



Integrated process design, techno-economic and environmental analysis of chokeberry pomace biorefineries: Phenolic compounds extraction with ethanol or energy production?

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ABSTRACT

Learning how to transform by-products or waste from the food industry instead of sending them directly to landfill is key to reducing food waste and obtaining new value-added products from them. This study carries out the environmental and economic assessment of the valorisation of chokeberry pomace for the extraction of phenolic compounds in a multi-product and circular biorefinery. For this purpose, two scenarios were analysed: scenario A, the remaining part of the pomace is used to obtain bioethanol and a lignin-rich stream; and scenario B, it is used for bio-energy production. The Life Cycle Assessment methodology is used to determine the environmental critical points, following a cradle-to-gate approach and considering impact categories such as Global Warming, Freshwater Eutrophication or Fossil Resource Scarcity, among others. The results show that scenario B performs better in all the impact categories analysed compared to scenario A. In both cases the main hotspot is the generation of the steam needed in the biorefinery, followed by the emissions in the agricultural stage and the demand for chemicals in the plant. Furthermore, this document presents a techno-economic analysis to assess the economic feasibility of both scenarios and a sensitivity analysis to determine the profitability factors of the platform, considering the total capital investment, operating costs and indicators such as Net Present Value or Internal Rate of Return. The results show that the scenario analysed is not profitable at any of the scales studied, requiring to optimise the production yield or a reduction in the plant's operating costs.

1. Introduction

One of the main challenges facing society is the generation and management of food by-products, which encompasses the environmental impacts of the upstream stages of their life cycle (e.g., cultivation) as well as at the disposal stage (if not properly treated). Food by-products are obtained throughout the different stages of the value chain, where the processing step represents 39 % of the

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waste produced (Cristóbal et al., 2018).

The juice production industry represents a notable contributor to the generation of food waste or by-products in Europe, accounting for approximately 3 % of the total food waste produced (Roda-Serrat et al., 2021). Among the Sustainable Development Goals (SDGs) (United Nations, 2019), better management of value chains in food production is included in SDG 12 (Responsible Consumption and Production). One of its targets is the reduction of food waste and the implementation of recycling and/or reuse strategies (United Nations, 2019). As current European legislation on the disposal of food waste (European Union, 2008) states that landfill disposal without pre-treatment should be the last option to be considered, novel ways of dealing with by-products from the food industry must be developed.

Considering the different characteristics and composition of these by-products, a special interest has grown in recent years about their valorisation to obtain high added-value products (Cristóbal et al., 2018; Roda-Serrat et al., 2021). By-products from the processing of fruits and vegetables are a source of specific untapped bioactive compounds, ranging from proteins to essential fatty acids and polyphenols (De Ancos et al., 2015). Consequently, the biorefinery concept emerges to move from traditional refineries to sustainable systems based on the valorisation of residual biomass, with the aim of producing value-added products such as food/feed, chemicals, biomaterials or energy (Solarte-Toro and Cardona Alzate, 2023).

Aronia melanocarpa berries (or chokeberry) and their products, such as juice and pomace, contain a high level of polyphenols with high antioxidant activity (Oszmianski et al., 2005). The cultivation of chokeberry is originally from North America but, nowadays, it is being cultivated in a great part of Europe (Markkinen et al., 2019), being Russia and Poland the most relevant producers (Ravichandran and Krishnaswamy, 2023). In general, berries are perishable, so much of berry crops are dried, frozen or processed into much durable products (Venskutonis, 2020). During the production of chokeberry juice, 20 % of the processed berry is converted into pomace (Vagiri and Jensen, 2017), a by-product consisting mainly of skins pulp, seeds and stems of the fruit (Venskutonis, 2020). Currently, large quantities of berry pomace are still discarded or used for composting and animal feed, although many reports address the recovery of phenolic compounds (which are not transferred to the juice) by various extraction and separation techniques (Shi et al., 2022; Tylewicz et al., 2018). Phenolic compounds are of great interest to different types of industries, whether food, cosmetics or pharmaceutical, due to their wide variety of applications, for example, antioxidants or anti-inflammatories. (Albuquerque et al., 2021). In addition, there is a growing interest in replacing synthetic antioxidants with natural ones, which are more beneficial to human health (Tylewicz et al., 2018).

Regarding phenolic compounds, various extraction techniques have been introduced using different extractive agents, the most frequent being organic solvents (e.g., ethanol and methanol) (Alara et al., 2021). However, if one of the final destinations of the phenolic compounds is one of the aforementioned (food, cosmetics or pharmaceuticals), certain organic solvents are not allowed. Only those that are accepted by the European Food Safety Authority (EFSA, 2012) and the European Commission Directive 2016/1855 (European Commission, 2016) can be used as an extractive agent, as is the case with ethanol. Traditionally, phenolic compounds are extracted by conventional techniques such as Soxhlet, shaking, maceration or steam distillation (Bitwell et al., 2023). However, there are many drawbacks to these extraction methods, such as long extraction times, low extraction yields and low quality of the obtained extract (Tylewicz et al., 2018). Therefore, new methods have been proposed for the extraction of phenolic compounds from natural matrices, such as extraction by microwave, pressurised liquids or supercritical fluids (Comunian et al., 2021; Paes et al., 2014; Tylewicz et al., 2018). Nevertheless, extraction using microwaves is notoriously complex when scaling up from laboratory-scale experiments due to its poor reproducibility and the competing heat transfer mechanism due to the low penetration depth of this technology (Li et al., 2013; Vinatoru et al., 2017). On the other hand, according to the study by Paes and colleagues (Paes et al., 2014), a lower extraction yield was observed with pressurised liquids than with supercritical fluid extraction of phenolic compounds from blueberry residues. Therefore, supercritical fluid extraction (SFE) has been considered as the main technique to obtain phenolic compounds from chokeberry pomace. SFE has several advantages, such as high selectivity, short extraction time and lack of toxic organic solvents (Khaw et al., 2017). In addition, carbon dioxide (CO₂) can be used as a supercritical fluid due to its low critical temperature and non-toxicity, as well as it can be mixed with other solvents, like ethanol, improving the extraction of some bioactive compounds (Comunian et al., 2021). Furthermore, SFE is considered a “green” extraction technique due to the reduction in solvent consumption and extraction time, which leads to reduced environmental impacts of the process (Chaves et al., 2020; Mondello and Salomone, 2019).

After the extraction of the phenolic compounds, the remaining organic part of the pomace is rich in fermentable sugars that can be used to produce bioethanol, which in addition to being used in the extraction process has a large market in the field of biofuels and bioenergy (Marcuzzo et al., 2024). The increase of greenhouse gases in the atmosphere, the saturation of the energy market and the changing oil market have increased the interest in biofuels decade after decade, being some of the advantages of them that they are biodegradable, do not contain sulphur or carcinogenic compounds and are non-toxic (Neupane, 2022). Global production capacity for these fuels reached 2072 thousand barrels of oil equivalent per day in 2023, of which biodiesel accounts 960 thousand barrels (Energy Institute, 2024). The four main waste feedstock groups for bioethanol production are sugar-based materials, lignocellulosic materials, starch-based materials and algal feedstocks (Barua et al., 2023).

Another option for utilising the remaining chokeberry pomace is to produce biogas through anaerobic digestion. In this process, the biodegradable feedstock is transformed in the absence of oxygen into biogas, a gas consisting mainly of methane and carbon dioxide (Bhatia, 2014). However, one of the difficulties with this is that a high percentage of carbohydrates in the digestate composition can act as a barrier to optimal digestion, so a good option to improve the methane ratio could be to mix different types of waste (Li et al., 2024). Finally, to obtain energy to power the plant, the biogas obtained is converted into bioenergy in a power generator unit (Kabeyi and Olanrewaju, 2022).

All these abovementioned actions would be framed within the perspective of a circular economy, which advocates a sustainable

system where the need for resources is separated from economic growth thanks to the recirculation of flows and reduction of energy consumption (Korhonen et al., 2018). The key aspects of the circular economy are the minimisation of waste that is generated throughout the entire process and treated as new raw materials for the creation of value-added products. However, this does not always translate into a direct reduction of environmental impacts, so a good tool to quantify the environmental viability of a bio-based system is Life Cycle Assessment (LCA) (Cortés et al., 2021; Niero and Kalbar, 2019), as it allows the identification of critical factors that could hinder the development of new biorefineries. This research evaluates the environmental and economic performance, based on the LCA and techno-economic assessment (TEA) methodologies, of two biorefinery designs for the valorisation of chokeberry pomace: i) phenolic compounds extraction with the production of ethanol and lignin by fermentative processes, and ii) phenolic compounds extraction with an anaerobic digestion to obtain biogas to produce bioenergy and the digestate. Thus, the main objective of this research is to compare which biorefinery design is more attractive under an environmental perspective, supporting the results from an economic point of view as well. This research contributes to give a new approach to a little studied waste in search of new economically and environmentally profitable alternatives from a biorefinery perspective. Secondary objectives derived from the investigation were: (i) to determine the main steps that contribute to the environmental profile, (ii) to assess the economic feasibility of each biorefinery design, and (iii) to identify, through a sensitivity analysis, the best possible option for implementing the designed biorefinery.

System boundaries

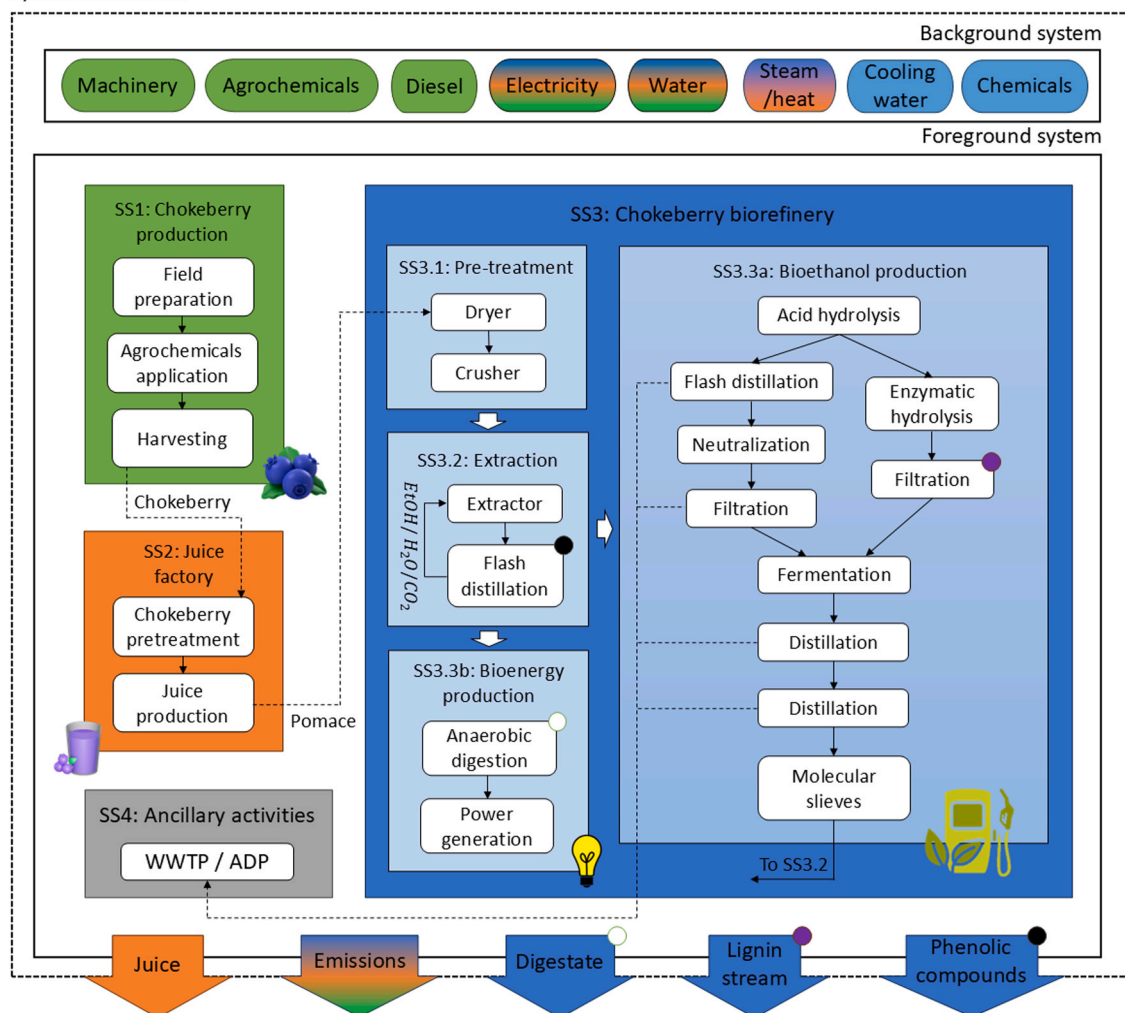


Fig. 1. System boundaries of the whole process with all the subsystems covered (WWTP: Wastewater Treatment Plant; ADP: Anaerobic Digestion Plant); the coloured circles of some of the outputs refer to the processes in which they occur.

2. Materials and methods

2.1. Life cycle assessment methodology

The LCA methodology assesses the environmental impacts of a process, product or service throughout their life cycle (ISO 14040, 2006). This methodology has been followed in detail, including its four phases: goals and scope definition, life cycle inventory, life cycle impact assessment and interpretation of results (ISO 14040, 2006; ISO 14044, 2006). Furthermore, it is considered an attributional LCA approach due to the use of average data in all scenarios analysed (Ekvall, 2020).

2.2. Definition of goal and scope

This study proposes the valorisation of a by-product obtained from the chokeberry juice production processes, as its pomace, under a biorefinery approach. However, biorefineries do not tend to produce a single target product, but in many cases, co-products and/or by-products are also obtained (Ekvall, 2020; Katakojwala and Mohan, 2022). Here, phenolic compounds have been considered as the main product of the platform. Nevertheless, throughout the valorisation process, side streams are generated, which can be further valorised, thus maximizing the use of the biomass. In this regard, two scenarios have been considered for the treatment of these side streams. On the one hand, to obtain bioethanol after a fermentative process and a lignin-rich stream as a by-product; and, on the other hand, to obtain bioenergy from the biogas generated by anaerobic digestion to feed the plant, obtaining as a by-product a digestate that can be used as biofertiliser after a previous treatment. Therefore, an environmental assessment will therefore be carried out on which of the proposed routes is best.

The scope in the LCA methodology considers the level of detail of the product system evaluated, which can vary considerably depending on the main goal of the environmental analysis (ISO 14040, 2006). When performing an LCA, the functional unit is one of the first steps to define. The ISO 14040 and 14044 standards describe the functional unit as the calculation basis that provides the input/output ratio of the system under study (ISO 14040, 2006; ISO 14044, 2006). In addition, it allows environmental impacts to be clearly expressed (Katakojwala and Mohan, 2022).

If there is a multi-product production in a biorefinery, the choice of the functional unit requires additional thought due to the added difficulty to identify the main function of the system (Katakojwala and Mohan, 2022). Considering that the objective of this environmental study is to identify the most environmentally friendly valorisation route for the by-products obtained in the chokeberry juice production industry, the functional unit selected is the amount of the chokeberry pomace processed per batch in the valorisation plant, that is 250 kg. This selected functional unit (i.e., the amount of biomass processed) is commonly used in LCA involving by-product management systems (Gullón et al., 2018; Sillero et al., 2021) and allows comparison between different schemes despite producing different high value-added products.

As shown in Fig. 1, the system boundaries follow a cradle-to-gate approach, widely accepted and frequently used in numerous LCA studies on biorefineries (Sillero et al., 2021; Rebolledo-Leiva et al., 2024b), including the aronia crop, juice factory, biorefinery plant, and ancillary activities such as wastewater treatment. The different valorisation scenarios proposed (scenario A and scenario B) are composed of different subsystems, depending on the scenario to be analysed: chokeberry cultivation (SS1), juice factory (SS2), and the chokeberry biorefinery (SS3). The latter distinguishes a pre-treatment stage (SS3.1), an extraction stage (SS3.2), a bioethanol production stage (SS3.3a) and a bioenergy production stage (SS3.3b), and ancillary activities (SS4). All scenarios consist of SS1, SS2, SS3.1 and SS3.2, while scenario A includes stages SS3.3a and SS4, and scenario B only includes section SS3.3b. The transport of the raw material (i.e. chokeberry pomace) to the biorefinery plant, as well as the production and transport of other inputs, have been included within the system boundaries. The assumed distance to the gate of the biorefinery was 300 km. This assumption was contemplated due to its accordance with the literature (Rebolledo-Leiva et al., 2024a). Besides, with an average distance of 700 km, the transport of chemicals has been considered (Pérez-López et al., 2014).

2.3. Chokeberry pomace composition

The berries generally consist of the skin, a soft, pasty pericarp, the intracellular juice and the seeds. Once the juice has been extracted, the composition of the pomace from the berries is reduced to skins and seeds, as well as the remains of stems, woody parts

Table 1
Composition of the chokeberry pomace (Struck et al., 2016).

Compound	Mass composition (%)
Ash	1.03
Cellulose	4.36
Fats	4.35
Hemicellulose	9.09
Lignin	21.44
Pectin	1.09
Phenolic compounds	0.71
Proteins	7.93
Water	50.00

and fragments of leaves that may be left over from the harvest (Struck et al., 2016). This pomace is rich in polyphenols, which are divided into 66 % proanthocyanins (mostly tannins), 25 % anthocyanins, 7.5 % chlorogenic and neochlorogenic acid and 1.3 % flavonols (Oszmiański and Wojdyło, 2005; Wawer et al., 2006). Due to the high initial moisture content of pomace (around 50 %) and the fact that it is rich in sugars and other digestible nutrients, it can be easily damaged by the action of microorganisms, making it necessary to apply treatments such as drying and milling to avoid contamination (Struck et al., 2016). After drying, the moisture content of the pomace is reduced to 5–6 %, also containing around 68 % fibre, in addition to 15 % protein and to a lesser extent lipids (Reque et al., 2014; Sójka et al., 2013; Sójka and Król, 2008). As there is no information about chokeberry, the data for blackcurrant pomace fibre was followed, which is composed of 59 % lignin, 25 % hemicellulose, 12 % cellulose and 3 % pectin (Nawirska and Kwaśniewska, 2005). Therefore, the final composition of the chokeberry pomace taken for the simulation is shown in Table 1.

2.4. Description of the biorefinery scenario under study

As mentioned above, two possible scenarios (scenarios A and B) have been designed to obtain different high value-added products from the perspective of a biorefinery of chokeberry pomace, under a circular economy approach. These scenarios are made up of two common subsystems (SS1 and SS2) referring to the cultivation and field operations of the crop and the juice factory. SS3 is where the differences begin: SS3.1 and SS3.2 are common to both subsystems, but SS3.3a belongs only to scenario A and SS3.3b corresponds only to scenario B. Finally, SS4 also applies only to scenario A. The flowchart is presented in Figures S1-S2 in the supplementary material (SM).

2.4.1. Subsystem 1: chokeberry production

This subsystem represents agriculture activities including all the field operations, infrastructure, fertilisers and pesticides applied for the cultivation of chokeberries. Due to lack of primary data related to chokeberry production, it was used data from a local production of blueberry in Spain, assuming that as both are berries, they have similar operations. The only data that was not provided by producers is that associated with the application of fertilisers. For this purpose, data on blueberry cultivation in Chile were used (Cordes et al., 2016), assuming the information collected by these authors on the orchard with predominantly sandy soil, as it is the one with the most similar characteristics to the field from which the primary data were obtained.

2.4.2. Subsystem 2: juice production

Once the chokeberries have been harvested, they are taken to a juice plant to generate chokeberry juice and obtain chokeberry pomace as a by-product. To simulate this plant, due to the lack of information on the production of juice from this fruit, the study of Cheng and collaborators on an apple juice production plant in China was used as a reference (Cheng et al., 2022). Therefore, the same input quantities of both water and fruit were assumed, as well as the energy consumption of the plant, changing only the juice-pomace ratio in the output of the plant, as there is information stating that for chokeberry this ratio is 80:20 (Vagiri and Jensen, 2017). The environmental loads attributed to the pomace were assessed using a mass allocation approach.

2.4.3. Subsystem 3: chokeberry biorefinery

2.4.3.1. Subsystem 3.1: pre-treatment stage. This subsystem includes the operation related to the removal of moisture from the raw material (chokeberry pomace), as well as its subsequent reduction size to facilitate the subsequent extraction process. The moisture is removed in an atmospheric dryer at 40°C until the moisture content is reduced to 5.5 % (Struck et al., 2016). Once this operation has been carried out, the dry pomace is introduced into a crushing unit (Struck et al., 2016). At the end of this stage, the dried and crushed pomace is stored and then introduced into the extraction equipment located in the next subsystem.

2.4.3.2. Subsystem 3.2: extraction stage. Supercritical fluid extraction is the technique used to extract the phenolic components from the pre-treated pomace. As an extractive agent, a mixture of ethanol, water and CO₂ in a composition of 10:10:80 (% v:v:v) and a feed stream to solvent ratio of 1:1.35 (w/w d.b.) was used (Seabra et al., 2010). The extraction process is carried out at 40°C and 20 MPa for 45 min (Seabra et al., 2010). After the extraction step, two streams are obtained. The first is made up of the mixture of the solvent and the target product (i.e., the phenolic compounds), while the second stream is made up of the solid remains of the pomace and a small amount of solvent. The liquid stream is processed to recover and recycle the maximum possible amount of solvent through flash distillation, recirculating 95 % of the solvent, assuming a 5 % loss with the product stream (Santiago et al., 2021; Santos et al., 2014). The target stream of this stage results in a flow rich in phenolic compounds, which could undergo different treatments depending on its destination and purpose in the market. On the other hand, the solid stream is treated by one of two possible treatments, either anaerobic digestion or fermentation. It is worth mentioning that a new residual solid stream is obtained from the filtration unit, mixing with the leftover pomace solids.

2.4.3.3. Subsystem 3.a: bioethanol production. The first process is an acid hydrolysis, using sulphuric acid, to improve the efficiency of conversion of cellulose and hemicellulose into glucose and xylose. The acid hydrolysis process is carried out for 1 hour in a stirred tank at 121°C and 1 bar with a solid-liquid ratio of 1:10 (w/w) and acid concentration of 2 % (v/v), as after this process enzymatic hydrolysis proceeds easily and efficiently (Dávila et al., 2017; Hasan Ba Hamid and Ku Ismail, 2020). In addition, furfural, 5-hydroxymethylfurfural and organic acids are formed due to the chemical decomposition of these compounds in small quantities (Ran et al.,

2014), so they are not considered as by-products and are neutralised later. The acid hydrolysis is followed by filtration to separate the liquid fraction (rich in hemicelluloses and the by-products formed) from the solid fraction. The liquid stream is sent to a flash unit, to reduce its water content, and then treated with sodium hydroxide (25°C, 1 bar) at a concentration of 2 % v/v, to neutralise the acid previously used (Dávila et al., 2017). This step is considered to reduce the concentration of by-products formed during acid hydrolysis, which are inhibitory compounds for further fermentation (Quintero et al., 2013). On the other hand, the solid stream (rich in cellulose and lignin) is treated with cellulases (25 mg/g cellulose) in an enzymatic hydrolysis process (50°C, 1 bar, 72 h) to convert the solid cellulose into glucose (Dávila et al., 2017; González-Rentería et al., 2011; Quintero et al., 2013; Shi et al., 2022). The estimation of the transformation of these lignocellulosic compounds was done stoichiometrically. Finally, the output streams of the enzymatic hydrolysis and neutralisation processes are treated in different filtration units. On the one hand, a lignin-rich stream (considered as a product of the biorefinery plant) and a residual stream that could be sent to an anaerobic digestion plant outside the plant are obtained. On the other hand, a glucose-rich stream is obtained which is subsequently fermented.

The fermentation process takes place at 33°C for 30 hours, using the recombinant bacterium *Zymomonas mobilis*, to convert the glucose-rich stream into bioethanol (Quintero et al., 2013). Once the fermentation is finished, the carbon dioxide, produced during this process, is discharged as exhaust gas and recirculated to SS2 to reduce the amount demanded for this input. The stream leaving the fermenter undergoes a double distillation to concentrate and recover as much ethanol as possible, with the maximum concentration by distillation corresponding to the azeotropic point (96 % wt.) (Quintero et al., 2013). Once this process is finished, the ethanol is dehydrated through molecular sieves, obtaining 99.8 % anhydrous bioethanol as the final product (Quintero et al., 2013). From the distillation and sieving processes, residual liquid streams are obtained, which will be treated in a water treatment plant outside the biorefinery. In this case, no process has been simulated, but the data has been obtained from the Ecoinvent® database version 3.9.1 (Ecoinvent, 2024).

Table 2

Inventory data per scenario of each subsystem. The data for SS1 are expressed per hectare of land, whereas SS2 and SS3 are expressed per batch (250 kg of chokeberry pomace).

Chokeberry production (SS1)					
Inputs	Value		Outputs	Value	
Diesel (kg)	38.17		<i>Product</i>		
Machinery (kg)	15.21		Chokeberry to SS2 (t)	20	
Implement (kg)	5.17		<i>Emissions from agrochemical use</i>		
Car (kg)	4.72		Dinitrogen monoxide (kg)	0.69	
Electricity (kWh)	4837		Ammonia (kg)	7.25	
Polyethylene (pipes) (kg)	0.12		Nitrogen dioxide (kg)	1.19	
PVC (pipes) (g)	54.80		Phosphate leaching (kg)	0.21	
Polypropylene (kg)	5.87		Phosphate run off (kg)	0.57	
Phytosanitary (kg)	11.00		Nitrate (kg)	85.39	
N (organic fertiliser) (kg)	29.86		Fungicide (water) (g)	1.34	
P ₂ O ₅ (organic fertiliser) (kg)	24.73		Fungicide (air) (g)	12.06	
K ₂ O (organic fertiliser) (kg)	7.00		Fungicide (soil) (kg)	0.12	
S (organic fertiliser) (kg)	61.77		Azadirachtin (water) (g)	0.26	
CaO (organic fertiliser) (g)	15.10		Azadirachtin (air) (g)	2.34	
MgO (organic fertiliser) (g)	1.30		Azadirachtin (soil) (g)	23.40	
Juice factory (SS2)					
Inputs	Value		Outputs	Value	
Chokeberry from SS1 (t)	3.46		<i>Product</i>		
Water (t)	3.46		Chokeberry juice (t)	1	
Electricity (kWh)	66.5		<i>By-product</i>		
Heat (MJ)	3853		Chokeberry pomace to SS3 (t)	0.25	
Chokeberry biorefinery (SS3)					
Inputs	A	B	Outputs	A	B
Pomace from SS2 (t)	0.25		<i>Product</i>		
Carbon dioxide (kg)	1.78		Phenolic compounds (kg)	1.77	
Sulfuric acid (kg)	3.02	-	<i>By-products</i>		
Sodium hydroxide (kg)	2.46	-	Lignin stream (kg)	56.32	-
Ethanol (kg)	79.79	89.28	Digestate (kg)	-	223
Water (kg)	151	-	<i>Emissions</i>		
Cooling water (m ³)	20.93	280.46	Nitrogen (kg)	4.58	3330
Electricity (kWh)	660	15.21	Oxygen (kg)	1.39	907
Steam (t)	3.62	3.34	Carbon dioxide (kg)	11.18	177
Air (t)	-	4.68	Water (kg)	-	445
			Ethanol (kg)	1.69	-
			WW to SS4 (m ³)	0.43	-

WW: Wastewater; A: Scenario A; B: Scenario B.

2.4.3.4. Subsystem 3.b: bioenergy production. In this subsystem, the solid stream leaving SS2 is treated by anaerobic digestion under mesophilic temperature ($\approx 40^{\circ}\text{C}$) because most of the methanogenic microorganisms are mesophiles, so at this temperature the conversion yield of organic matter to biogas is higher and the process is faster (Rashed, 2014; Vazifekhoran et al., 2016). Since no literature has been found that refers to the digestion of this type of components, the methodology based on the study by Vazifekhoran et al. (2016) has been applied to estimate the amount of methane and carbon dioxide content in the biogas produced by the anaerobic digestion of the remaining chokeberry pomace. This methodology is described in the SM. Finally, the biogas generated is transformed into bioenergy in a power generation unit with the idea of recirculating it to the plant to try to satisfy part of its energy requirement.

2.4.4. Subsystem 4: ancillary activities

In this subsystem are included a wastewater treatment plant (WWTP) and an anaerobic digestion plant (ADP) for treating the waste flows generated in Subsystem 3.3a. Since the objective of the manuscript is to treat the streams generated in the process, rather than to design these facilities, the data for them were taken from the Ecoinvent® database version 3.9.1 (Ecoinvent, 2024).

2.5. Life cycle inventory

This LCA stage summarises the input and output data of the systems proposed for the environmental assessment. In this research, the treatment capacity of the biorefinery in both scenarios is 250 kg per batch of chokeberry pomace. Additionally, inventory data, such as energy requirements (electrical and thermal) of all equipment, chemical consumption and process water have been obtained from process simulations using SuperPro Designer® version 11.0 (Intelligen, 2020), taking as input data the experiments conducted at laboratory scale developed by Quintero et al. (2013) and Dávila et al. (2017). The mass and energy balances resulting from process simulation are used as the basis for the lifecycle inventory (see Table 2) of each scenario.

In the environmental analysis, heat and cooling water generated in the process is going to be recirculated. For the remaining demand of these heat transfer agents, the Ecoinvent® database version 3.9.1 (Ecoinvent, 2024) was used, considering cooling water from Spain and steam from Europe market. Inventory data associated with their production were taken from the Ecoinvent® database but updated considering the Spanish electricity mix for 2019 (Spanish Electrical Network, 2019). For the anaerobic digestion processes mentioned in scenario B and the wastewater treatment in scenario A, the inventory data were taken from the Ecoinvent® database version 3.9.1 (Ecoinvent, 2024). As indicated above, anaerobic digestion produces biogas that can be converted into energy through a generator unit. The methodology for the calculation of the biogas produced and the energy obtained can be found in the supplementary material. The computational implementation of the life cycle inventory data was carried out using the SimaPro v9.0.0 software (PRÉ Sustainability, 2024).

An uncertainty analysis was carried out on the inputs obtained from the Ecoinvent® database version 3.9.1 for both scenarios. The Monte Carlo simulation was performed in SimaPro® software with 2000 iterations and 95 % confidence interval to propagate the uncertainties and assess their impact to the final results, which are presented in Table S1 in SM. For the input data, the distribution used was log-normal, with deviations estimated based on default values from Ecoinvent® database.

2.6. Life cycle impact assessment methodology

Two impact assessment methods were considered to carry out the environmental analysis. Firstly, the hierarchical midpoint method of ReCiPe 2016 V1.04 World (2010) (Huijbregts et al., 2016) was used to perform the environmental profile of both scenarios. The characterisation factors reported by this method were considered to estimate the environmental burdens in terms of the following impact categories: global warming (GW), stratospheric ozone depletion (SOD), terrestrial acidification (TA), freshwater eutrophication (FE), marine eutrophication (ME), terrestrial ecotoxicity (TET), freshwater ecotoxicity (FET), marine ecotoxicity (MET) and fossil resource scarcity (FRS). On the other hand, the hierarchical Endpoint method of ReCiPe 2016 V1.04 World (2010) H/H (Huijbregts et al., 2016) was considered to compare the two valorisation profiles. With this endpoint approach it is possible to have a single score of the general impacts, allowing a better dissemination of the environmental results to the stakeholders (Arias et al., 2020).

2.7. Techno-economic analysis

2.7.1. Total capital investment

The biorefinery has been modelled by entering the units sequentially and setting the parameters of the input or output streams, as well as other operating parameters such as pressure, temperature and operating time. After this, material and energy balances are calculated for each unit. The initial scale selected was 250 kg/batch of chokeberry pomace, as the annual production in Poland (the largest producer) reaches about 50,000 tons per year (Wronka et al., 2021), of which 20 % is processed into pomace. Assuming that half is used for juice production, this results in approximately 5,000 tons of chokeberry pomace annually, meaning the biorefinery would be capable of processing 1 % of that amount with a total of 200 batches per year. Additionally, this scale closely aligns with that chosen in a similar study focused on the valorisation of food waste for the extraction of bioactive compounds (Santiago et al., 2021). Moreover, larger scales of 12,500 and 25,000 kg/batch were analysed in the sensitivity analyses to assess the influence of plant size. The data obtained are then used to calculate the size of the equipment and its costs using the programme's data. Once these costs have been determined, the direct and indirect costs of the plant are determined to estimate the necessary investment capital and the economic performance of the designed plant (Humbird et al., 2011). The currency used as a reference for all economic estimates is the US dollar and is already updated to 2024 by the software's own database.

The total direct plant cost (TDPC) is therefore the sum of the equipment cost and its installation, control and instrumentation, piping, insulation, electrical systems, building, yard improvement and auxiliary facilities. On the other hand, the total indirect plant cost (TIPC) is the sum of engineering and supervision, contractor's fee & contingency cost (Humbird et al., 2011). Both direct and indirect costs were estimated based on the mass and energy balances, from which the costs of equipment and instrumentation procurement, piping preparation, auxiliary facilities, as well as contractor and supervision fees are calculated according to the software's database related to 2024. The fixed capital investment (FCI), finally, is the sum of the TDPC and TIPC (Humbird et al., 2011). FCI together with working capital (WC) (5 % of fixed capital investment) make up the total capital investment (TCI) (Brown et al., 2013; Humbird et al., 2011; Ladakis et al., 2022).

2.7.2. Total operating cost

The total operating cost (TOC) is composed of variable operating costs (VOC), those that depend on plant activity, and fixed operating costs (FOC), which are those that are incurred regardless of whether the plant is operating or not (Humbird et al., 2011). Variable costs are composed of the chemical compounds used (e.g., NaOH, sulphuric acid, ethanol, among others) and the energy demands of the plant (electricity, steam, cooling water), which are obtained from in-country or global industry quotations or chemical price reports; while fixed cost include salaries, labour burden, maintenance and property insurance. The cost of chokeberry pomace was taken from literature, assuming the same cost as for grape pomace due to the lack of information about the cost of this pomace, assuming 32 USD/ton (Jin et al., 2021). Transportation costs of this pomace to the biorefinery are not contemplated within the study, assuming zero cost. The labour cost was estimated by multiplying the number of operators by the annual wage of the workers. Firstly, is needed to calculate the number of operators per shift (N_{OL}) following the Eq. (1) (Alkayat and Gerrard, 1984):

$$N_{OL} = (6.29 + 31.7P^2 + 0.23N_{np})^{0.5} \quad (1)$$

Where P is the number of process steps involving handling solids and N_{np} is the number of process steps not involving handling solids. The number of operators needed is rounded to the next integer. Finally, to calculate the labour cost, it is assumed that the plant needs operators 365 days a year including maintenance, that there are 3 shifts in a day, that an employee makes 5 shifts per week and that an operator works 49 weeks a year. About the salary is assumed that the annual salary per person is 50,000 USD/year (Huang et al., 2016).

In addition, labour burden is assumed to be 90 % of total salaries (Humbird et al., 2011). On the other hand, the cost of maintenance materials is calculated as 3 % of equipment costs and property insurance as 0.7 % of fixed capital investment (Humbird et al., 2011). Depreciation is calculated using the Modified Accelerated Cost Recovery System (MACRS) for 7 years (Ladakis et al., 2022). Finally, distribution and market costs are 10 % of the total operating Cost cost, while research and development costs represent 5 % of it (Max et al., 2003).

2.7.3. Revenues and profitability analysis

Once the capital and operating costs are obtained, the revenues from product sales are then calculated. The selling price for phenolic compounds is set at 20 USD/kg, based on literature (Jin et al., 2021). For the scenario A, the price for lignin is set at 1300

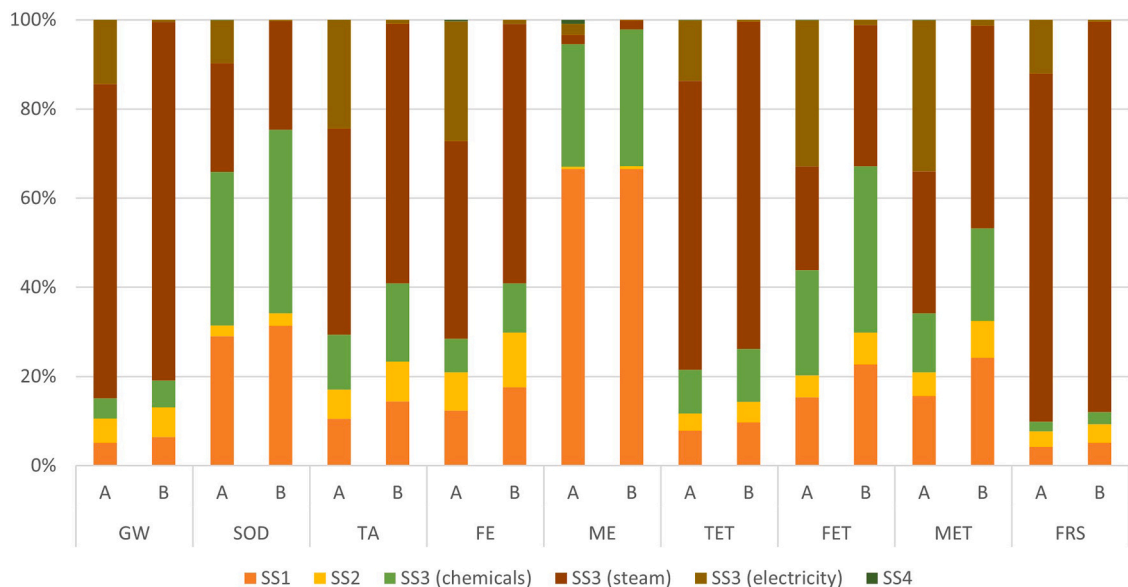


Fig. 2. Relative environmental profile for (A) Scenario A and (B) Scenario B (GW: Global Warming; SOD: Stratospheric Ozone Depletion; TA: Terrestrial Acidification; FE: Freshwater Eutrophication; ME: Marine Eutrophication; TET: Terrestrial Ecotoxicity; FET: Freshwater Ecotoxicity; MET: Marine Ecotoxicity; FRS: Fossil Resource Scarcity).

USD/ton (De Guzman, 2020), while for scenario B, the price for digestate is set at 9.58 USD/ton (Tröster, 2023). A discount rate of 10 % and a plant lifetime of 30 years are assumed, inclusive of the equipment, with an additional three years allocated for construction and start-up. The total capital investment is distributed over these initial three years, with 8 % in the first year, 60 % in the second year, and 32 % in the third year (Huang et al., 2016; Ladakis et al., 2022). Additionally, the analysis assumes 100 % equity financing. A summary with the main data used for the profitability analysis can be found in Table S2 in SM.

The economic performance of the process is evaluated by using two common indicators: net present value (NPV) and internal rate of return (IRR). The former is defined as the sum of the present values of the future cash flows for a given period (Towler and Sinnott, 2021), while the latter is the discount rate at which the NPV is zero after tax (Humbird et al., 2011).

3. Results and discussion

3.1. Environmental impact analysis (midpoint approach)

The environmental results of the chokeberry pomace biorefinery, including the juice factory and berry cultivation, according to both scenarios evaluated are presented in Fig. 2. The main hotspots in both scenarios are the generation of the steam needed to supply the energy demand for the operation of the biorefinery, followed by the emissions from the field operations for chokeberry production, mainly due to the high diesel consumption, and the chemical demand in SS3, especially due to the ethanol demand for the supercritical fluid extraction. The following is a category-by-category analysis of the main contributors to this environmental profile, being finally better in almost all impact categories the bioenergy production scenario.

3.1.1. Global warming

This category values the integrated infrared radiative forcing increase of greenhouse gas (GHG) in terms of kg CO₂ eq (Huijbregts et al., 2017). In both cases, the main impact comes from steam production in SS3, which exceeds 70 % of the total impacts. This is due to the need to heat large quantities of liquid to remove most of the moisture from the chokeberry pomace and for extraction with supercritical fluids, or, in the case of scenario A, also by acid hydrolysis. The total amount for scenario A is 1481 kg CO₂ eq, while for scenario B it is 1196 kg CO₂ eq, indicating that in this impact category, the impacts of scenario B are approximately 20 % lower. On the other hand, GHG emissions from the chokeberry biorefinery mainly come from fossil CO₂, and to a lesser extent, from N₂O and CH₄. The standard deviation obtained in the uncertainty analysis for scenarios A and B was 0.14 and 0.13 t CO₂ eq per batch, respectively, demonstrating that this variable significantly influences the environmental profile.

3.1.2. Stratospheric ozone depletion

SOD is formed because of the photochemical equilibrium between oxygen molecules, oxygen atoms and solar radiation, and it is this ozone layer that protects life on the earth's surface from the sun's ultraviolet B radiation (wavelength 280–310 nm), with this category measuring the impacts that occur on it (EEA, 2016). Here the impacts are more evenly distributed, with the main contributor for both scenarios being the production of the chemicals needed in SS3, with 41 % of the impacts for scenario A and 34 % for scenario B, followed by the impacts from agricultural production, with around 30 % of the impacts in both scenarios, and the production of the steam needed in the biorefinery, with 24 % of the impacts in both cases. For scenario A, the total emissions are 0.0011 kg CFC₁₁ eq, while for scenario B, they are 0.0010 kg CFC₁₁ eq, so as can be seen there is hardly any difference between the two, with CH₄ and N₂O being the substances that contribute most to this category.

3.1.3. Terrestrial acidification

In TA category, the main impact of both scenarios comes again from the steam production, with 46 % of the total impacts for scenario A and 58 % for scenario B. Another prominent impact in the case of the biofuel production scenario is the energy demand of the biorefinery, contributing up to 24 % of the total impacts. The main impacts come from NH₃, NO₂ and SO₂, being the total emissions 5.08 and 3.72 kg SO₂ eq for scenarios A and B respectively.

3.1.4. Freshwater and marine eutrophication

In terms of FE, in both cases the results are very similar to those obtained in the previous category, with the production of steam in SS3 being the main cause of the impacts, with 44 % of the total for scenario A and 58 % for scenario B. In addition, again in the case of the first scenario, the production of the necessary electricity has an important weight with 27 % of the impacts. In this category, the main contributors are BOD₅, COD and PO₄, being the total impacts for scenario A 0.31 kg P eq and 0.21 kg P eq for scenario B.

Moving to ME, in both cases there is one main contributor to this category, which is the emissions in the SS1 field, accounting for about 67 % of the impact in both of them. The total amount for each scenario is the same for both cases, 0.3 kg N eq, caused mainly by the effect of NH₄⁺ and NO₃⁻.

3.1.5. Terrestrial, freshwater and marine ecotoxicity

Starting with TET, the impacts come mainly in both cases from steam generation, with more than 64 % of the total contributions. In FET, for scenario A, the impacts are more or less equally distributed, with the generation of the electricity needed in the biorefinery accounting for 33 % of the total impact. On the other hand, for scenario B, the main contributor is the production of the ethanol needed in the biorefinery for extraction, followed by the production of steam, with 37 % and 32 % of the loads respectively. Finally, for MET, the main contributor to the impacts in scenario B is steam generation again, with 46 % of the total, while in scenario A these are

divided between electricity and steam production, with 34 % and 32 % of the total impacts respectively. For scenario A, the total amount issued are 2387 kg 1,4-DCB for TET, 21.5 kg 1,4-DCB for FET and 27.1 kg 1,4-DCB for MET, while for scenario B these amounts were 1943, 14.6 and 17.5 kg 1,4-DCB respectively. This is mainly due to the emission of certain metals such as copper, zinc and vanadium during the manufacture of machinery.

3.1.6. Fossil resources scarcity

Finally, in the case of FRS, for both cases the main contributor, with more than 75 % of the total impacts, is the generation of the steam needed in SS3. The main resources that contribute to this category are coal, natural gas and oil, being the total amount 465 kg oil eq for scenario A and 382 kg oil eq for scenario B, i.e. the latter scenario is almost 20 % better from an environmental point of view.

3.2. Environmental impact analysis (endpoint approach)

In this section, the environmental results are expressed as a single overall score to better compare the two scenarios evaluated. The endpoint level analysis presents results through three indicators that quantify the relative severity in three categories: Human Health (HH), Ecosystems (E) and Resources (R). These endpoint indicators are derived from an aggregation process that integrates midpoint categories using specific endpoint characterisation factors. In this study, only the impact categories previously selected for the environmental assessment at the midpoint level (GW, SOD, TA, FE, ME, TET, FET, MET and FRS) will be considered for the estimation of the single environmental score, considering the corresponding weighting and normalisation score. Among these, SOD contributes to HH, GW contributes to both HH and E, FRS contributes to R, while the remaining impact categories contribute to E.

The 'Human health' category is measured in the unit of "disability-adjusted life years" (DALYs). This refers to the sum of the years of life lost and disabled due to that disease with a uniform weighting factor for all ages and according to the best health care practices in 1990 (Goedkoop et al., 2013). The impacts for scenario A are little higher, with a value of $1.38 \cdot 10^{-3}$ DALYs for scenario A and $1.11 \cdot 10^{-3}$ DALYs for scenario B. Nearly 100 % of this contribution is due to the impact of GW, accounting for 99.95 % of the total, while the contributions of SOD are practically negligible.

In the 'Ecosystems' category, damage is calculated by multiplying the density of species on the planet by the number of species that are potentially endangered, considering 1.6 million terrestrial, 100,000 freshwater and 250,000 marine species (Goedkoop et al., 2013). Once again, the differences between the two are small, with an amount of $5.47 \cdot 10^{-6}$ species/year for scenario A, while scenario B represents $4.31 \cdot 10^{-6}$ species/year. Regarding the distribution, approximately 76 % of the impacts are also caused by GW, making it the category with the highest impact in the obtained profile, followed by TA (18–20 %) and FE (3–4 %), while the remaining impact categories contribute less than 1 % to the overall total.

Finally, for the 'Resources' category, its contribution is based on the damage in the impacts of metal and fossil fuel depletion (Goedkoop et al., 2013) and is expressed in US dollars per cost of extracting them in 2013. This is the category where the biggest difference between the two scenarios can be seen, with a value of 152.2 USD for scenario A and 129.7 USD for scenario B.

The results are illustrated in Fig. 3, where the size of the circles represents the magnitude of the impact generated by each subsystem, expressed in points (Pt). The score for Scenario B is 3.87 points lower than that of Scenario A (20.31 Pt). It can also be observed that the distribution of impacts is nearly identical for both scenarios, with 85 % corresponding to HH, 7 % to E, and 8 % to R.

This approach therefore reinforces the findings obtained previously using the midpoint methodology, demonstrating that, from an environmental perspective, Scenario B performs better across all three analysed categories.

3.3. Analysis of the environmental profile of phenolic compounds (midpoint approach)

The environmental profile of the phenolic compounds is compared with those available in the literature in which the environmental

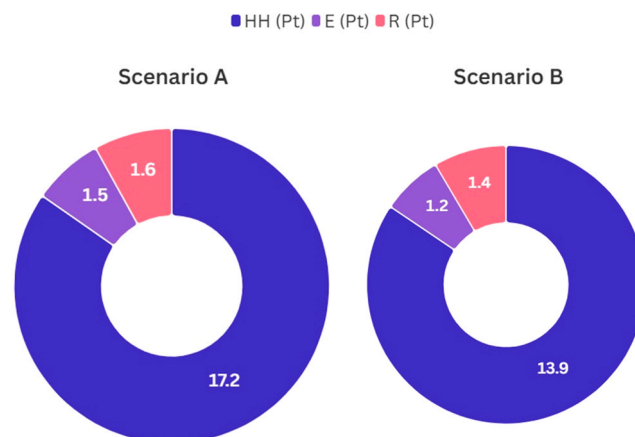


Fig. 3. Endpoint damage profile for each scenario (HH: Human Health; E: Ecosystems; R: Resources).

analysis per gram or kilogram of these compounds is made (Arias et al., 2022; Carlqvist et al., 2022; Croxatto Vega et al., 2021; Santiago et al., 2021). For this purpose, a mass allocation of environmental loads has been applied to the products obtained in Scenario B, phenolic compounds (0.79 %) and digestate (99.21 %). It should be noted that only one study carried out by Santiago et al. (2021) has been found in which a mass allocation was done (0.30 % of the loads associated with this target product and the remaining 99.70 % with digestate), while in the rest of the studies, it is the only product considered. Scenario A has not been considered in this comparison because it presents a worse environmental performance compared to scenario B.

Only one study has been found in the literature that includes the agricultural phase and the food processing stage of biomass generation (Carlqvist et al., 2022), while the other three studies include only the biorefinery simulation (Arias et al., 2022; Croxatto Vega et al., 2021; Santiago et al., 2021). The study developed by Arias et al. (2022) was discarded because it only gives percentage values, not the total impact for each category. The other studies focus on the phenolic compounds extraction from asparagus by-product (Santiago et al., 2021), spruce bark (Carlqvist et al., 2022) and from red wine pomace (Croxatto Vega et al., 2021). In the paper of Carlqvist et al. (2022) was considered the scenario where the extraction of the product is done with the SFE technology, because is the same that is used in this article, while in the work of Croxatto Vega et al. (2021) was selected only the scenario where the extraction was done by pressurized liquid extraction with a 10 % of solvent ratio, due to it is close to the simulated biorefinery. Finally, in the work of Santiago et al. (2021) has taken the data obtained in scenario 3 with the mass allocation approach. Table 3 displays the comparison of the environmental profiles of phenolic compounds.

Since the environmental analysis in this article follows a ‘cradle to gate’ approach, including the cultivation and processing stages up to the extraction of the product of interest, it might be expected that the impacts would be higher than in the other articles, but when doing the mass distribution between both biorefinery products the loadings associated with phenolic compounds are very low. According with the data collected in Table 3, in the paper of Santiago et al. (2021) the results obtained are higher in all impact categories than in the rest of the studies, maybe due to the large amount of electrical energy required in the extraction stage. In Carlqvist et al. (2022), all impacts are very low, which may be due to the fact that the energy used comes from renewable energies, because as the document states if it were to come from the European Energy Association, where 70 % comes from fossil resources, this impact could be up to 16 times higher on climate change, in addition to the fact that the composition of the raw material is different, which also influences the way it is treated. Croxatto Vega et al. (2021), reported that for extraction with pressurised fluids one of the main causes of the impact on global warming is the energy required for the heating process in distillation, and could see the importance of energy generation in all the papers reviewed. For TA, FE and ME categories, the results are like those obtained in the rest of the literature reviewed, close to 0, being the largest impacts obtained in GW and TET, which is due to the high vapour requirements of SS3, which comes from fossil fuels.

About the hotspots of the systems, Santiago et al. (2021) report that the main hotspot in the selected scenario is the high amount of electricity required, which is effectively also a contributor to this study, although not as important. Carlqvist et al. (2022) identified that the high amounts of ethanol required were the dominant factor for most environmental impact categories, which has also been identified as one of the main hotspots in this paper. Finally, Croxatto Vega et al. (2021) identify the high solvent demand again and the energy used for heating and cooling as the main hotspots, both of which are also identified as two of the main impacts of this study. Also, the work of Arias et al. (2022) report the energy requirements as the main hotspot, so it can be stated that the data obtained are in line with those reported in previous works.

Regarding the yield in the mentioned studies, Santiago et al. (2021) reported an amount of 68.6 g of rutin per 300 kg of residue and Carlqvist et al. (2022) talked about a yield of 96 g GAE/kg dry bark, while the own yield is 1.77 kg of phenolic compounds per 250 kg of pomace. Although the raw materials have different composition, in the case of Santiago et al. (2021) the moisture content is 90 % compared to 50 % in this study, it can be said that the yield is much higher. On the other hand, per kg of dried chokeberry pomace 13.38 g of phenolic compounds would be obtained, which although it is less than what Carlqvist et al. (2022) found, it can be said that it is in the same order of magnitude, so based on the articles using the same technology, the yield obtained is not bad.

3.4. Techno-economic analysis

Fig. 4 shows the results obtained for the total capital investment in both scenarios. Both share two subsystems and only one is different in each, but nevertheless the total direct and indirect costs of the plant are quite different, with the investment needed for scenario A being about USD 2600,000 more.

Table 3

Comparison of environmental profile of phenolic compounds obtained in this study with literature (FU: 1 kg of product).

Category	Unit	This study	(Santiago et al., 2021)	(Carlqvist et al., 2022)	(Croxatto Vega et al., 2021)
GW	kg CO ₂ eq	5.34	357.70	5.80	36.44
TA	kg SO ₂ eq	0.02	n/d*	0.06	0.07
FE	kg P eq	0**	n/d*	0**	0.01
ME	kg N eq	0**	n/d*	0**	0**
TET	kg 1,4-DCB	8.67	n/d*	0.01	52.39
FET	kg 1,4-DCB	0.06	21.10	0.11	0.44
MET	kg 1,4-DCB	0.08	n/d*	0.11	0.65
FRS	kg oil eq	1.70	n/d*	1.70	12.04

Note: *no data, **a value of 0 has given.

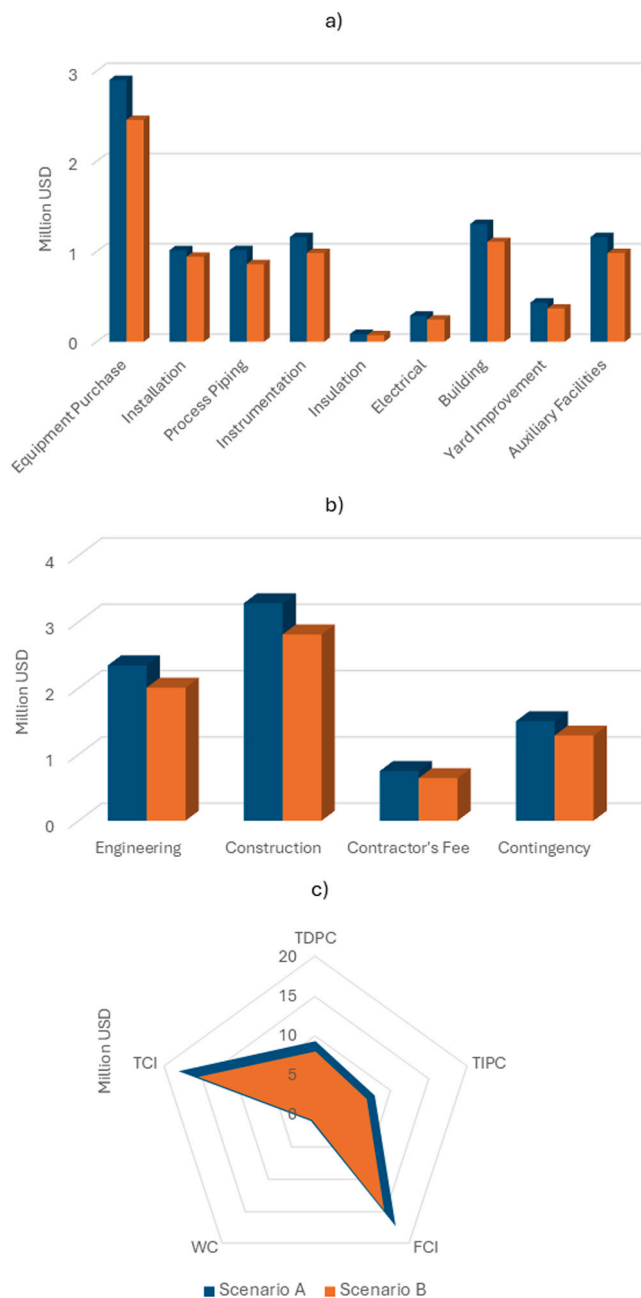


Fig. 4. Cost distribution for each scenario. a) TDPC (TDPC: Total Direct Plant Cost); b) TIPC (TIPC: Total Indirect Plant Cost); c) Capital Investment estimated for each scenario (FCI: Fixed Capital Investment; WC: Working Capital; TCI: Total Capital Investment).

These data alone do not tell the whole story, as operating costs are also very important for the economic viability of the plant. Table 4 shows the prices taken for each of the chemical compounds used in the facility, as well as the results of the fixed operating costs for each scenario and the total operating costs for each plant. Most of the cost in both plants is spent on salaries, although in scenario A the expenditure is even higher, as due to the higher amount of equipment in the plant it is needed to pay for the salaries of the employees. Then, labour costs are also important and depend directly on wages, so the higher the wages, the higher the labour costs will be. In addition, a notable difference between the two scenarios is the cost of purchasing raw materials, where the expenditure for scenario B is 30 % higher than for scenario A, which can be important when scaling up the plant's production. The sum of all these parameters is again higher in scenario A than in scenario B due to the costs related to the higher number of employees required in this scenario.

Regarding the material and energy balances obtained, for every 250 kg of wet chokeberry pomace, 1.77 kg of phenolic compounds

Table 4
Variable operating costs, fixed operating costs and total operating costs.

Variable Operating Costs (VOC) (Scenario A/Scenario B)	Value
Electricity	0.1 USD/kWh
Steam	12 USD/ton
Cooling water	0.05 USD/ton
Chilled water	0.4 USD/ton
Carbon dioxide	23 USD/ton
Chokeberry pomace	32 USD/ton
Ethanol	70.75 USD/hL
Nitrogen	0.17 USD/m ³
Oxygen	0.22 USD/m ³
Sodium hydroxide	0.41 USD/kg
Sulphuric acid	0.13 USD/kg
Water	0.35 USD/ton
Fixed Operating Costs (FOC) (Scenario A/Scenario B)	
Number of operators	18/14
Total Labor salaries	900,000 / 700,000 USD
Labor burden	810,000 / 630,000 USD
Maintenance	87,060 / 73,770 USD
Property insurance	120,722 / 103,369 USD
Total Operating cost (TOC) (Scenario A / Scenario B)	
TOC (USD/year)	2282,676 / 2027,326

are obtained. Additionally, in Scenario A and B, 56.32 kg of lignin and 222.91 kg of digestate are produced, respectively. As for the main utility demand in the process, the highest consumption is electricity with 173,282 kWh annually in Scenario A, with more than 92 % demanded by the crusher to reduce the biomass size and the acid hydrolysis process. In Scenario B, the main consumption is related to cooling water with 58,897 metric tons annually.

Finally, based in the revenue of each scenario, it can be said that none of them is profitable, as the gross annual revenues are, for both scenarios, much lower than the annual expenses. This is primarily due to the low yield of the main product, which results in low profits insufficient to cover wages and utility costs. Additionally, the selling prices of the other compounds produced in each scenario are too low to contribute meaningfully to overall profitability. Focusing on scenario B, expenses are up to 90 % higher than the plant's revenues at this scale, mainly due to the high amount of steam and cooling water required. Furthermore, the direct and indirect costs of scenario B are lower, as the valorisation process involves fewer equipment units, resulting in lower acquisition, instrumentation, and operational costs, as well as a reduced need for personnel to operate the equipment. Due to this, a sensitivity analysis will be carried out for scenario B (as it is the best from an environmental and economic point of view) in the following section to try to make the plant economically viable. This will involve adjusting parameters such as plant scale, among others, in an attempt to ensure that sales revenue can offset the necessary initial investment.

3.5. Sensitivity analysis

The sensitivity analysis is carried out under different scenarios by making changes regarding the scale of the industry, the initial investment required, or the selling prices established, as there are the main critical points derived from the TEA. For alternative 1, the initial investment required is reduced assuming that the costs related to the construction of the building and the land are zero, since the company already has the building acclimatized, considering only the costs of equipment and its installation. For alternative 2, the selling price of the products increases threefold. Attending to alternative 3, the initial scale of the plant, 250 kg/batch of chokeberry pomace, is assumed to change, with a raw material quantity 50 times greater in order to assess the influence of the scale change. For alternative 4, it is decided to increase the scale a little more and assume that the amount of chokeberry pomace per batch is 100 times higher. In alternative 5, the same assumptions regarding the initial investment assumed for alternative 1 are considered the scale selected in alternative 3, and finally, for alternative 6, the same assumptions were made as in alternative 1 but for the scale selected in alternative 4, to assess whether the exclusion of land and construction costs with the scale change results in better outcomes.

Despite the numerous modifications made, none of the alternatives analysed result in a positive revenue level. This indicates that to become economically viable, the amount of products obtained would need to increase significantly by exploring other technologies with higher extraction yields, or by reducing the operating costs drastically. Increasing the selling prices does not help either, as the quantity of phenolic compounds is mainly low and with the highest price of the products elaborated. Consequently, in all scenarios, the NPV remains negative and the IRR does not yield a positive value. This clearly demonstrates that, despite being the most environmentally favourable option and requiring the least capital investment, it is not economically profitable. The NPV results for alternatives 1–6 are as follows: - 28,930,559 USD, -28,752,774 USD, -167,829,820 USD, -291,780,315 USD, -72,993,718 USD, and -129,288,348 USD, respectively.

4. Future research prospects

Future studies could improve the biorefinery system's environmental and economic feasibility by exploring two key strategies. Firstly, to improve production yields, the co-digestion of chokeberry pomace with other substrates could be implemented, or alternative technologies to enhance phenolic extraction yields could be explored. Combining pomace with complementary organic materials may boost biogas production through improved nutrient balance and synergistic microbial interactions, thereby increasing energy output. Additionally, enhancing the yields of phenolic compounds would help balance income and expenses, thereby improving the economic viability of the plant, although it would also be necessary to consider other factors such as the seasonality or logistics of the biomass.

Secondly, transitioning to environmentally sustainable steam generation methods could significantly reduce the biorefinery's environmental impact, as steam production is a major hotspot across most impact categories. Alternatives such as biomass boilers or solar-thermal systems could be implemented, aiming to lower operational costs and improve the environmental footprint. Another option could be to use energy from hydrogen, the only clean energy source that does not cause any adverse environmental impacts during its production or throughout the supply chain, as it can be produced from renewable resources (Yukesh Kannah et al., 2021). These strategies offer scalable and sustainable solutions for the valorisation of chokeberry pomace and similar biorefinery systems.

5. Conclusions

This study assesses the environmental and economic sustainability of a biorefinery for chokeberry pomace valorisation, comparing two scenarios: i) bioethanol via fermentation and ii) bioenergy via anaerobic digestion. The bioenergy scenario demonstrated enhanced environmental performance across all impact categories, except marine eutrophication category. Steam production required for biorefinery operations was identified as the main environmental hotspot, accounting for over two-thirds of impacts in GW, TET, and FRS, followed by agricultural phase, chemical production and electricity consumption. Techno-economic analysis indicated that neither scenario is economically viable under conditions analysed. Sensitivity analysis confirmed that profitability would only be achieved with significant increases in production yields or substantial reductions in operational costs of the plant and initial capital investment.

CRedit authorship contribution statement

Adrián Agraso-Otero: Investigation, Methodology, Software, Visualization, Writing – original draft. **Ricardo Rebolledo-Leiva:** Investigation, Supervision, Writing – review & editing. **Eduardo Entrena-Barbero:** Investigation. **Sara González-García:** Funding acquisition, Investigation, Supervision, Writing – reviewing and editing.

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. Supporting information

Supplementary data associated with this article can be found in the online version at [doi:10.1016/j.eti.2025.104165](https://doi.org/10.1016/j.eti.2025.104165).

Data availability

Data will be made available on request.

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