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Environmental performance of different water bottles with different compositions: A cradle to gate approach

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Highlights

- Virgin PET (vPET) production had higher environmental impacts.
- Recycled PET (rPET) flake had lower impacts, due to a simpler industrial process.
- Produce the vPET bottle had lower impacts due to less weight than reusable ones.
- To bottle production, the injection step was the highest contributor to the impacts.

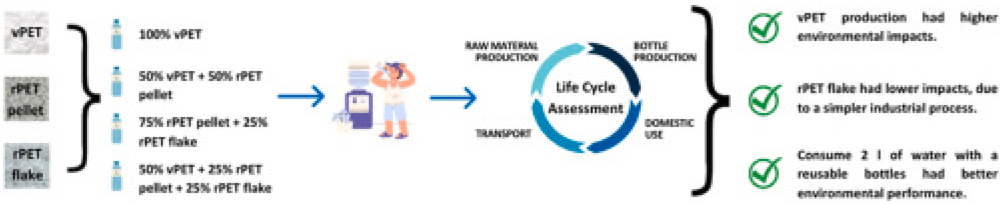
- To consume 2l of water, the reusable bottles had a better environmental performance.

Abstract

Plastic production has increased over the years and the packaging industry was responsible for 44% of the total plastic production. Polyethylene terephthalate (PET), due to its favorable properties, is one of the most used polymers in this sector.

This study first aimed to compare the environmental performance related to the production of a novel recycled PET (rPET) form, namely, rPET flake, and then compare it with the production of virgin PET (vPET) and rPET pellet. Secondly, this study aimed to compare the environmental impacts of four water bottles with different compositions, namely, option A composed with only vPET, option B made with 50% vPET and 50% rPET pellet, option C made with 75% rPET pellet and 25% rPET flake, and option D made with 50% vPET, 25% rPET pellet and 25% rPET flake. Option A was designed as a single-use water bottle, while the remaining options (Options B, C and D) were thought to be reusable bottles, and for that reason were heavier and more robust compared to Option A. The environmental impact assessment followed the International Standard Rules of Life Cycle Assessment (LCA), and the impact assessment method used was the Environmental Product Declaration. Ecoibéria and Logoplaste provided the majority of the required data, and three functional units were considered. The first one was the production of 1 kg of PET, the second was the production of different water bottles, and finally, the third one was the consumption of 2l of water with different water bottles. As a result, it was first observed that the production of rPET flake in comparison to vPET reduces, on average, 79% of the impacts, and rPET pellet reduces 10% of the impacts. Secondly, in the production of the different water bottles, Option A, the single-use bottle, presented the lowest environmental impacts in almost all categories. Finally, when taking into account the reusable factor, the use of single-use bottles presented the higher environmental impact in all categories, probably because of the dilution of the environmental impacts associated with the production of heavier and robust reusable bottles by the multiple times of uses of these bottles.

Graphical abstract



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1. Introduction

Plastic production has been increasing over the years to satisfy the human population's requirements. In 2022, global plastic production increased by 4% compared to 2021, with China as the biggest producer, responsible for 32%, and Europe with only 15% of the global production (Plastics Europe, 2022a). In 2021, the packaging industry, including plastic water bottles production, was responsible for 44% of the total plastic produced (Plastics Europe, 2022a), and one of the most used polymers in this industry seems to be polyethylene terephthalate (PET) due to its favorable properties such as strength, versatility, chemical and thermal stability, durability, transparency, and cost-effectiveness (Marathe et al., 2019; Nisticò, 2020; Olatayo et al., 2021; Tsironi et al., 2022; Vallejos et al., 2022). However, some of these advantages, such as durability, could also be considered disadvantages since the disposal of these bottles could have significant environmental and social impacts. According to Plastics Europe (2022b), in 2020, only 46% of plastic packages produced in Europe were recycled, ending the remaining amount in energy recovery treatments (37%) or in landfills (17%). However, the plastic recycling rate has been increasing mainly due to the scarcity and the rising price of fossil fuel resources by-products, and also because of the sought of new alternatives, such as including more recycled materials or looking for alternative materials, such as bio-based polymers (Nisticò, 2020). It is estimated that in 2021, the number of recycled plastics used in the packaging industry raised to 8.5%, indicating an upward trend compared to the previous year (Plastics Europe, 2022a). In this context, several studies evaluated the environmental impact of using rPET in the production of plastic bottles. Stefanini et al. (2021) conducted a study comparing the environmental impact of PET, recycled (r)PET, glass, and returnable glass bottles used for packaging milk, concluding that the rPET bottles have the lowest environmental impact. Benavides et al. (2018) also evaluated and compared the environmental impact of the production of PET bottles from different sources, namely virgin fossil fuel feedstocks, rPET, and cellulosic biomass, and concluded that bio-derived and rPET bottles offered both lower greenhouse gas (GHG) emissions and fossil fuel consumption than fossil fuel-derived PET bottles. A similar conclusion was taken by Shen et al. (2012), where recycled and bio-based materials also offered superior environmental benefits over single-use petrochemical PET bottles, and by Horowitz et al. (2018), where the rPET and Environmental Solution (ENSO) bottles were generally better than the polylactic acid (PLA) and regular PET bottles. ENSO bottle is a relatively new alternative created to increase biodegradability of the regular plastic bottles in landfills, where it was added an additive that makes the bottles more enticing to the microorganisms responsible for the degradation of the plastic bottles (ENSO Bottles, 2009). However, only a few studies focus on the environmental comparison of using different recycled PET forms, such as pellet and flake forms, and to our knowledge, none focuses on their usage in plastic bottle production. Shen et al. (2010) demonstrated that fibers produced directly from rPET flakes had a lower environmental impact than when rPET was used in pellet form. Previously, Arena et al. (2003) also confirmed that from the several scenarios evaluated, the recycled flakes production scenario was always environmentally preferable. Additionally, Bataineh (2020) recently found that the processing stage for the conversion of plastic wastes into rPET flake was the life cycle step with the highest environmental impact when compared with collection, sorting, and separation. Finally, Chilton et al. (2010) also noted that in the comparison of environmental emissions associated with extracting value from post-consumer PET through recycling and thermal recovery routes, the recycling option demonstrated an overall decrease in environmental impact.

The majority of the studies focusing on the environmental approach use the Life Cycle Assessment (LCA) tool. This tool allows the evaluation and quantification of the environmental impacts of a product, process, or system throughout its entire life cycle, from raw material extraction to disposal or recycling (Gracida-Alvarez et al., 2023; Saleem et al., 2023; Stefanini et al., 2021; Zhou et al., 2023). In the present study, an LCA was conducted to evaluate the environmental performance across three dimensions. First, the environmental performance of different PET forms, namely, virgin PET (vPET) and recycled PET (rPET). Second, to evaluate the environmental performance of producing four water bottles, with different weights and compositions; and third to measure the environmental significance of the use of reusable bottles versus the single-use.

2. Methods

To evaluate the environmental performance of the different PET forms or different PET bottle compositions the International Standard Rules of LCA were used, as detailed in the sections below (ISO14040, 2006, ISO14044, 2006). SimaPro software (version 9.4.0.1, PRé Sustainability, Amersfoort, The Netherlands) was applied to model the life cycle impact, through the Environmental Product Declaration (EPD, 2018) method.

2.1. Goal and scope definition

This study aims to assess the integrated environmental performance across three dimensions. First, the aim is to evaluate the environmental impact of raw material production, by comparing the production of vPET with two rPET variants (flake and pellet). Second, the study aims to scrutinize the application of the previously studied materials in the production of water bottles with different compositions; and finally, the study aims to measure the environmental significance of the use of reusable bottles versus the single-use.

2.1.1. Production of different PET forms (rPET flake, rPET pellet, and virgin PET)

The present section focuses on the environmental performance of different PET forms, including vPET, rPET flake, and rPET pellet, being this last one the most traditional form of rPET.

The LCA approach followed the concept "from cradle to gate", and for that reason, the system boundaries included several steps until the final product production, which was 1 kg of rPET. Briefly, the production of the rPET flake included residue reception, sorting, crushing, washing, drying, homogenization, and rPET food grade validation, as described in Fig. 1. During sorting, labels, bottle caps, and other products made from more than one type of plastic were separated, and the PET residues were also separated by colour. Subsequently, were ground into small fractions, passed through a hot wash system to remove contaminants, and thereafter by a drying process to minimize the water content of the flakes. Next, a homogenization step took place to promote a better standardization of the mixture. Finally, an optical separation step was applied to ensure that all contaminants were eliminated and all flakes were separated by color and grade as much as possible. A more detailed description of the production and certification of rPET flakes to food grade can be found in EFSA Panel on food contact materials flavourings and processing aids (2016).

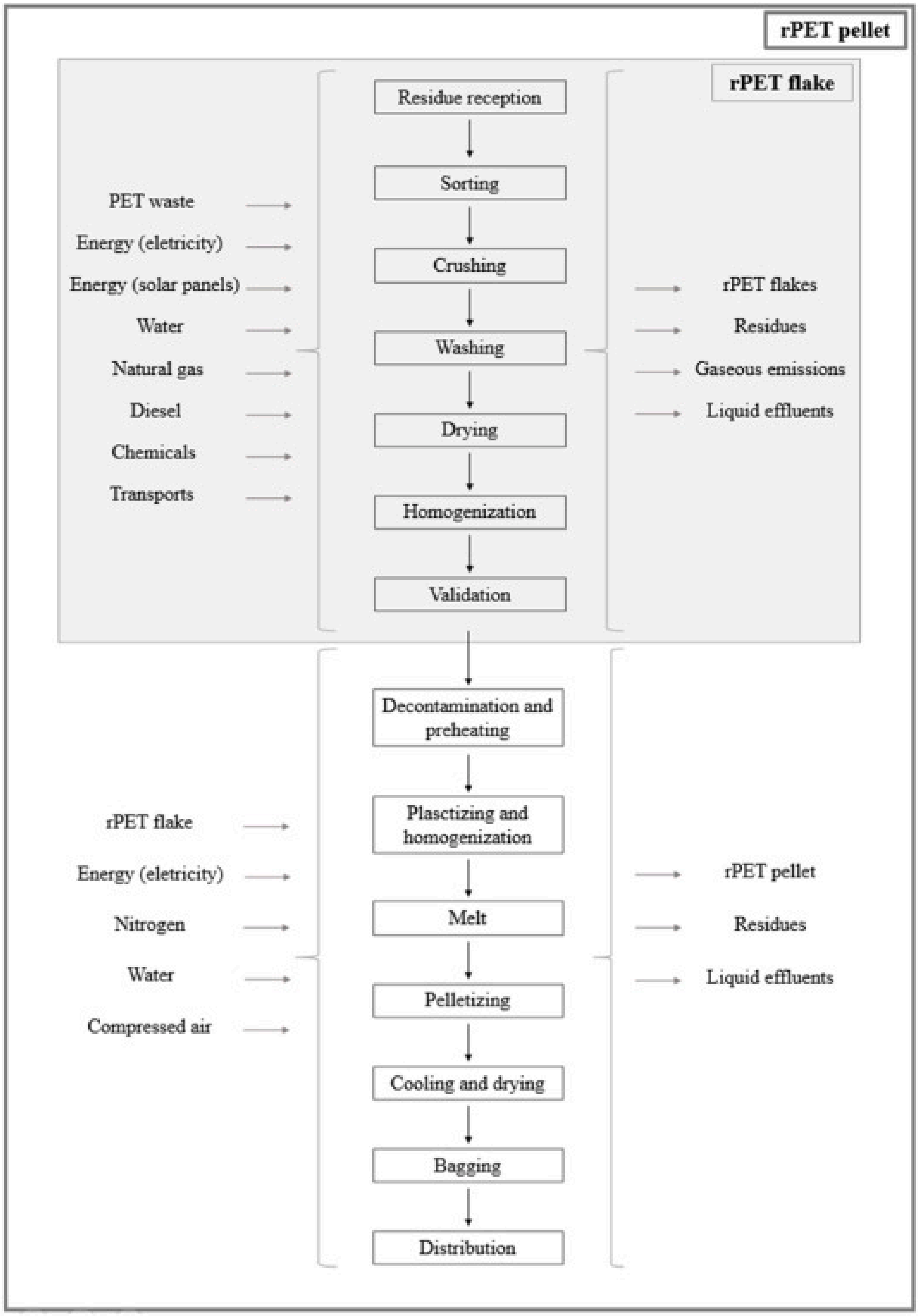

Fig. 1. System boundary considered to the production of rPET flake (grey zone) and pellet (white and grey zones).

The production of rPET pellet used rPET flake as a raw material. For this reason, the first step of the rPET pellet production started with the transportation of the rPET flake to a subsequent section within the same manufactory plant. Here, the material entered the vacuum lock and reactor filling, where decontamination and preheating took place. The material was then discharged into an extruder, where plasticizing and homogenization occurred. Still during the extrusion phase, the material was melted, and thereafter, transformed into spherical granules. Finally, the granules were cooled and dried in the cooling unit for later transportation to a bagging station. The main system boundaries considered for the production of rPET pellets are presented in Fig. 1.

Both rPET forms, flake and pellet, were produced by Ecoibéria company (Vila Nova de Famalicão, Portugal), which provided all the required data for the present study. However, the data provided was not segregated for each production step, constraining the evaluation of the environmental impact of each one of the steps previously described. Also, as vPET was not produced by Ecoibéria company and no longer was possible to find a main producer, the present study considered the production flowchart available in the Ecoinvent database (version 3.7.1.).

The production of vPET started with the esterification of purified terephthalic acid (PTA) and mono ethylene glycol (MEG) to bishydroxyethyl (BHET). Then, BHET is sent to pre-polycondensation in a reactor under vacuum, further to a melt polycondensation reactor at a higher temperature. The final step involved a solid-state polymerization during the polymerization phase. Fig. 2 illustrates the primary system boundaries taken into account for the production of vPET.

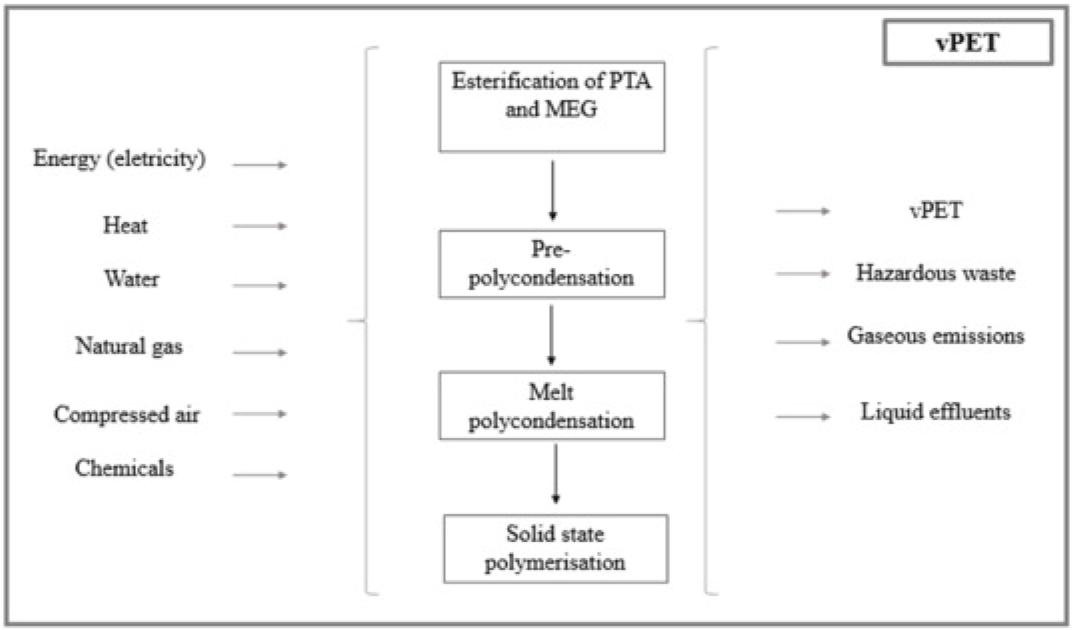

Fig. 2. System boundary considered to the production of vPET, according to the Ecoinvent database. PTA: purified terephthalic acid; MEG: mono ethylene glycol.

The present study excluded from the analysis the construction of infrastructures and equipment, maintenance of the equipment, end-of-life of capital goods, and wastes from administration, laboratory, canteen, or offices.

The functional unit (FU) was defined as 1 kg of produced granulate for further use in bottle production, which means 1 kg of rPET flake, 1 kg of rPET pellet, or 1 kg of vPET.

The present study used an attributional approach and mass allocation since the majority of the studies available in the literature use mass allocation, which allows easier comparison between studies (Bataineh, 2020; Benavides et al., 2018; Horowitz et al., 2018; Olatayo et al., 2021; Shen et al., 2010, 2012). Furthermore, the high price fluctuations for recycled material would not allow a steady economic allocation in time, and energy allocation is not useful for PET producers and their stakeholders, since these used mass units as trade units.

2.1.2. Production of four PET bottles with different compositions and use

This section focuses on comparing the production of plastic bottles with different compositions and their use. The first bottle was made with 100% vPET (option A), the second bottle with 50% vPET and 50% rPET pellet (option B), the third bottle with 75% rPET pellet and 25% rPET flake (option C) and the fourth bottle with 50% vPET, 25% rPET pellet and 25% rPET flake (option D), as described by Table 1. Additionally, the bottle produced with only vPET (option A) was designed as a lighter bottle to be used only once, while the remaining bottles were designed with more material to be used more than once. Because of that, the present study will, first, evaluate and compare the environmental performance related to the production of the four water bottles, considering the production of 0.5l water bottles as FU; and secondly, evaluate and compare the environmental performance of consuming 2l of water using the different water bottles design, to take into account the reusable potential of the options B, C and D. Thus, consuming 2l of water using the single-use bottle (option A) will implicate the production of four 0.5l water bottles. On the other hand, the consumption of 2l of water using the reusable bottles (options B, C, and D) involved only the production of one 0.5l water bottle, due to their reuse potential, with an additional step domestic use which includes washing and refilling processes.

Table 1. Detailed composition of each one of the plastic bottles studied and their weight.

Bottle	Composition	Weight
Option A	100% virgin PET (vPET)	11 g
Option B	50% vPET and 50% recycled PET (rPET) pellet	25 g
Option C	75% rPET pellet and 25% rPET flake	25 g
Option D	50% vPET, 25% rPET pellet and 25% rPET flake	25 g

Regarding the comparison between the production of the different water bottles, it was considered the system boundary described in Fig. 3, which included raw material production, preform injection, stretch blow molding, filling and packaging. The preform injection process consisted on the manufacturing of the preforms, which are cylindrically shaped injection molded components that already have the neck of the final package. The stretch blow molding process began with the heating of the preforms until they became slightly malleable. After this heating, they were transferred into the mold, where the mechanical stretching process of the preform in its axial direction took place while compressed air was injected into the preform. Finally, the bottle was demolded and forwarded to the machine exit (Duarte et al., 2017). To take into account the usage of reusable bottles, the FU defined was the consumption of 2l of water, and the system boundary described by Fig. 3, included an extra step, namely domestic use, which covers washing and filling processes. The consumption of 2l of water per day is a recommendation of the World Health Organization (Tsindos, 2012).

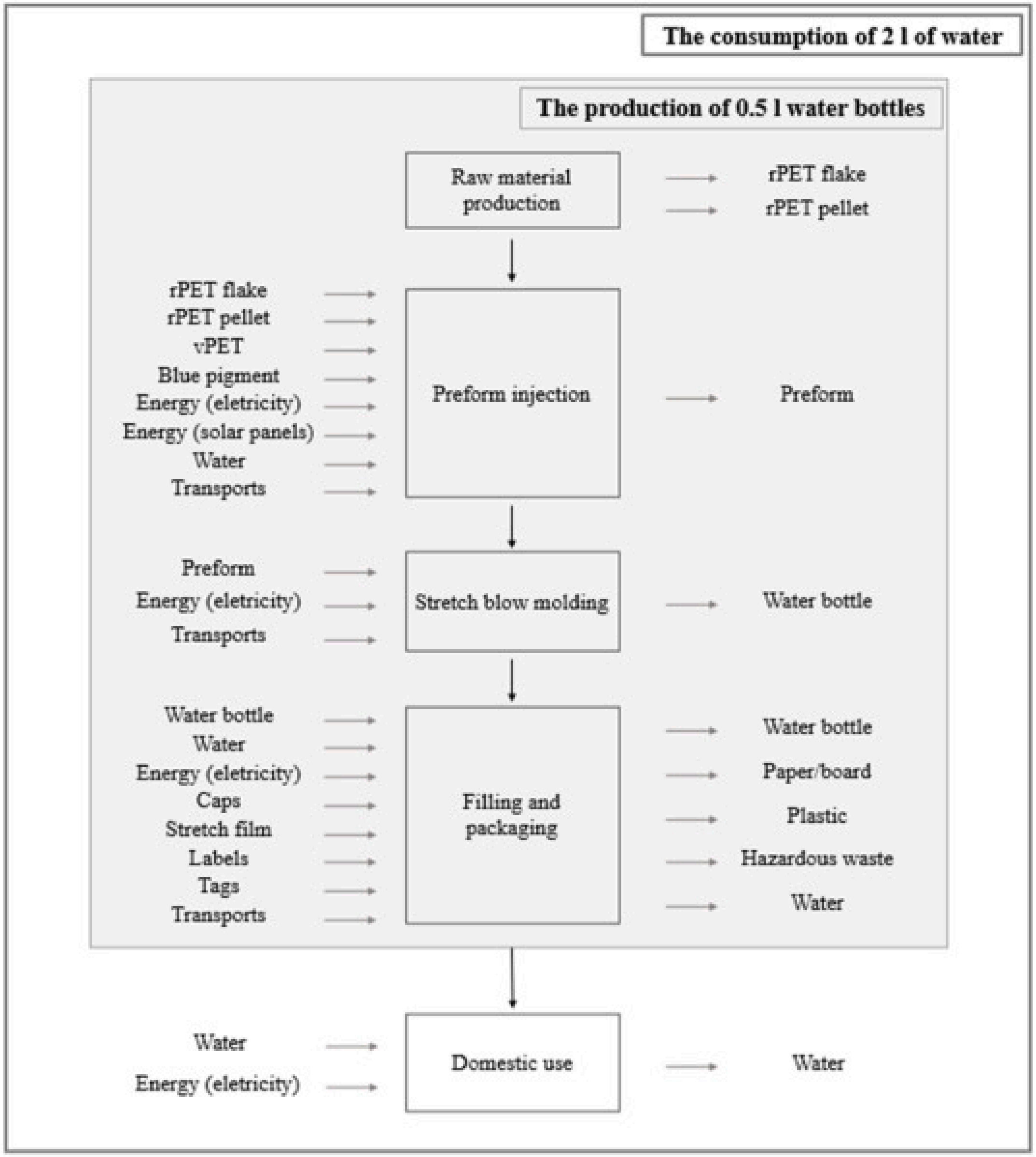

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Fig. 3. System boundary considered to the production of 0.5l plastic bottles (grey zone) and to the consumption of 2l of water (white and grey zones).

At this stage, any type of transportation from the warehouse to the consumer's home is excluded.

The data for the production of the raw material was either provided by Ecoibéria, for rPET, or taken directly from the Ecoinvent database, for vPET. For the injection and stretch blow molding steps, the data was provided by Logoplaste, and for the filling and packaging stage it was provided directly by a company, which could not be shared due to confidentiality issues. In this study the distribution and end-of-life steps, mold manufacturing used in the preform injection step, construction of infrastructures and equipment, maintenance of the equipment, end-of-life of capital goods, and wastes from administration, laboratory, canteen, or offices, were excluded from the analysis.

2.2. Life cycle inventory (LCI)

The inventory analysis aimed to collect the necessary data and organize it by FU. Generally, primary data were used, however, when the same was not available, background data from the Ecoinvent database (version 3.7.1) and related literature was employed. The Ecoinvent database used the mass allocation per cutting unit ("Cut-off, U") and the electricity as the Portuguese electricity mix. Whenever possible and applicable, it was used the data from Europe ("RER"). In the cut-off approach, the primary (or previous) products, such as vPET, do not get any credit or burden from recycling, and therefore the recycled product is derived from non-economically valued waste, allowing it to utilize a burden-free feedstock (Corona et al., 2019).

2.2.1. Production of different PET forms (rPET flake, rPET pellet, and virgin PET)

Table A1 and Table A2, in appendix, describe the inventory list for the production of rPET flake and rPET pellet, respectively. Table A5 (appendix) outlines the detailed composition of the chemicals used in the rPET flake production, Table A6 (appendix) provides the detailed composition of the gaseous emissions and Table A7 (appendix) describes the detailed composition of the liquid effluents. All the data about rPET production was made available by Ecoibéria. In rPET flake production, most of the data were calculated through the weighted average of the Ecoibéria company's monthly consumption during 2021, except for gaseous emissions characterization, where the only data available were related to December 2019. In contrast, for the production of rPET pellet, the majority of data was based on theoretical or preindustrial values, since the plant is still in the start-up phase. In both rPET forms production, it was considered that liquid effluents were routed to the nearest wastewater treatment plant. Data related to the transportation of residues and/or raw materials were obtained also from Ecoibéria company, and the distances between Ecoibéria plant and their stakeholders were calculated through Google Maps (https://www.google.pt/maps/ ↗). When road transport was needed, the present study considered the use of 16–32 metric ton lorry belonging to the EURO6 class, since this load capacity represented around 78% of all trucks circulating in Europe, in 2021 (Eurostat, 2021).

In the production of vPET, the Ecoinvent database was used, as it was not feasible to identify a local producer.

2.2.2. Production of four PET bottles with different compositions and use

The inventory data for the production of 0.5l water bottles with different compositions were described in Table A3 (appendix). All the data about bottle production was made available by Logoplaste. The energy consumption data for the filling and packaging stage was provided directly by a company, which required anonymity. In the water bottle production, most of the data were calculated through the weighted average of the Logoplaste company's annual consumption during 2021. In the context of energy consumption, the efficiency of the installed solar panels was assumed to be 3.5% relative to the overall energy consumption. Data related to the transportation of raw materials were obtained also from Logoplaste company, and the distances between the Logoplaste plant and their stakeholders were calculated through Google Maps (https://www.google.pt/maps/ ↗). When road transport was needed, the present study considered the use of a 16–32 metric ton lorry belonging to the EURO6 class, since according to the information provided, the average quantity transported was 26 tons.

With respect to the consumption of 2l of water with the different bottles, the inventory data were described in Table A4 (appendix). Briefly, to fulfil the FU requirements, the production of four 0.5l water bottles was necessary from option A, while options B, C, and D only required the production of one bottle each. The water bottle production phase followed the previously described, where the majority of the data was made available by Logoplaste. The domestic washing and filling step took into consideration the use of a washing machine with the reference SMD6ZDIO8E (Bosh, Stuttgart, Germany), and the technical specifications can be found in Table A8 (appendix).

2.3. Data quality analysis

The data quality analysis ensures greater reliability of the study's results and was conducted following the International Reference Life Cycle Data System (ILCD) developed by the European Commission (Wolf et al., 2010). This analysis consists of six indicators: precision, completeness, temporal representativeness, geographical representativeness, and technological representativeness. A score from 1 to 5 was assigned to each indicator, with 1 representing the highest degree of quality and 5 the lowest quality level, as shown in Table 2. In addition to identifying the quality levels of various indicators, the overall quality of the dataset is assessed, using the Data Quality Rating (DQR). Table 3 represents the data obtained for the data quality analysis, where it was found that the DQR was equal to 1.6, indicating **high-quality data**.

Table 2. Pedigree matrix used for the data quality analysis, following the International Reference Life Cycle Data System (ILCD) developed by the European Commission (Wolf et al., 2010).

Indicator score	1	2	3	4	5
Precision	Verified data based on measurements	Verified data partly based on assumptions or non-verified data based on measurement	Non-verified data partly based on qualified estimates	Qualified estimate (e.g., by industrial expert)	Non-qualified estimate
Completeness	Representative data from all sites relevant to the market considered, over an adequate period to even out normal fluctuations	Representative data from >50% of the sites relevant for the market considered, over an adequate period to even out normal fluctuations	Representative data from only some sites <50% of sites but from shorter periods	Representative data from only one site relevant for the market considered or some sites but from shorter periods	Representativeness unknown or data from a small number of sites and from shorter periods
Temporal correlation	Less than 3 years of difference to the time period of the dataset	Less than 6 years of difference to the time period of the dataset	Less than 10 years of difference to the time period of the dataset	Less than 15 years of difference to the time period of the dataset	Age of data unknown or more than 15 years of difference to the time period of the dataset
Geographical correlation	Data from area under study	Average data from larger area in which the area under study is included	Data from area with similar production conditions	Data from area with slightly similar production conditions	Data from unknown or distinctly different area

Indicator score	1	2	3	4	5
Technological correlation	Data from enterprises, processes and materials under study	Data from processes and materials under study (i.e. identical technology) but from different enterprises	Data from processes and materials under study but from different technology	Data on related processes or materials	Data on related processes on laboratory scale or from different technology

Table 3. Data quality of the present study using Pedigree Matrix detailed in Table 6.

Indicator score	Description	Condition	Rate
Precision (P)	Measure of the data variability values for each data expressed	Data is measured for most of the products. Some of the data is based on assumptions and qualified estimates and calculations	2 Good
Completeness (C)	Percentage of flow that is measured or estimated	All relevant data within the system boundary are included in the study, following the cut-off rules	1 Very good
Temporal representativeness (TiR)	Date of the data and the minimum time period during which the data should be collected	Less than 3 years of difference to the year of study	1 Very good
Geographical representativeness (GR)	Geographical area from which data on unit processes should be collected	Data was collected from companies based in Portugal	1 Very good
Technological representativeness (TeR)	Specific technology or combination of technologies	The current technological setup of a site-specific production unit	1 Very good
Data Quality Rating (DQR)[a)]		**1.6 – "High quality"**	

a)

DQR = (TeR+GR+TiR+C+P+X_w * 4)/(i+4), X_w: weakest quality level obtained among the data quality indicators; i: number of applicable data quality indicators.

2.4. Limitations of the study

In the current study, some limitations should be highlighted. Regarding the rPET production, firstly, the data collected in Ecoibéria was aggregated and not detailed by each life cycle stage of production as it happened in the production of the water bottles. Secondly, the data related to gas effluent characterization was reported from 2019, instead of 2021 as the remaining data. Moreover, the data collected for the production of rPET pellet was, in the majority, based on theoretical or pre-industrial values, since the plant is still in the start-up phase. Finally, since no primary data was found for vPET production, this study considered a secondary database, comparing the production of vPET from a secondary database with the production of rPET assessed through primary data.

In regards to the consumption of the 2l of water, the considered limitation is related to the bottle production, since the data available is linked the production of 0.5l water bottles, and not for the production of a 2l water bottle. This limitation increases the probability of bias error since in single-use bottles this study considers the use of 4 water bottles instead of using only one, with a capacity of 2l of water.

2.5. Life cycle impact analysis (LCIA)

SimaPro (version 9.4.0.1, PRé Sustainability, Amersfoort, The Netherlands) was used to model the life cycle impact, through the Environmental Product Declaration (EPD, 2018) method. Most impact categories were taken directly from the CML-IA baseline method, such as eutrophication, global warming, ozone depletion, and abiotic resource depletion, or from the CML-IA non-baseline method, such as acidification. The water scarcity category was based on the AWARE method and photochemical oxidation was based on the ReCiPe 2008 method (PRé-Sustainability, 2020). A detailed description of each environmental impact category considered in the present study can be found in Table 4. This method is especially important to those who want to create an Environmental Product Declaration, as could be the case of Logoplaste and other water bottle producers, but also allows us a correct comparison with those who choose the CML method since both use the same impact categories. The CML method is one of the most used in the academic field in several areas (Aryan et al., 2019; Briassoulis et al., 2023; Gear et al., 2018; Humbert et al., 2009; Shen et al., 2010; Silva et al., 2018).

Table 4. Environmental impact categories considered in the present study.

Impact category	Unit	Description
Acidification	kg SO_2 eq.	The acidification potential describes the fate and deposition of acidifying substances.
Eutrophication	kg PO_4^{3-} eq.	Eutrophication includes the impacts due to excessive levels of macronutrients (nitrogen and phosphorus) in the surface water caused by the emission of nutrients to the air, water, and soil, which promotes a rapid growth of aquatic plants.
Global warming	kg CO_2 eq.	The global warming category is essentially affected by greenhouse gases.
Photochemical oxidation	kg NMVOC	Photochemical oxidation consists of the formation of reactive substances (mainly ozone) which are harmful to human health and ecosystems.
Abiotic depletion. elements	kg Sb eq.	Abiotic depletion indicates the potential impact of reducing the amount of non-renewable raw materials and is determined according to the extraction of minerals and fossil fuels.
Abiotic depletion. fossil fuels	MJ	
Water scarcity	m^3 eq.	The water scarcity category quantifies the relative scarcity of one cubic meter of water captured in a region, on a scale of 0.1–100 where a value of 1 corresponds to the global average.
Ozone layer depletion	kg CFC-11 eq.	The ozone layer depletion category is related to ozone layer destruction. This destruction can cause harmful effects on human and animal health as it would allow a greater fraction of ultraviolet radiation (UV–B) to reach the Earth's surface.

3. Results

Regarding the production of different PET forms, the environmental impacts are summarized in Table 5. The production of rPET flake appeared to have the lowest environmental impact in all analyzed impact categories, while the production of vPET presented the highest environmental results in the majority of the categories, except eutrophication and water scarcity, where the rPET pellet presented the highest environmental impact. Table A9 (appendix) details the specific input in the production of rPET flake and rPET pellet that has the most significant environmental impact within each evaluated impact category. Here, in the production of rPET flake, the primary contributor to overall impacts was the PET waste, in the majority of the environmental impact categories. While, regarding the production of rPET pellet, the input with the most significant contribution to the majority of environmental impacts was the rPET flake.

Table 5. Summarized environmental impacts of the production of 1 kg of raw material and variation rate between the production of the different PET forms. The environmental impacts were assessed using the Environmental Product Declaration (EPD, 2018) method.

Impact category	**Unit**	**vPET**	**rPET flake**	**rPET pellet**	**rPET flake vs vPET**[a]	**rPET pellet vs vPET**[b]	**rPET flake vs rPET pellet**[c]
Acidification	kg SO_2 eq	8.11E-03	2.13E-03	4.32E-03	−74% ↓	−47% ↓	−51% ↓
Eutrophication	kg PO_4^{3-} eq	8.63E-04	2.68E-04	2.74E-03	−69% ↓	218% ↑	−90% ↓
Global warming	kg CO_2 eq	2.52E+00	4.92E-01	7.94E-01	−81% ↓	−69% ↓	−38% ↓
Photochemical oxidation	kg NMVOC	7.63E-03	1.62E-03	2.63E-03	−79% ↓	−66% ↓	−38% ↓
Abiotic depletion. elements	kg Sb eq	3.39E-04	1.27E-07	1.34E-07	−100% ↓	−100% ↓	−5% ↓
Abiotic depletion. fossil fuels	MJ	6.19E+01	5.70E+00	9.20E+00	−91% ↓	−85% ↓	−38% ↓
Water scarcity	m^3 eq	1.33E+00	2.70E-01	3.01E+00	−80% ↓	126% ↑	−91% ↓
Ozone layer depletion	kg CFC-11 eq	9.98E-06	4.14E-06	4.23E-06	−59% ↓	−58% ↓	−2% ↓
Average[d]					**−79%** ↓	**−10%** ↓	**−44%** ↓

The filling ( ) indicates the smallest, the ( ) the intermediary, and the ( ) the highest impact value related to each environmental impact category assessed when comparing all raw materials; Arrows (↓)or (↑)noted the decrease or increase of the environmental impact value when comparing two raw materials.

a

Variation rate between rPET flake and vPET = (rPET flake – vPET)/vPET.

b

Variation rate between rPET pellet and vPET = (rPET pellet − vPET)/vPET.

c

Variation rate between rPET flake and rPET pellet = (rPET flake − rPET pellet)/rPET pellet.

d

(sum of the differences of the categories/number of categories).

In the comparison between the different raw materials production, the rPET flake allows an average decrease of 79% in environmental impacts when compared to vPET and 44% when compared to rPET pellet. In the comparison between the rPET pellet and vPET, the rPET pellet represented a decrease of 10%, in average, of the environmental impacts.

Regarding the production of four PET bottles with different compositions, Table 6 and Fig. 4 show the environmental impacts of each option considered in the study. Table 7 describes the variation rate between the production of single-use bottles (option A) with the production of reusable bottles (options B, C, and D). In general, reusable bottles had higher environmental impacts than single-use bottles, and whatever the water bottle option considered, the preform injection seemed to be the step with the highest contribution to the environmental impacts in the majority of the impact categories. The stretch blow molding step was the one that presented the lowest environmental impact in all the options considered in the study, and also in all impact categories, representing on average, less than 7% of the total impacts. Table A10 (appendix) outlines the key stages and specific inputs that exert the most significant influence on environmental impacts within the evaluated impact categories during the production of the four water bottles under study. Thus, in Option A the use of vPET and electricity were the key inputs with the greatest impact on overall environmental impact categories. In Options B and D, vPET consistently emerged as the primary contributor across the majority of categories. In contrast, Option C emphasized the leading role of rPET pellet as the key input to the environmental impact.

Table 6. Environmental contribution (%) by life cycle stage to each one of the options studied and overall net value to each environmental impact category. The environmental impacts were assessed using the Environmental Product Declaration (EPD, 2018) method, and the functional unit is equal to the production of one 0.5l water bottle.

Impact category	Unit	Life cycle stages	Option A	Option B	Option C	Option D
Acidification	kg SO_2 eq	Preform injection	42%	52%	42%	50%
		Blow injection	10%	15%	19%	16%
		Filling	48%	33%	39%	34%
		Overall	2.83E-04	4.16E-04	3.47E-04	4.03E-04
Eutrophication	kg PO_4^{3-} eq	Preform injection	43%	73%	75%	65%
		Blow injection	8%	7%	7%	10%
		Filling	49%	20%	18%	26%
		Overall	2.84E-05	6.94E-05	7.64E-05	5.39E-05
Global warming	kg CO_2 eq	Preform injection	49%	56%	38%	55%
		Blow injection	6%	11%	15%	11%
		Filling	44%	33%	46%	34%
		Overall	7.41E-02	9.99E-02	7.12E-02	9.80E-02
Photochemical oxidation	kg NMVOC	Preform injection	50%	58%	42%	57%
		Blow injection	7%	11%	16%	12%
		Filling	43%	31%	42%	32%
		Overall	2.03E-04	2.82E-04	2.07E-04	2.76E-04
Abiotic depletion. elements	kg Sb eq	Preform injection	100%	100%	52%	100%
		Blow injection	0%	0%	1%	0%
		Filling	0%	0%	46%	0%
		Overall	3.74E-06	4.25E-06	6.78E-09	4.25E-06
Abiotic depletion. fossil fuels	MJ	Preform injection	59%	63%	34%	63%

Impact category	Unit	Life cycle stages	Option A	Option B	Option C	Option D
		Blow injection	4%	8%	14%	8%
		Filling	37%	29%	52%	30%
		Overall	1.36E+00	1.72E+00	9.69E-01	1.70E+00
Water scarcity	m^3 eq	Preform injection	30%	60%	62%	52%
		Blow injection	2%	2%	2%	3%
		Filling	68%	37%	36%	45%
		Overall	5.23E-02	9.49E-02	9.88E-02	7.78E-02
Ozone layer depletion	kg CFC-11 eq	Preform injection	97%	98%	97%	98%
		Blow injection	0%	0%	1%	0%
		Filling	3%	2%	3%	2%
		Overall	1.14E-07	1.83E-07	1.09E-07	1.82E-07

The filling ( ) indicates the smallest, the ( ) the second smallest, the ( ) second highest, and the ( ) the highest impact value related to each environmental impact category assessed when was compared all water bottle options.

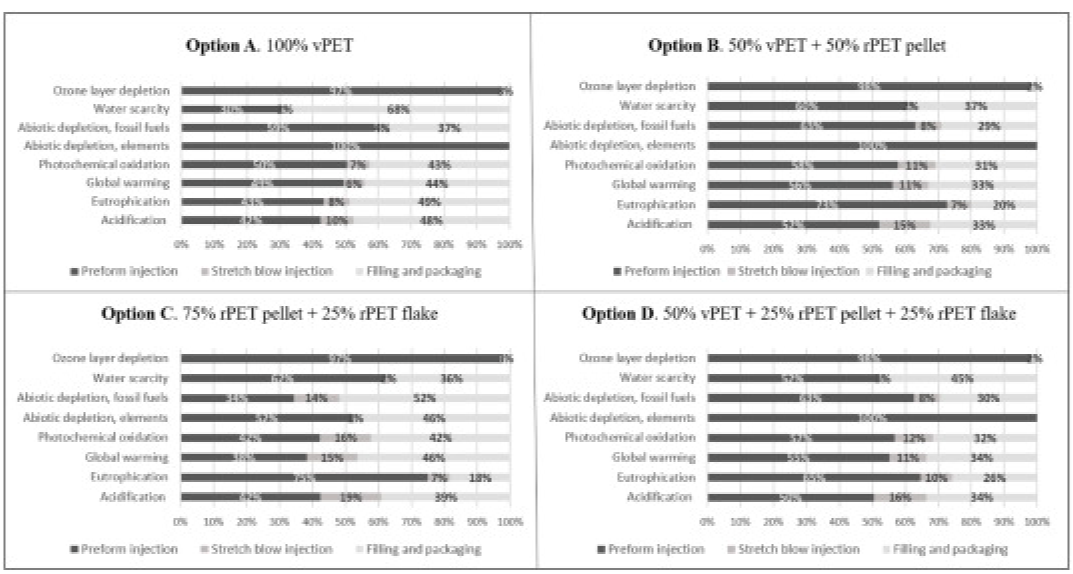

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Fig. 4. Graphical representation of environmental contribution by life cycle stage for the production of the four water bottles under study. The environmental impacts were assessed using the Environmental Product Declaration (EPD, 2018) method, and the functional unit is equal to the production of one 0.5 l water bottle.

Table 7. Variation rate between option A (bottle produced with 100% vPET) and the other bottles.

Impact category	Option B *vs* Option A[a]	Option C *vs* Option A[b]	Option D *vs* Option A[c]
Acidification	47% ↑	22% ↑	42% ↑
Eutrophication	144% ↑	169% ↑	90% ↑
Global warming	35% ↑	−4% ↓	32% ↑
Photochemical oxidation	39% ↑	2% ↑	36% ↑
Abiotic depletion. elements	14% ↑	−100% ↓	14% ↑
Abiotic depletion. fossil fuels	27% ↑	−29% ↓	25% ↑
Water scarcity	82% ↑	89% ↑	49% ↑
Ozone layer depletion	60% ↑	−4% ↓	60% ↑
Average[d]	**56% ↑**	**18% ↑**	**43% ↑**

The arrows (↓) or (↑) noted the decrease or increase of the environmental impact value in comparison to Option A.

a

Variation rate between Option B and Option A = (Option B – Option A)/Option A.

b

Variation rate between Option C and Option A = (Option C– Option A)/Option A.

c

Variation rate between Option D and Option A = (Option D – Option A)/Option A.

d

(sum of the differences of the categories/number of categories).

In comparison to option A (bottle produced with only vPET), option B had an increment of the environmental impacts on an average of 56%, while option C only represented an increase of an average of 18%, and option D of 43%.

The results of the consumption of 2 l of water utilizing different water bottles are described in Table 8 and in Fig. 5. Table 9 describes the variation rate between the use of single-use bottles (option A) with the use of reusable bottles (options B, C, and D). Analyzing the various life cycle stages considered in the current study, the preform injection stage accounted for an average of 59% of the environmental impacts. The domestic use of reusable bottles was responsible for 8% of the environmental impacts, on average. Furthermore, it was noted that the stretch blow molding stage exhibited significantly lesser impacts, accounting for only 7% of the environmental impacts, on average. For this part of the study, a table with the most significant stages and inputs was not generated, as the results presented are the same as those shown for the production of 0.5 L of water in Table A10 (appendix). Thus, it can be observed that the additional household use stage included in this part of the study has a relatively insignificant contribution to the overall process. Comparing the four options under study, in the majority of the environmental impact categories, the use of option C (water bottle fully produced by recycled material and reusable) presented the lowest environmental impact. In contrast, the use of option A, the bottle produced with only vPET and for single-use, was the option with the highest environmental impacts for all impact categories. In comparison with option A, the use of option B represented a decrease of the environmental impact by an average of 56%, option C, a reduction of an average of 65%, and option D was noted for a reduction of an average of 59%.

Table 8. Environmental contribution (%) by life cycle stage to each one of the studied options and overall net value to each environmental impact category. The environmental impacts were assessed using the Environmental Product Declaration (EPD, 2018) method, and the functional unit is equal to the consumption of 2 l of water with the different bottles studied.

Impact category	**Unit**	**Life Cycle stages**	**Option A**	**Option B**	**Option C**	**Option D**
Acidification	kg SO_2 eq	Preform injection	42%	50%	40%	48%
		Blow injection	10%	15%	18%	15%
		Filling	48%	31%	37%	32%
		Domestic use	–	4%	5%	4%

Impact category	Unit	Life Cycle stages	Option A	Option B	Option C	Option D
		Overall	1.13E-03	4.34E-04	3.64E-04	4.20E-04
Eutrophication	kg PO_4^{3-} eq	Preform injection	43%	53%	56%	44%
		Blow injection	8%	5%	5%	6%
		Filling	49%	15%	14%	18%
		Domestic use	–	27%	25%	32%
		Overall	1.14E-04	9.50E-05	1.02E-04	7.96E-05
Global warming	kg CO_2 eq	Preform injection	49%	55%	37%	54%
		Blow injection	6%	11%	15%	11%
		Filling	44%	32%	45%	33%
		Domestic use	–	2%	3%	2%
		Overall	2.96E-01	1.02E-01	7.34E-02	1.00E-01
Photochemical oxidation	kg NMVOC	Preform injection	50%	56%	41%	55%
		Blow injection	7%	11%	15%	11%
		Filling	43%	30%	41%	31%
		Domestic use	–	4%	4%	3%
		Overall	8.13E-04	2.90E-04	2.14E-04	2.84E-04
Abiotic depletion. elements	kg Sb eq	Preform injection	100%	100%	52%	100%
		Blow injection	0%	0%	1%	0%
		Filling	0%	0%	46%	0%
		Domestic use	–	0%	0%	0%
		Overall	1.49E-05	4.25E-06	6.81E-09	4.25E-06

Impact category	Unit	Life Cycle stages	Option A	Option B	Option C	Option D
Abiotic depletion. fossil fuels	MJ	Preform injection	59%	62%	33%	62%
		Blow injection	4%	8%	13%	8%
		Filling	37%	29%	51%	29%
		Domestic use	–	1%	2%	1%
		Overall	5.44E+00	1.75E+00	9.95E-01	1.73E+00
Water scarcity	m^3 eq	Preform injection	30%	46%	48%	38%
		Blow injection	2%	2%	2%	2%
		Filling	68%	29%	28%	33%
		Domestic use	–	23%	22%	27%
		Overall	2.09E-01	1.23E-01	1.27E-01	1.06E-01
Ozone layer depletion	kg CFC-11 eq	Preform injection	97%	98%	97%	98%
		Blow injection	0%	0%	1%	0%
		Filling	3%	2%	3%	2%
		Domestic use	–	0%	0%	0%
		Overall	4.57E-07	1.83E-07	1.10E-07	1.82E-07

The filling ( ) indicates the smallest, the ( ) the second smallest, the ( ) second highest, and the ( ) the highest impact value related to each environmental impact category assessed when was compared all water bottle options.

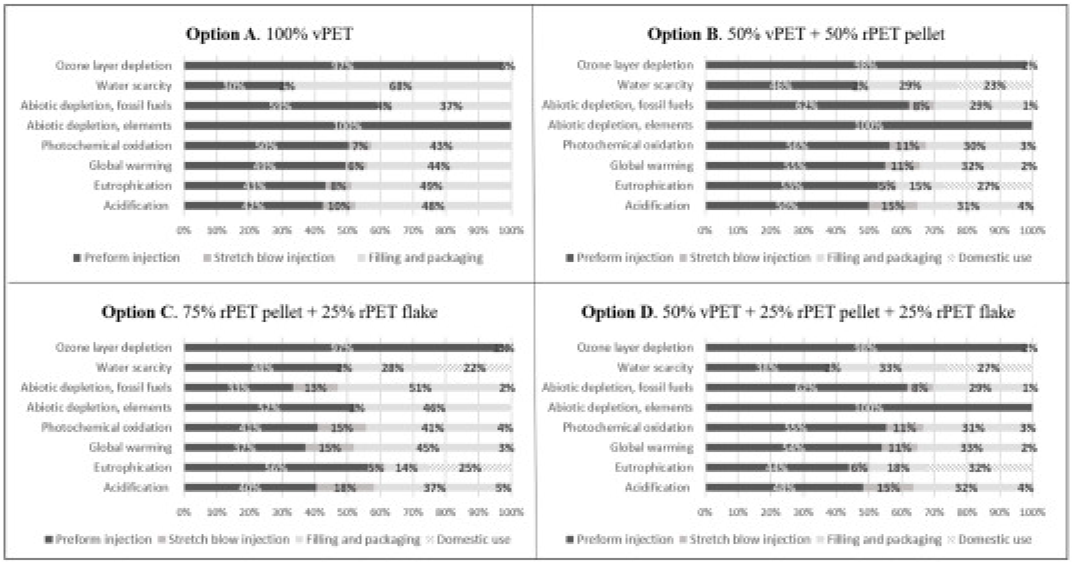

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Fig. 5. Graphical representation of the environmental contribution by life cycle stage for the consumption of 2 l of water with the four bottles under study. The environmental impacts were assessed using the Environmental Product Declaration (EPD, 2018) method, and the functional unit is equal to the consumption of 2 l of water with the different bottles studied.

Table 9. Variation rate between the consumption of 2 l of water using option A (bottle produced with 100% vPET) or the other bottles.

Impact category	**Option B *vs* Option A**[a]	**Option C *vs* Option A**[b]	**Option D *vs* Option A**[c]
Acidification	−62% ↓	−68% ↓	−63% ↓
Eutrophication	−16% ↓	−10% ↓	−30% ↓
Global warming	−66% ↓	−75% ↓	−66% ↓
Photochemical oxidation	−64% ↓	−74% ↓	−65% ↓
Abiotic depletion. elements	−72% ↓	−100% ↓	−72% ↓
Abiotic depletion. fossil fuels	−68% ↓	−82% ↓	−68% ↓
Water scarcity	−41% ↓	−39% ↓	−49% ↓
Ozone layer depletion	−60% ↓	−76% ↓	−60% ↓
Average[d]	**−56%** ↓	**−65%** ↓	**−59%** ↓

The arrow (↓) noted the decrease of the environmental impact value to consumed 2 l of water using Options B, C, and, D, in comparison to Option A.

a

Variation rate between the use Option B and Option A = (Option B – Option A)/Option A.

b

Variation rate between the use Option C and Option A = (Option C– Option A)/Option A.

c

Variation rate between the use Option D and Option A = (Option D – Option A)/Option A.

d

(sum of the differences of the categories/number of categories).

4. Discussion

In general, the production of rPET flake appeared to have a lower environmental impact in all impact categories analyzed than the production of vPET, which presented the highest environmental results in the majority of the categories, except for eutrophication and water scarcity. Despite some authors pointing out the impacts of recycled products as strongly influenced by the choice of the allocation method applied (Bataineh, 2020; Shen et al., 2010, 2012), the results of the present study were in line with the majority of the literature available, where the production of rPET resulted in an important environmental saver over the production of vPET (Bataineh, 2020; Franklin Associates, 2018; Shen et al., 2012). Indeed, Sinha et al. (2010) previously suggested that the recycling of PET not only serves as a partial solution to the solid waste problem but also contributes to the conservation of raw petrochemical products, saving 50–60% of energy when compared to making the same product from vPET. As in Franklin Associates (2018), the present study showed that the water consumption was higher for the production of rPET pellet than for produced vPET or rPET flake. This higher consumption probably explains the higher impacts observed for the eutrophication and water scarcity categories, since water scarcity quantifies the relative scarcity of one cubic meter of water captured in a region, and eutrophication is related to excessive levels of macronutrients in the surface water causing the rapid growth of aquatic plants (PRé-Sustainability, 2020). In the comparison between the rPET flake and rPET pellet, the rPET flake seemed to be the better environmental choice, since it presented lower environmental impacts. This result was expected and can be easily explained by the fact that the production of the rPET pellet included all the life cycle steps to produce the rPET flake plus extra steps, such as preheating, plasticizing and homogenization, pelletizing, cooling, and drying. However, despite the lower impacts related to the production of rPET flake, the utilization of this material is currently restricted due to its heterogeneity which may affect the injection process. Indeed, the production of rPET flake is an innovative and relatively recent technology, having obtained approval from Logoplaste in 2016. In the future is expected that the technology can be improved and more rPET flake content can be included in the final products.

Regarding the production of the four different water bottles, the results were the opposite of what is available in the literature (Benavides et al., 2018; Horowitz et al., 2018; Marathe et al., 2019; Shen et al., 2011, 2012), since in the present study the bottle with the vPET was the one that presented the lowest environmental impact. This can be explained by the fact that the vPET water bottle was designed as a single-use bottle, while the remaining bottles, with rPET, were thought of as reusable ones, being heavier and thereby consuming more raw material and energy in their production. Even so, independently of these results, looking at the life cycle steps contribution, Horowitz et al. (2018) observed that either in rPET or vPET bottles, it was the manufacturing, packaging, and distribution steps that had a higher contribution to the environmental impacts. Although the distribution step was not evaluated in the present study, these results are still in accordance with their study, since the manufacturing step, which includes preform injection and stretch blow molding, was the one that presented the higher contribution to the environmental impacts. A similar conclusion was also taken recently by other authors (Kouloumpis et al., 2020; Marathe et al., 2019).

Another aspect to be taken into account is related to the abiotic depletion category, where the bottle made only of recycled materials (option C) had a much lower environmental impact than the other bottles. This can be attributed to the fact that this impact category relies on the extraction of new materials, and this bottle was made exclusively from recycled content.

Similar to the present study, Olatayo et al. (2021) evaluated the life cycle impact of single-use PET bottles and reusable PET bottles based on consumption patterns in South Africa and concluded that single-use bottles have a higher environmental impact than reusable ones. This means that the higher environmental impact associated with the production of heavier and robust reusable bottles was diluted by the multiple numbers of uses of these same bottles. Additionally, it is also important to note that, the domestic use step, added to the system boundary of the reusable bottles did not spend enough energy and resources to invert the worst-case scenario of using only single-use water bottles to consume 2 l of water.

It's noteworthy that for the environmental impacts of the reusable bottle to outweigh those of the single-use bottle, the reusable option only needs to be used twice. Additionally, in general, when considering the consumption of 2 l of water as FU, the major environmental contributor step was bottle manufacturing. This is consistent with what was reported by other studies (Kouloumpis et al., 2020; Olatayo et al., 2021).

Finally, it is important to agree with other authors, not only the search for new and alternative materials is needed, but also equal attention should be given to new designs and production processes that could save consumption of more energy and resources (Olatayo et al., 2021; Tsironi et al., 2022), as explored by Steenis et al. (2018).

5. Conclusions, limitations, and future research

This study was conducted to promote sustainable decision-making in new products or industrial processes. In the presented study, it was first concluded that the production of vPET presented a higher environmental impact in almost all categories, while the production of rPET flake appeared to be the most successful alternative due to its simpler production process when compared to the rPET pellet.

Regarding the production of the four water bottles studied, the bottle with the vPET presented the lowest environmental impact. This happened, as expected, due to this bottle weighing less than reusable ones, 11 g compared to 25 g. Moreover, regardless of the specific bottle under consideration, the manufacturing phase, encompassing preform injection and stretch blow molding, emerged as a significant contributor to the overall environmental impacts.

Considering the consumption of 2 l of water, reusable bottles had a better environmental performance than single-use bottles, even considering an extra stage of domestic washing and refilling. This only happened due to the reusable factor, where the higher environmental impact associated with the production of heavier and more robust reusable bottles was diluted by their multiple numbers of uses.

This article provides a notable advantage by enabling comprehension and interpretation across all segments of the value chain. Bottle producers may find the results about 0.5 l water consumption more relevant, whereas consumers or policymakers may prioritize data related to 2 l water consumption.

To minimize the environmental footprint related to water bottle production a targeted approach should be taken focusing on stages that have a higher influence on the overall impact. In the case of the present study, the preform injection stage emerges as a key player in environmental repercussions, and because of that, should be strategically selected to be included in the decarbonization strategies. These decarbonization strategies should include a strategy to reduce the consumption of energy, by implementing, for instance, a routine for machine maintenance, or enhancing the harnessing of solar panel energy.

However, the current study had also some limitations. Firstly, related to the rPET production systems and secondly when considering the consumption of the 2l of water. For the rPET production system, the data provided was aggregated instead of being detailed stage by stage as the remaining data collected; additionally, the data related to gas effluent characterization was from 2019 and not from 2021 as the remaining data; lastly, the majority of the data was collected based on theoretical or pre-industrial values since the rPET plant is still in the start-up phase. Regarding the consumption of the 2l of water, the data available was for the production of 0.5l water bottles, and not for the production of the 2l water bottle. This limitation can increase the probability of bias error since in single-use bottles this study considers the use of 4 water bottles instead of the use of only one bottle with a capacity of 2l of water.

In the future, the inclusion of other life cycle steps should be planned, such as distribution routes and waste disposal. The quest for new and alternative materials remains urgent, as does the exploration of innovative designs and production processes aimed at conserving energy and resources.

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Europe (2022b); Previously, Finally, EPD, 2018; Panel (2016); ReCiPe 2008; Associates (2018); .

CRediT authorship contribution statement

Bruno Silva: Supervision, Project administration, Funding acquisition, Conceptualization. **Inês Costa:** Writing – original draft, Software, Methodology, Investigation, Formal analysis, Data curation. **Pedro Santana:** Validation, Resources, Investigation, Conceptualization. **Maria E. Zacarias:** Visualization, Validation, Resources, Investigation. **Bruno Machado:** Visualization, Validation, Resources, Investigation. **Pedro Silva:** Visualization, Validation, Resources, Investigation. **Sandra Carvalho:** Visualization, Validation, Resources, Investigation. **Filipa Faria:** Visualization, Methodology, Investigation, Formal analysis. **Catarina Basto-Silva:** Writing – review & editing, Validation, Supervision, Software, Project administration, Methodology, Investigation, Formal analysis.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

The following is the Supplementary data to this article:

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Multimedia component 1.

Data availability

Data will be made available on request.

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