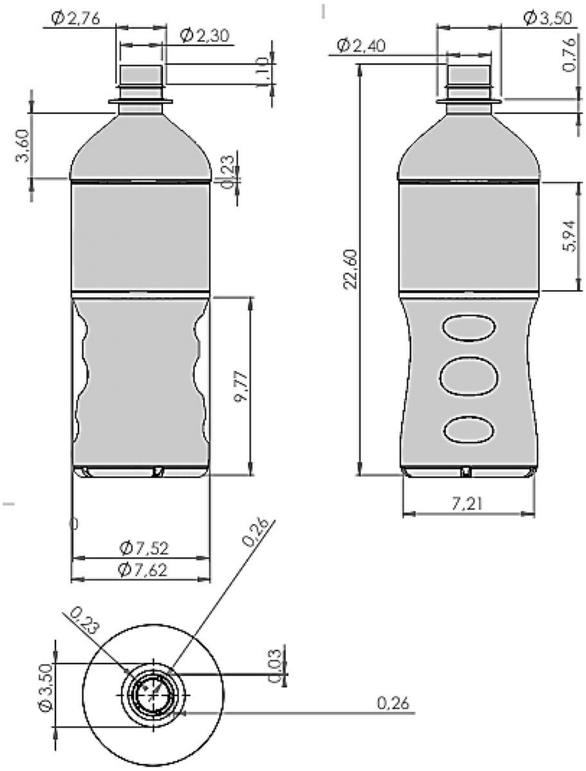

Fig. 2. 3D model and bottle dimensions (units in cm). Source: Prepared by the authors.

Table 1
Product requirements. Source: Prepared by the authors.

Product requirements	
Characteristic	Requirements vs. Reference value
Mass	+20% −30%
Resistance	+20% −30%
Cost/volume	0% −20%
Elasticity	+20% −30%
Water resistance	Good water resistance
Financial impact	≤0.20 USD
Environmental impact	
Carbon footprint	≤0.31 kg CO_2e
Total energy consumption	≤5.2 MJ
Atmospheric acidification	≤7 E−4 kg SO_2e
Water eutrophication	≤1.4 E−4 kg PO_4e

used is PET. The content of the product is drinking water.

Table 1 shows the requirements in quantitative terms of the material that is currently being used. This is used to define selection criteria and the allowable tolerances of the characteristics and/or properties of the new material in comparison to PET.

3.2. Parametric analysis and preliminary selection of the new material

Based on the requirements, a parametric analysis is performed on each product property or characteristic for the current material. Fig. 3 displays Young's modulus and the densities of the different families of materials. A higher Young modulus means that the material is more rigid, and higher density implies greater weight. From Fig. 3, It is concluded that the best candidates are polymers and natural materials, taking into consideration the parameters of density, weight and elasticity. Metals, foams, elastomers and composites do not fulfill the requirements.

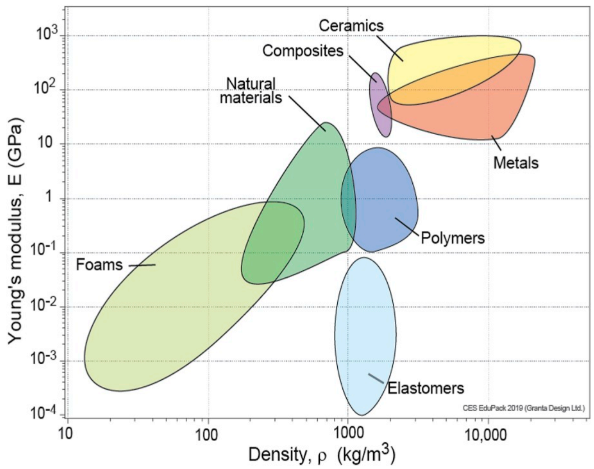

Fig. 3. Young's modulus and density by type of material (Chart created using CES EduPack 2018, Granta Design Ltd.) [13].

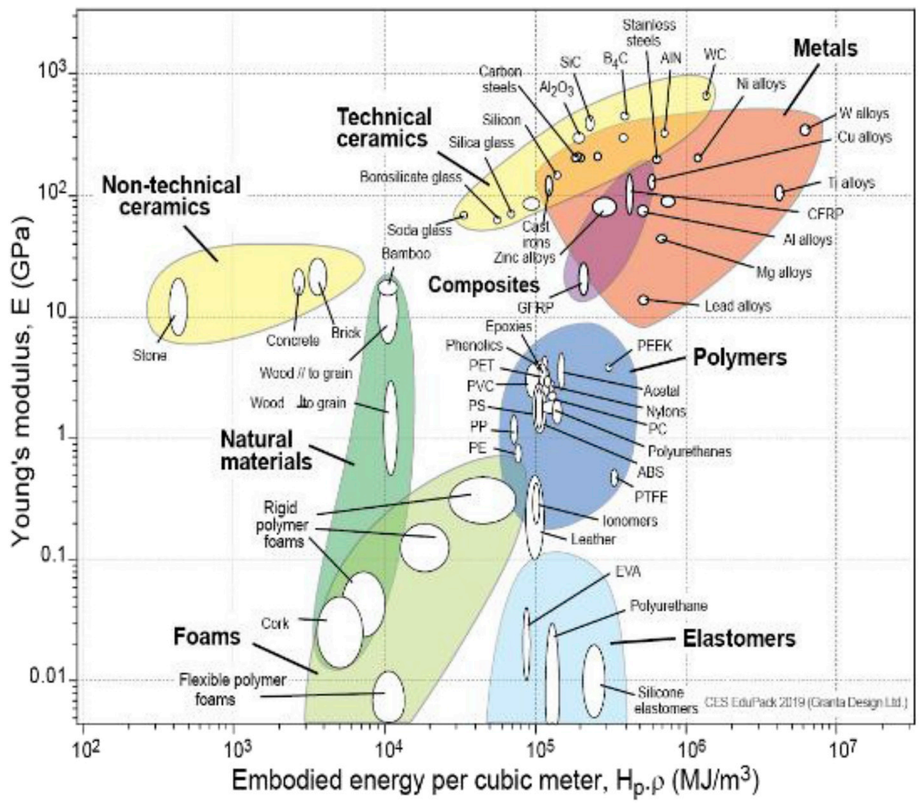

Fig. 4. Young's modulus and energy consumed by cubic meter in manufacturing for different materials (Chart created using CES EduPack 2018, Granta Design Ltd.) [13].

Fig. 4 displays Young's modulus and energy used per cubic meter during manufacturing. In this case, the suitable materials with similar Young Modulus values and energy consumption per cubic meter, according to the requirements are: polymers (ABS, PVC and PS) and natural materials (Wood//to grain). Wood//to grain is ruled out because it may be affected by moisture and water.

Fig. 5 displays flow resistance and relative cost per unit of volume. The two materials that stand out are ABS and PS. The one material out of these, which cost range per unit is relatively lower than PET is ABS. Even though its flow resistance is lower, according to the requirements ABS is within the allowable tolerance for flow resistance.

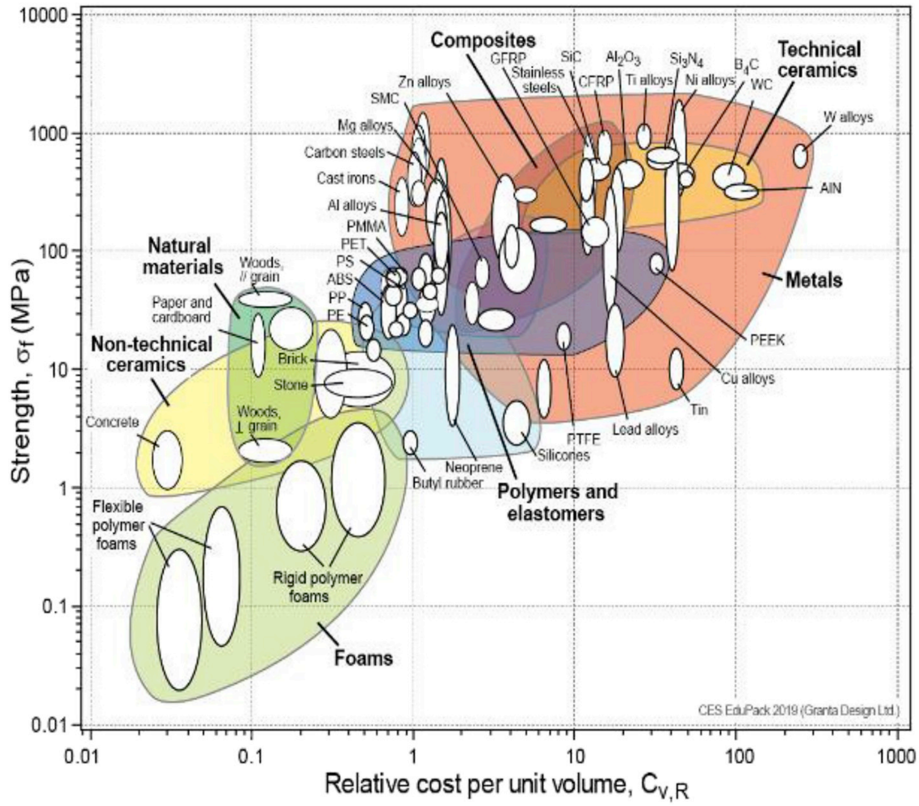

Fig. 5. Flow resistance vs. relative cost per unit of volume for various materials (Chart created using CES EduPack 2018, Granta Design Ltd.) [13].

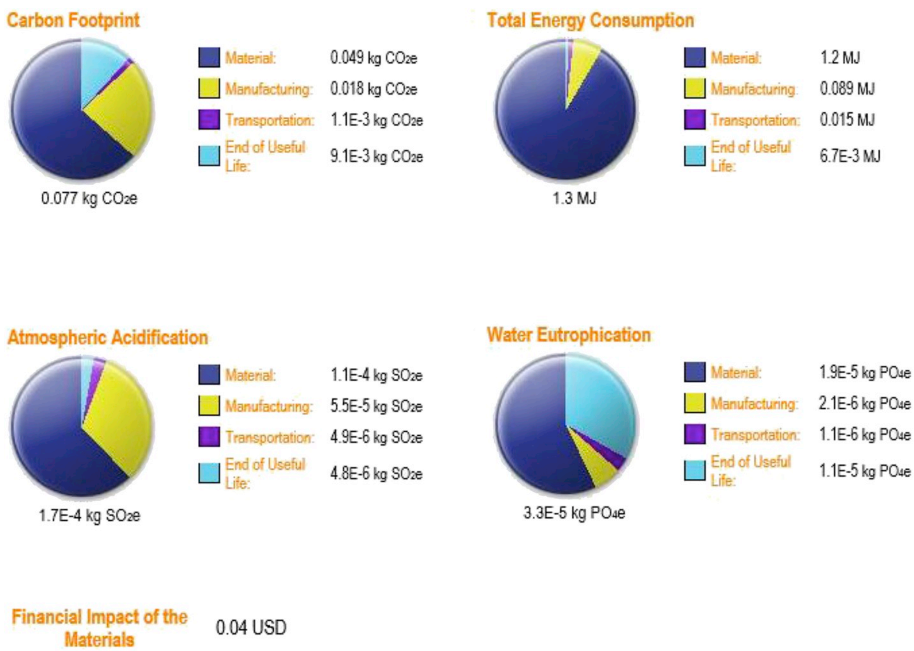

Fig. 6. Environmental impact of the product with ABS, calculated using the CML impact assessment methodology. Source: Prepared by the authors.

Table 2
Sustainability report over the life cycle of the product (ABS).

Sustainability Report						
Model name:	ABS Bottle	Material:	ABS	Mass:	13.58 g	Manufacturing Process:
				Surface area:	1.07E+5 mm^2	Injection molding
		Recycled content:	0.00%	Made to last:	1.0 year	
				In use during:	1.0 year	
Material cost per unit:		2.90 USD/kg				
Manufacturing			Use			
Region:		South America	Region:	South America		
Process:		Injection molding	In use during	1.0 year		
Electricity consumption:		1.8 kWh/lbs				
Natural gas consumption:		0.00 BTU/lbs				
Scrap rate:		2.0%				
Made to last:		1.0 year				
Painted part:		No Paint				
Transportation			End of useful life			
Distance by truck:	1600 km		Recycled:	20%		
Distance by train:	0.00 km		Incinerated:	18%		
Distance by ship:	0.00 km		Landfill:	62%		
Distance by air:	0.00 km					

Table 3
Product life cycle sustainability report (PET). Source: Prepared by the authors.

Sustainability Report						
Model name:	Bottle	Material:	PET	Mass:	18.9 g	Manufacturing process:
				Surface area:	1.07E+5 mm^2	Injection molding
		Recycled content:	0.00%	Made to last:	1.0 year	
				In use during:	1.0 year	
Material cost per unit	2.20 USD/kg					
Manufacturing		Use				
Region:	South America	Region:	South America			
Process:	Injection molding	In use during:	1.0 year			
Electricity consumption:	1.8 kWh/lbs					
Natural gas consumption:	0.00 BTU/lbs					
Scrap rate:	2.0%					
Made to last:	1.0 year					
Painted part:	No Paint					
Transportation		End of useful life				
Distance by truck:	1600 km	Recycled:	20%			
Distance by train:	0.00 km	Incinerated:	18%			
Distance by ship:	0.00 km	Landfill:	62%			
Distance by air:	0.00 km					

3.3. Environmental and financial impact over the life cycle of the product

In order to determine the environmental and financial impact over the life cycle of the product with the new pre-selected material (ABS), we must take into consideration the material, the manufacturing technologies, the region of use, the transportation of the product from the manufacturing location to the region of use, energy consumption during the manufacturing process, water consumption and the useful life of the product, among others.

Fig. 6 displays the environmental impact of the product according to the specifications described in Table 2. The analysis of the environmental impact over the life cycle of the product indicates that the component of greatest incidence in the carbon footprint is the material, equivalent to 63.39% of the total carbon footprint. From the total of energy consumption, the material has the greatest incidence, accounting for 92.15% of the total. The material is also the component with highest impact on atmospheric acidification and water eutrophication.

The data used for the environmental and financial impact assessment of the product manufactured in PET are displayed in Table 3.

Fig. 7 displays the environmental and financial impact assessment of the product in the PET material. For the environmental impact calculation, the same energy values were used as for ABS.

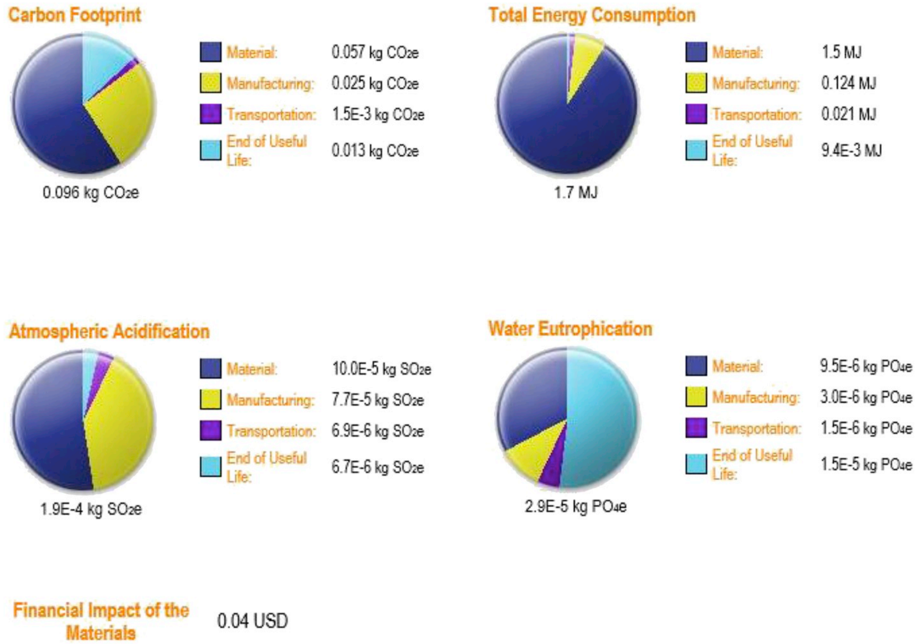

Fig. 7. Environmental impact of the product with the PET material, calculated using the CML impact assessment methodology. Source: Prepared by the authors.

Table 4
Verification and assessment of product requirements with the new material. Source: Prepared by the authors.

Product requirements				
Characteristics	Requirements vs. reference	Fulfills requirement	ABS	PET
Mass (g)	+20% −30%	Yes	13.58	18.9
Resistance (Mpa)	+20% −30%	Yes	43.6	59
Cost/volume (Cv,R)	+0% −20%	Yes (Depends on the local provider)	0.88	0.88
Elasticity (kN/mm)	+20% −30%	Yes	2.3	2.4
Water resistance	Good water resistance	Yes	Good water resistance	Good water resistance
Financial impact (USD)	≤0.20 USD	Yes	0.04	0.04
Environmental impact				
Carbon footprint (kg CO_2e)	≤0.31 kg CO_2e	Yes	0.077	0.096
Total energy consumption (MJ)	≤5.2 MJ	Yes	1.3	1.7
Atmospheric acidification (kg SO_2e)	≤7 E−4 kg SO_2e	Yes	1.9 E−4	1.7. E−4
Water eutrophication (kg PO_4e)	≤1.4 E−4 kg PO_4e	Yes	2.9 E−5	3.3 E−5

3.4. Initial assessment of the requirements

Table 4 displays the evaluation of the requirements following the environmental and financial impact assessment. In this case, the new material with the original design meets the specifications.

Fig. 8 displays the improvement in each of the bottle's characteristics by using ABS rather than PET. In conclusion, the carbon footprint of the bottle is reduced by approximately 19.5% using ABS instead of PET; total energy consumption is reduced by approximately 24% by using ABS; atmospheric acidification decreases by 9% and water eutrophication increases by 18%. However, the financial impact is very similar in both materials, the acquisition cost/kg ABS 1.8 times than cost/kg PET (After having quoted the materials with different local providers) [14]. The cost of purchasing the material for an ABS bottle is 29.3% higher than that of PET, however, throughout its life cycle, the financial impacts are similar. Normally, this life cycle analysis is not performed because only the purchase cost of the material is taken into account. Even so, replacing PET with ABS implies significant technological changes in the industry dedicated to the manufacture of water bottles and their investment may not be justified with this financial analysis, even if their environmental impact has diminished. Another alternative that may allow better results would be the use of polystyrene (PS) or biodegradable bioplastics with PET.

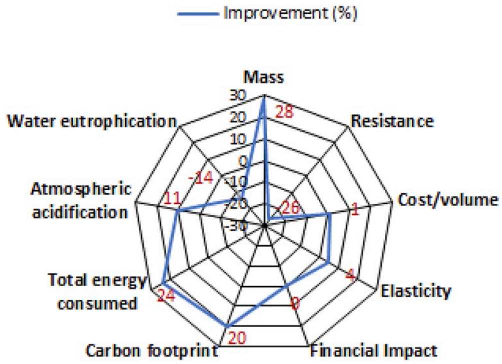

Fig. 8. Improvement from using ABS as the bottle material rather than PET.
Source: Prepared by the authors.

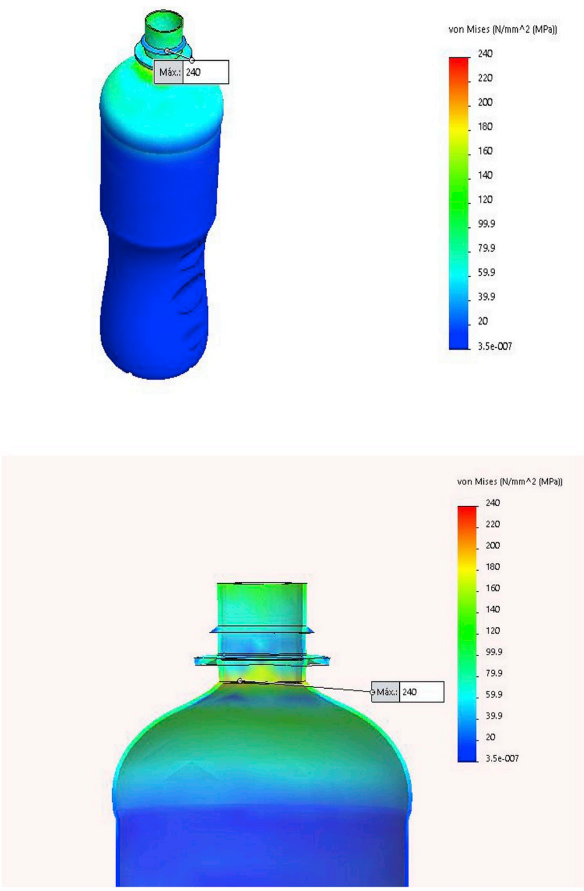

Fig. 9. Stress effects on the ABS bottle. Source: Prepared by the authors.

The weight of the bottle decreases by 28.2%, which is the characteristic that produces the greatest benefits. However, more detailed studies would be required to stress the effects on the bottle, because of the allowable range, the lower resistance of ABS compared to PET and the characteristics of the model.

3.5. Evaluation of product requirements using specialized finite element software

Figs. 9–11 display the results of the simulation of stress effects based on an impact on the bottle at a speed of 50 m/s. The impact is on the upper part of the bottle, specifically on the bottle neck surface. Fig. 9 indicate the areas with greatest stress effect. The greatest

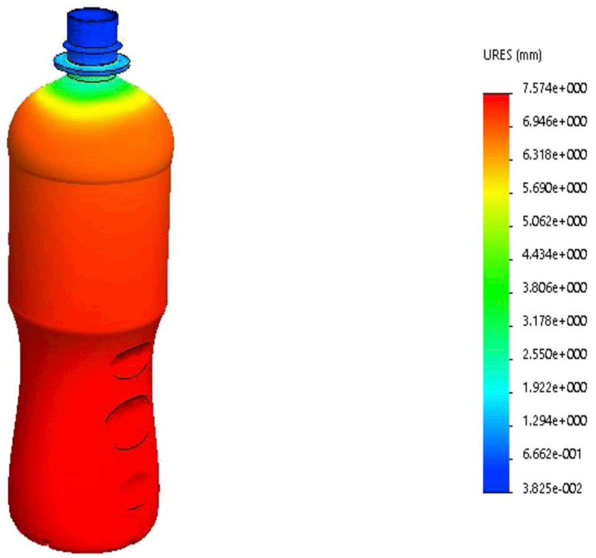

Fig. 10. Deformation of the ABS bottle. Source: Prepared by the authors.

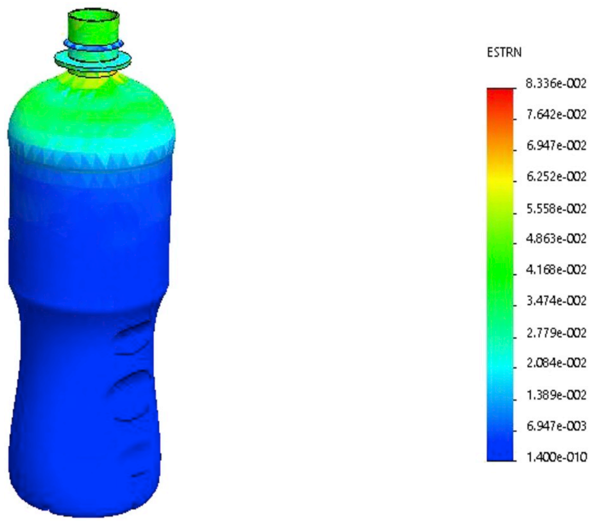

Fig. 11. Unit deformation throughout the bottle.

stress from the impact on the product occurs at the base of the bottle spout, with a value of 240 Mpa.

It is advisable to reinforce the neck section; however, since the polymer is subject to plastic deformation without actually breaking, more detailed tests and simulations should be carried out; in the event it does not fulfill the requirement, the product must be redesigned.

Fig. 10 displays the deformation of the bottle in ABS material and Fig. 11 displays unit deformation throughout the bottle. In these (Figs. 10 and 11), the largest deformation occurs on the base of the bottle neck, which is due to the concentration of stress effects in this area. The deformation values indicate that the bottle can continue to function without problems, because these deformations are not significant in this application. The design time of this product, based on this methodological approach, was approximately one-fourth the design time using the traditional approach.

4. Conclusions

The following conclusions arise from this study.

1. It is economically and environmentally viable to use the ABS material as a substitute for PET in water bottles.

2. The replacement of PET for ABS has a negative effect on water eutrophication.
3. The stress on the bottle from an impact at 50 m/s is concentrated in the base of the bottle spout.
4. An ABS bottle weighs less than a PET bottle with the same design and dimensions.
5. The material is the component that has the greatest environmental impact on this product over its life cycle.
6. Use of ABS instead of PET in water bottles reduces the carbon footprint by 20%.
7. Fluency resistance decreases by 26%, but the amount of deformation of the ABS bottle is acceptable.
8. The proposed methodology produces practical and simple results that help reduce the time required for sustainable design taking into consideration the product's life cycle.
9. Additional detailed simulations are required in order to detect and compare other types of product failure, such as cracking and wear, and for finding the security factor for the conditions presented in this study.
10. Additional future research should focus on manufacturing times of each product in each material and its effects, in view of recent new developments and substantial progress in technologies related to 3D printing and blow molding, among others. This study only takes into consideration the injection molding manufacturing process.

After using the proposed methodology and according to the results, in the life cycle there are different favorable aspects to replace PET with ABS. The economic impacts of the ABS implementation are acceptable in relation to the reduction of the environmental impact diminished by the non-use of ABS, which makes it an effective material for the application. On the other hand, production and technology must be detailed so that it does not affect the competitiveness and productivity of companies. Also, this analysis can be used to analyze and compare PET with other similar materials and find one that best suits the needs of market.

Declaration of competing interest

The authors declare no conflicts of interest.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.csite.2019.100561.

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