Science of the Total Environment 955 (2024) 177038

Contents lists available at ScienceDirect

Science of the Total Environment

journal homepage: www.elsevier.com/locate/scitotenv

# Life cycle assessment and yield to optimize extraction time and solvent: Comparing deep eutectic solvents vs conventional ones

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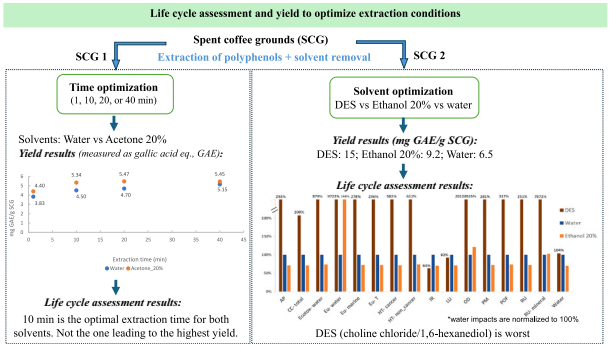
## HIGHLIGHTS

- Life cycle assessment as a tool to optimize extraction conditions (ex. polyphenols)
- The aim should be to obtain higher yield with lower environmental impact
- Polyphenol yield increase from 10 to 40 min doesn't offset the environmental impact
- Polyphenol yield increase with DES isn't enough to replace water as a solvent

## GRAPHICAL ABSTRACT




## ARTICLE INFO

Editor: Jacopo Bacenetti

*Keywords:*
Total polyphenols extraction
Spent coffee grounds
Eco-friendly solvents
Life cycle assessment
Environmental impacts

## ABSTRACT

Deep eutectic solvents (DES) are gaining interest as eco-friendly alternatives for extracting bioactive compounds, but their environmental benefits remain unclear and need further evaluation. In this work, a case study of total polyphenols (TPC) extraction from spent coffee grounds (SCG) was environmentally evaluated using life cycle assessment (LCA). First, the most convenient extraction time (1, 10, 20, or 40 min) for water and acetone 20 % from an environmental perspective was identified. Second, a comparison of different solvents—DES (choline chloride-1,6-hexanediol), water, and ethanol 20 %—under their optimal extraction yield conditions was performed using literature data. Results from the first study revealed that the environmentally optimal extraction time (10 min) was not the one leading to the highest yield. The main contributors to the impacts were the use of acetone and electricity consumption.

For the second study, DES performed worse in all studied environmental impact categories compared to both ethanol 20 % and water. Ethanol 20 % was the better option compared to water due to its higher extraction yield (9.2 mg vs. 6.5 mg TPC/g SCG, respectively). The environmental impacts associated with the DES system were primarily attributed to the DES preparation step, which requires virgin raw materials (e.g., dimethyl hexanediol), and the adsorption stage involving the use of resins. A sensitivity analysis was also conducted by optimizing the DES system to the best possible described conditions (90 % reuse of DES and maximum reduction of the

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https://doi.org/10.1016/j.scitotenv.2024.177038
Received 16 July 2024; Received in revised form 21 September 2024; Accepted 16 October 2024
Available online 20 October 2024

macroporous resin used to adsorb the TPC after extraction). Nevertheless, the DES system still performed worse than water or ethanol 20 % systems, in 11 out of 16 impact categories.

The study highlights the importance to consider environmental impacts and yield when optimizing extraction processes, especially at the laboratory scale, as the insights gained are valuable for improving eco-efficiency on an industrial scale.

## 1. Introduction

The annual production of spent coffee grounds (SCG) is approximately 8 million tons, which is disposed of mainly via landfilling (Atabani et al., 2023). On the other hand, it has been reported that SCG contains valuable components such as polyphenols (TPC), which exhibit important bioactivities, including antioxidant and anti-inflammatory effects. As a result, adopting environmentally friendly extraction methods for bioactive compounds extraction has become increasingly prominent in recent years (Atabani et al., 2023).

Currently, new solvents are being developed to further reduce environmental impacts and avoid the use of more harmful options. Among these emerging solvents, ionic liquids (IL) and deep eutectic solvents (DES) have emerged as promising alternatives. Ionic liquids are salts that remain liquid near room temperature and exhibit unique properties such as high thermal stability, low vapor pressure, high dissolving capacity, low flammability, and high electrical conductivity. They have been found to be applicable in various fields such as catalyst recovery, electrochemistry and chemistry. However, their widespread use has been limited by certain challenges, including their high cost, difficulty in large-scale synthesis, as well as toxicity and biodegradability limitations (Greer et al., 2020; Ijardar et al., 2022; Płotka-Wasylka et al., 2020). In contrast, deep eutectic solvents (DES) are mixtures of two or more solid components that melt together at a temperature lower than the individual melting points of the components. When the components are derived from natural substances such as sugars, sugar alcohols, organic acids, or amino acids, they are known as natural deep eutectic solvents (NADES) (Paiva et al., 2014).

Traditional classifications of DES include Type I, consisting of a quaternary ammonium salt and a metal chloride, Type II, which combines a quaternary ammonium salt and a hydrated metal chloride, Type III, involving a quaternary ammonium salt as both a hydrogen bond donor and hydrogen bond acceptor, and Type IV, combining a metal chloride and a hydrogen bond donor (Ijardar et al., 2022).

Compared to IL, DES/NADES are cost-effective, easy to produce, biodegradable, and less toxic (Płotka-Wasylka et al., 2020) (Paiva et al., 2014; Syakfanaya and Saputri, 2019). Their primary drawbacks lie in their high density and viscosity (Płotka-Wasylka et al., 2020). Nonetheless, DES have gained interest and found application in various fields, including chemical catalysis, organic synthesis (Zaib et al., 2022), extraction of bioactive compounds, electrodeposition and enzymatic reactions (Peng et al., 2016). Despite these applications, the real potential of DES as an environmentally friendly solvent remains unclear. This highlights the need for DES environmental evaluation.

Life Cycle Assessment (LCA) emerges as a comprehensive approach, examining the environmental effects associated with each phase of a product's lifecycle, extending from resource extraction to disposal. It is a universally recognized and standardized method for evaluating the environmental sustainability of various processes, including emerging technologies and new materials. The environmental comparison of DES with conventional solvents using LCA has not been extensively researched (Murugan et al., 2021; Vinci et al., 2023; Wang et al., 2024). However, some studies on bioactive compounds' extractions were reported (Vinci et al., 2023; Wang et al., 2024). Regarding the extraction of bioactive compounds from plant materials, Vinci et al. (Vinci et al., 2023) have compared between MeOH 60 % and different DES types (Betaine/Fructose, Betaine/Triethylene-glycol, Choline Chloride/Fructose, Choline Chloride/ Triethylene-glycol) for the extraction of polyphenols from dark chocolate. The comparative LCA study highlighted that MeOH 60 % had a 60 % higher impact than DES especially in terms of mineral and fossil resources availability.

Wang et al. (Wang et al., 2024) also conducted a comparative study on three distinct extraction methods: heat reflux extraction (HRE), ultrasound-assisted extraction (UAE), and magnetic agitation in a water bath (DESE). These methods were applied to extract flavonoids from *Ginkgo biloba* leaves, using ethanol 70 %, ethanol 65 %, and DES (a mixture of choline chloride/glycerine), respectively. Ethanol 65 % using UAE was the eco-friendliest in all 8 impact categories. Both studies by Wang et al. (Wang et al., 2024) and Vinci et al. (Vinci et al., 2023) mainly focus on the extraction process only, excluding the processes to obtain the pure active substance from the extract. Therefore, an environmental impact evaluation for DES, including all processes, is essential to fully understand their potential and feasibility for large-scale applications.

The present study aims to perform, for the first time, a life cycle environmental assessment comparing water-based solvents and deep eutectic solvents (DES) using the same extraction method and including the subsequent step (solvent removal) to obtain the bioactive substances for further applications. Furthermore, this paper also addresses the optimization of extraction processes using not only extraction yield, but also the environmental impact. The hypothesis to be proved is that the optimum extraction conditions are those that do not require intensive use of resources to obtain adequate yield. This hypothesis will be tested using two different comparative analysis: study A (comparison of different extraction times) and study B (comparison of DES with conventional solvents). The chosen case study for both comparative analysis was the extraction of polyphenols (TPC) from spent coffee grounds (SCG).

## 2. Materials and methods

Life cycle assessment (LCA) methodology according to ISO 14044 (International Organization for Standardization, Environmental management — Life cycle assessment — Principles and framework, 2006) was used to assess the environmental comparison of the extraction methods. A functional unit of 100 mg of TPC extracted from SCG was defined as reference unit for the comparisons. As mentioned earlier, two different comparative analyses were performed: study A (comparison of different extraction times) and study B (comparison of DES with conventional solvents). The link between the two studies lies in the fact that the optimization considers both the TPC yield and the environmental impact. However, the two analyses are treated separately because the yields obtained are not comparable, as different SCG samples were used as raw material. As previously reported by Bouhzam et al. (Bouhzam et al., 2023), SCG samples can vary significantly in composition (e.g., TPC content) due to factors such as origin, coffee variety (e.g., arabica, robusta, etc.), grain preparation (e.g., roasting), and the infusion preparation process. The scope and system boundaries of each study are detailed in Sections 2.1 and 2.2, respectively.

The processes were modelled using Gabi software v10.6.135 (2023), and the Environmental Footprint (EF) 3.1 method, recommended by the European Commission (European Commission, 2017), was used for the impact assessment. The evaluation was based on sixteen impact categories including acidification potential (AP, mole of $H^+$ eq), climate change total (CC, kg $CO_2$ eq), freshwater ecotoxicity (Ecotox-water, CTUe), freshwater eutrophication (Eu-water, kg P eq), marine

eutrophication (Eu-marine, kg N eq), terrestrial eutrophication (Eu-T, mole of N eq), human toxicity-cancer (HT- cancer, CTUh), human toxicity-non_cancer (HT- non_cancer, CTUh), ionizing radiation-human health (IR, kBq U235 eq), land use (LU, Pt), ozone depletion (OD, kg CFC-11 eq), particulate matter (PM, disease incidences), photochemical ozone formation (POF, kg NMVOC eq), resource use-fossils (RU-fossils, MJ), resource use-mineral and metals (RU-mineral, kg Sb eq), and water use (water, $m^3$ world equivalent).

### 2.1. Study A: Comparison of different extraction times

The first study aimed to conduct an environmental comparison of different extraction times (1, 10, 20, and 40 min) using water and a 20 % mixture of acetone/water as solvents for the extraction of total polyphenols (TPC). These comparisons would enable visualizing the effect of the extraction time (and yield obtained) on the environmental performance of the extraction process.

Total polyphenols extracted was measured using the Folin–Ciocalteu method, and results were expressed in mg of gallic acid equivalent (GAE) per g of spent coffee ground (SCG). These results were derived from previous experiments performed by our research team and published by Bouhzam et al. (Bouhzam et al., 2023) (see Fig. 1). As evidenced by the results presented in Fig. 1, the use of acetone 20 % significantly enhances the extraction yield, with a gradual increase from 4.40 to 5.47 mg GAE/g SCG in 20 min. To assess the impact of time on the environmental performance of the extraction process, a comparative analysis will be performed using water as solvent, aiming to identify the duration that optimizes environmental efficiency. A similar study will be conducted for acetone 20 % as the solvent. Finally, a comparison involving both solvents at their optimal extraction times will be conducted to identify the environmentally better solvent for TPC extraction, thereby providing a comprehensive understanding of both yield efficiency and environmental implications.

To conduct the environmental comparison, the functional unit (FU) was defined as: “100 mg of TPC extracted from spent coffee grounds”. Two processes were evaluated: Extraction and filtration, followed by evaporation of the solvent. The first one consists of the extraction of TPC from SCG, followed by a filtration step to separate the extract from the solid SCG. The evaporation process involves the complete evaporation of the solvent.

The remaining wet SCG from the extraction and filtration processes was considered to be treated in a composting plant. Additionally, 90 % of the distilled water resulting from the evaporation process was reused in the extraction process, while the remaining 10 % was sent for incineration. Similarly, 90 % of the distilled acetone was reused in the extraction process.

The system boundaries of the study using acetone 20 % as solvent for 1 min are detailed in Fig. 2. The system boundaries remain the same whether using water, or acetone 20 % as the solvent. Nevertheless, the inventory data presented in Fig. 2 correspond to the one using acetone 20 %. This inventory data will be explained in the following sections.

### 2.2. Study B: Comparison of DES with conventional solvents

To compare DES with conventional solvents, a literature review was performed to identify extraction methods to obtain polyphenols (TPC) and/or chlorogenic acid from spent coffee grounds (SCG). Only a limited number of studies have investigated the use of deep eutectic solvents (DES) for the extraction of TPC and chlorogenic acid from SCG. Specifically, six studies were identified in the literature using DES extraction, five of them measuring total polyphenols extracted, and only two measuring chlorogenic acid. Table 1 presents these studies showing, for each study, the best results obtained with DES extraction. The total polyphenols (TPC) is expressed as milligrams of gallic acid equivalent (GAE) per gram of SCG, while chlorogenic acid was measured as the amount of one or more of its isomers. For example, in study 6, the isomers 3-CQA, 4-CQA, and 5-CQA were quantified collectively, and the results were expressed in mg 3-CQA eq per g SCG. On the other hand, in study 5, the results were presented in mg chlorogenic acid (CA) per g of SCG without specifying the particular isomer being quantified.

The reported results of total polyphenols and chlorogenic acid using DES ranged from 0.46 to 31.67 mg GAE/g SCG, and from 4.6 to 5 mg CA/g respectively using different molar ratios and liquid to solid ratios, with extraction times ranging from 15 to 150 min, and extraction temperature varying from ambient to 120 °C. The results from different authors presented in Table 1 cannot be compared because they are greatly affected by the diversity in composition of the spent coffee grounds used as raw material in the various studies. This variation in both SCG and the extraction methods ensures that TPC yields obtained using DES cannot be directly compared among different studies. On the contrary, direct comparison between them would be unsuitable and inaccurate, as previously reported by Bouhzam et al. (Bouhzam et al., 2023).

Table 1 also presents the results obtained using various conventional

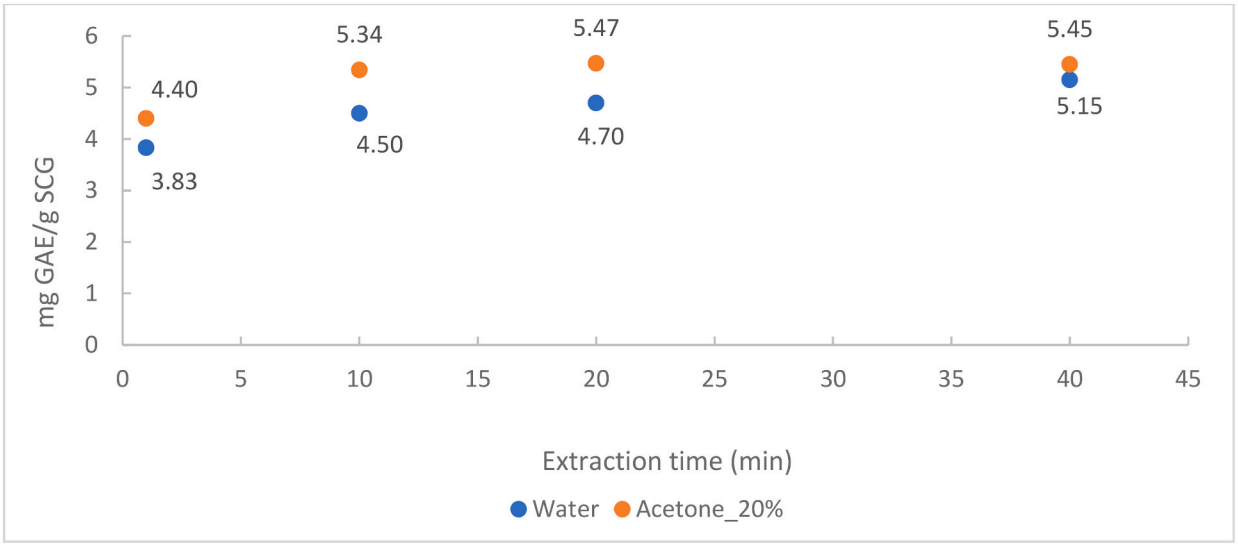


**Fig. 1.** Kinetic curves of total polyphenols at room temperature using water and acetone at 20 % (m/m) as the extraction solvents. (Bouhzam et al. (Bouhzam et al., 2023)).

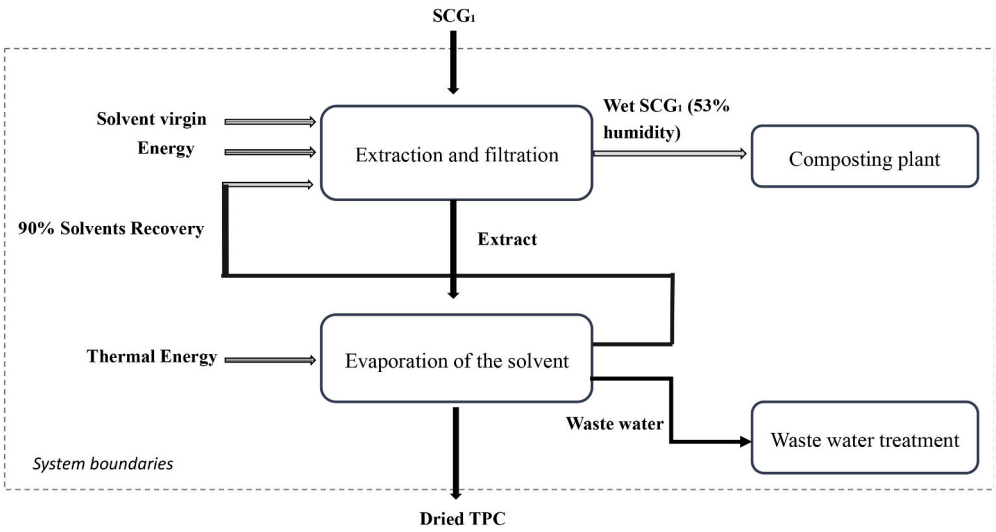


**Fig. 2.** System boundaries for total polyphenols (TPC) extraction using water or 20 % acetone/water mixtures as solvent.

**Table 1**
Comparison of deep eutectic solvents and conventional solvents for the extraction of total polyphenols, and chlorogenic acid from SCG.

| Study n° | Solvent | Molar ratio for DES | Extraction method | Time | T (°C) | Liquid solid ratio | TPC (mg GAE /g) | Chlorogenic acid (mg/g) | References |
|---|---|---|---|---|---|---|---|---|---|
| 1 | Betaine - 1,2-butanediol | [1:7] | Magnetic agitation | 60 min | 50 | 10 g/g | 31.67 | – | (Krisanti et al., 2019) |
| | Ethanol 96 % | – | – | – | – | – | 4.24 | – | |
| 2 | Water | – | Magnetic agitation-water bath | 1 h | 100 | 8 mL/g | 9.5 | – | (García-Roldán et al., 2023) |
| | Ethanol 60 % | – | Magnetic agitation-water bath | 2 h | 60 | 8 mL/g | 13 | – | |
| | Chlorine chloride: 1,2-propanediol and water | [1:2] with 50 % water | Magnetic agitation-water bath | 150 min | – | 15 mL/g | 14 | – | |
| 3 | Betaine: Glycerol and water | [1:2] with 10 % water | Ultrasound | 40 min | – | 3 % (S/L) | 28.65 | – | (Tzani et al., 2023) |
| | Betaine: Glycerol and water | [1:2] with 50 % water | Microwave | 60 min | 90 | 1 % (S/L) | 30.9 | – | |
| | Ethanol 50 % | – | Microwave | 60 min | 90 | 1 % (S/L) | 22.67 | – | |
| 4 | Choline chloride: glycerol and water | [1:2] | Microwave | 15 min | 120 | 10 % (*w*/*v*) | 0.46 | – | (López-Linares et al., 2021) |
| | Ethanol 25 % | – | Microwave | 15 min | 60 | – | 0.3 | – | |
| 5 | Betaine–Triethylene glycol and water | [1:2] with 30 % water | Ultrasound | 20 min | 65 | 15 mL/g | – | 4.6 mg CA/g | (Fanali et al., 2020) |
| **6** | **Choline Chloride-1,6-hexanediol** | **[1:2]** | **Ultrasound** | **45 min** | **Ambient** | **17 mL/g** | **15** | **5 mg 3-CQA/g** | (Yoo et al., 2018) |
| | **Ethanol 20 %** | **–** | **Ultrasound** | **45 min** | **Ambient** | **17 mL/g** | **9.2** | **4.9 mg 3-CQA/g** | |
| | **Water** | **–** | **Ultrasound** | **45 min** | **Ambient** | **17 mL/g** | **6.5** | **4.8 mg 3-CQA/g** | |

solvents. It's noteworthy that direct comparisons between deep eutectic solvent (DES) extraction and conventional solvents are limited in the literature. Specifically, only two studies (n° 3 and n° 6) have employed identical extraction conditions for both DES and conventional solvents, making them suitable for comparison. The study 6 (described by Yoo et al. (Yoo et al., 2018)) will be considered in the comparative analysis (study B) since it is the only study that includes water in addition to DES and ethanol, using the same SCG. Results obtained in study n° 6 revealed that the TPC contents obtained using DESs were 63 %–130 % higher than those with ethanol 20 % and water, respectively. Nevertheless, an in-depth LCA is needed to determine the environmental impact of these extraction processes. Such an assessment would identify the significant environmental burdens and provide a clearer understanding of the extent to which DES can be considered truly green solvent in the context of TPC extraction.

Hence, the environmental comparison of DES (choline chloride/hexanediol) with conventional solvents (water and ethanol 20 %) will be performed with the experiments described by Yoo et al. (Yoo et al., 2018) (study n° 6) in Table 1. The comparison will be performed by using the total polyphenols (TPC) as the valuable substance that we want to obtain.

The functional unit (FU) for this comparison was also defined as "100 mg of total polyphenols (TPC) extracted from spent coffee grounds". The processes considered for the extraction with DES were the ones reported by Yoo et al. (Yoo et al., 2018), although to complete the inventory data needed, additional data was collected from other studies. Five processes were identified: preparation of DES, extraction and separation, adsorption, desorption, and evaporation of solvents (see Fig. 3).

DES was prepared by mixing choline chloride with 1,6-hexanediol in a molar proportion of 1:2. The extraction and separation processes

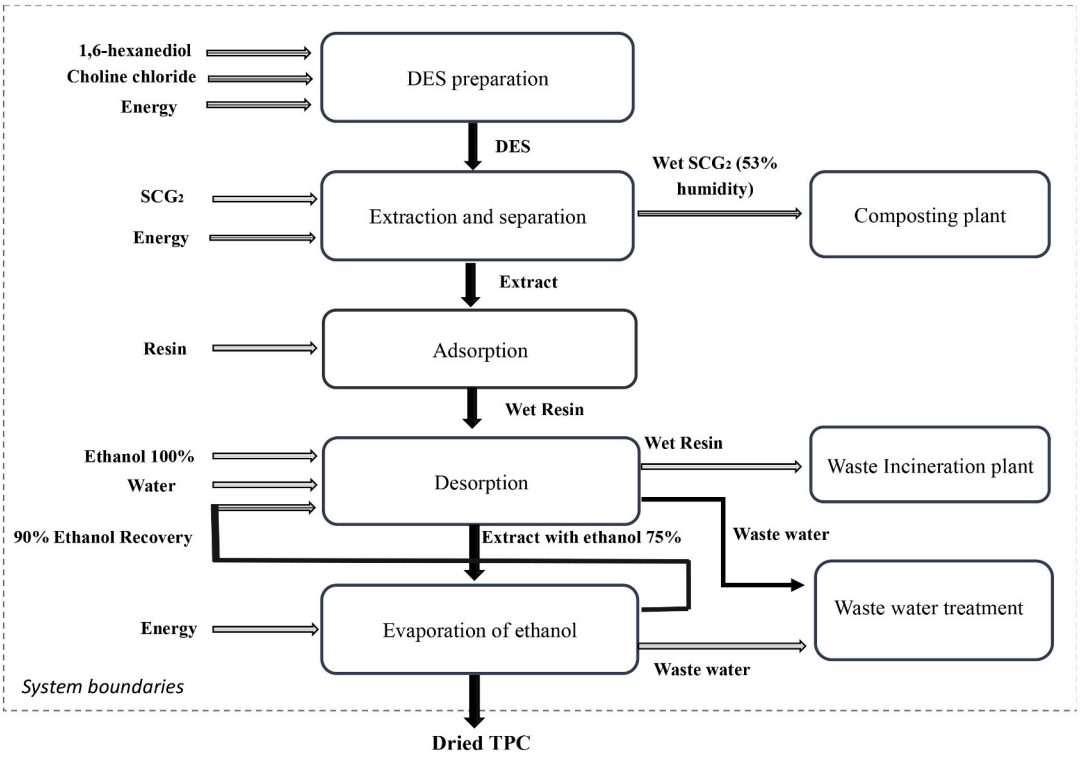


**Fig. 3.** System boundaries for DES extraction.

consist of the extraction of total polyphenols from SCG followed by filtration to isolate the extract from the SCG. The extract was then passed through an adsorption column filled with macroporous resins (in which TPC were retained). Then, the resins were washed with water (to remove DES from the resin), followed by a 50 % ethanol/water mixture, and finally ethanol 100 % to recover total polyphenols (TPC). The resulting ethanolic mixture was subjected to evaporation to obtain the final product (TPC). It was assumed that 90 % of the ethanol regenerated was reused in the desorption process.

The system boundaries of the study are detailed in Fig. 3. The inventory data will be explained in the following section.

### 2.3. Modelling in the software

The modelling of both studies is primarily based on the use of various chemicals (1,6-hexanediol, choline chloride, resin, water, ethanol), along with the consumption of electricity and thermal energy. The data for resin, water, ethanol, electricity, and thermal energy were obtained from the ecoinvent database. Electricity and thermal energy were modelled using the Spanish medium voltage electricity grid mix (1–60 kV), and the Spanish thermal energy from natural gas respectively. 1,6-hexanediol was substituted by dimethyl hexanediol, as a proxy, due to the lack of data in the database. Choline chloride production process was modelled based on the methodology detailed in the literature (Zaib et al., 2022). This process involves the use of primary reagents needed to obtain choline chloride. Hence, the inputs considered were hydrochloric acid (HCl), trimethylamine (TMA), deionized water (DI water) and ethylene oxide (EO), all of them obtained from the ecoinvent database. Waste treatments were implemented as follows: wet SCG (53 % humidity) was composted, wet resin (53 % humidity) was incinerated, and wastewater was treated in a municipal water treatment, where the sludge obtained was meant for incineration.

## 3. Inventory data

The data for the comparison of different extraction times (section 2.1) were collected from Bouhzam et al. (Bouhzam et al., 2023) as said before (see Fig. 1). The results obtained (total polyphenols yield) at each extraction time were used to determine the different inputs and outputs required to obtain the functional unit for the comparison, defined as 100 mg TPC.

The data for the comparison of DES with conventional solvents (section 2.2) were collected from Yoo et al. (Yoo et al., 2018). Based on this previous study, 0.75 mg GAE, 0.46 mg GAE, and 0.325 mg GAE were obtained using DES, ethanol 20 %, and water extraction methods, respectively. These results were used to determine the different inputs and outputs required to obtain the functional unit for the comparison, thus 100 mg TPC. The inputs and outputs are given as the amount per experiment.

### 3.1. Study A: Inventory data for the comparison of different extraction times

In this section, the necessary calculations to obtain the inventory data for the first study are explained. Tables 2 and 3 present the inventory data using water and acetone 20 % as solvents, respectively, with an extraction time of 1 min. Similar calculations are required to obtain the data for the various extraction times (1, 10, 20, and 40 min) considering the different yields in TPC obtained. The only factor that changes with extraction time is electricity consumption, which increases from 24 kJ for 1 min, to 30 kJ for 10 min, 36 kJ for 20 min, and 48 kJ for 40 min, respectively.

#### 3.1.1. Extraction and filtration

A 0.7 g sample of dry SCG was mixed with 4 mL of water or acetone 20 % and vortex-stirred for the following different times: 1, 10, 20, and 40 min for water extraction and 1, 10, 20 min for acetone 20 % extraction (Bouhzam et al., 2023).

Subsequently, the mixture was centrifuged for 30 min and filtered. The power of the vortex (Velp Scientifica F202A0176, Usmate, MB, Italy) was 10.3 W. The centrifuge (J.P. Selecta 7,002,575, Barcelona, Spain) could support a capacity of 16 tubes with a power of 210 W.

**Table 2**
Inventory data to extract total polyphenols from 0.7 g of SCG in 1 min using water as solvent.

| Stage | Inputs | Amount/ experiment with 90 % reused solvent (g) | Outputs | Amount/ experiment with 90 % reused solvent (g) |
|---|---|---|---|---|
| **Extraction and filtration** | Water | 1.11 | Wet $SCG_1$ (53 %) | 1.49 |
| | $SCG_1$ | 0.70 | | |
| | Electricity[a] (kJ) | 24.2 | Extract (with polyphenols) | 3.20 |
| **Evaporation of solvent** | Extract (with polyphenols) | 3.20 | Water for reuse | 2.88 |
| | | | Waste water | 0.320 |
| | Thermal energy (kJ) | 8.30 | Total polyphenols (measured as GAE[b]) | $2.68\ 10^{-3}$ |

[a] Electricity consumption was estimated from the power and use-time of each equipment. Vortex: 10.3 W and 1 min per experiment. Centrifugation: 210 W and 30 min considering a capacity of 16 tubes (one tube is one experiment).
[b] GAE: gallic acid equivalent.

**Table 3**
Inventory data to extract total polyphenols from 0.7 g of SCG in 1 min using acetone (20 %) as solvent.

| Stage | Inputs | Amount/ experiment with 90 % reused solvent (g) | Outputs | Amount/ experiment with 90 % reused solvent (g) |
|---|---|---|---|---|
| **Extraction and filtration** | Acetone 20 % | 0.211 | Wet $SCG_1$ (53 %) | 1.49 |
| | Water | 0.844 | | |
| | $SCG_1$ | 0.700 | Extract (with polyphenols) | 2.65 |
| | Electricity[a] (kJ) | 24.2 | | |
| **Evaporation of solvent** | Extract (with polyphenols) | 2.65 | Water for reuse | 1.91 |
| | | | Acetone for reuse | 0.477 |
| | | | Waste water | 0.265 |
| | Thermal energy (kJ) | 5.83 | Total polyphenols (measured as GAE[b]) | $3.08 \times 10^{-3}$ |

[a] Electricity consumption was estimated from the power and use-time of each equipment. Vortex: 10.3 W and 1 min per experiment. Centrifugation: 210 W and 30 min considering a capacity of 16 tubes (one tube is one experiment).
[b] GAE: gallic acid equivalent.

Hence, the energy consumption per experiment was calculated using the power corresponding to one tube and the operating time of the equipment. The wet SCG has 53 % humidity (determined using vacuum filtration followed by drying at 100 °C) and was considered to be processed in a composting plant.

#### 3.1.2. Evaporation of solvent

The evaporation process consisted of the complete evaporation of the solvent, either water or acetone 20 %, to obtain the bioactive substance (TPC). Approximately, 90 % of the evaporated solvent was recycled and reused in the extraction process. The thermal energy required for the solvent evaporation was estimated theoretically by heating to its boiling point and accounting for the subsequent phase change from liquid to vapor.

### 3.2. Study B: Inventory data for the comparison of DES with conventional solvents

In this section, the inventory data for the comparison of DES with conventional solvents (water and ethanol 20 %) are presented and explained. Tables 4 and 5 provide inventory data for DES and ethanol 20 %, respectively. Similar calculations, as performed for ethanol 20 %, are necessary to obtain the inventory data for water. The data presented here is for total polyphenols extraction. Inventory data in Tables 4 and 5 was calculated according to the experiments and yields described by Yoo et al. (Yoo et al., 2018). Some additional information was also needed to obtain the complete mass and energy balance. All these calculations are explained below.

#### 3.2.1. DES preparation

Choline chloride and 1,6-hexanediol were mixed in a 1:2 M ratio and stirred at 80 °C. The reference article did not provide a specific time for preparing DES. Therefore, a duration of 90 min was adopted based on the work of Zahrina et al. (Zahrina et al., 2018). The density of DES was estimated to be 1.057 g/cm$^3$, referring to choline chloride and butanediol (Mirza et al., 2015).

The energy consumption associated with the preparation was calculated by considering the power of stirring and heating and the operating time of the equipment. The stirring and heating power was the one from IKA magnetic stirrer (IKA C-MAG HS7, Staufen im Breisgau, Germany), with an estimated capacity of 10 L.

#### 3.2.2. Extraction and separation

The extraction process involved the recovery of total polyphenols from SCG, followed by a filtration process to isolate the liquid extract from the solid SCG. A liquid/solid ratio of 17 mL/g SCG was used for the extraction process, as reported by Yoo et al. (Yoo et al., 2018) (for 0.05 g SCG, 0.85 mL are required). The extract was then subjected to the adsorption process. The wet SCG, having a 53 % humidity, was considered to be processed in a composting plant.

To estimate the power required per experiment for the extraction (ultrasound) and separation (centrifuge & filtration), other equipments were used due to the lack of data for the devices used by Yoo et al. (Yoo et al., 2018). Specifically, the power of the J.P. Selecta 3,000,866 ultrasound bath (180 W, 24 tube capacity) (Barcelona, Spain) and the lab centrifuge FC5714 centrifuge (300 W, 24 tube capacity) (Atkinson, Nebraska, USA) were considered for the respective processes. The energy consumption per experiment was then calculated using the power corresponding to one tube and the operating time of each equipment (45 min and 20 min respectively).

#### 3.2.3. Adsorption

The adsorption process involved the recovery of total polyphenols (TPC) from the DES solvent assisted by macroporous resins. According to Yoo et al. (Yoo et al., 2018), 5.18 g of resin, specifically selected for polyphenols extraction, were used with 0.84 mL of extract (hence a low ratio of 0.16 mL of extract per g of resin), but no reuse of the resin was mentioned. Nevertheless, different studies in the literature reported that macroporous resins could be reused several times. A summary of the studies found in the literature involving macroporous resins for the extraction of total polyphenols using DES is presented in Supplementary Materials (see Table S6 in SM1). Some of these studies have evaluated the reusability capacity of these resins. Specifically, four studies reported that resins could be effectively reused between five to six cycles when employing DES as the extraction solvent. These resins may have a significantly extended lifecycle, being reusable up to twelve times when solvents such as ethanol 60 % are used. Based on study 14 (Wang et al., 2022), six cycles were adopted to assess the reusability of the resin in the present study.

The recovery ratio of the adsorption and desorption processes is considered to be 92.3 %, as reported by Yoo et al. (Yoo et al., 2018).

**Table 4**
Inventory data to extract total polyphenols (TPC) from 0.05 g SCG in 45 min using DES (choline chloride/1,6-hexanediol) as solvent (adapted from Yoo et al. (Yoo et al., 2018).

| | Inputs | | Outputs | |
|---|---|---|---|---|
| | | Amount/ experiment with ethanol reuse (g) | | Amount/ experiment with ethanol reuse (g) |
| **DES Preparation** | 1,6-hexanediol | 0.565 | DES | 0.898 |
| | Choline chloride | 0.333 | | |
| | [a]Electricity (1) (kJ) | 0.496 | | |
| **Extraction and separation** | DES | 0.898 | Extract | 0.842 |
| | $SCG_2$ | 0.05 | Wet $SCG_2$ (53 %) | 0.106 |
| | [a]Electricity (2) (kJ) | 35.3 | | |
| **Adsorption** | Extract | 0.842 | Wet resin | 1.71 |
| | Macroporous Resin | 0.863 | | |
| **Desorption** | Wet resin | 1.71 | Wet Resin | 1.80 |
| | Water | 7.99 | Wastewater | 8.83 |
| | Ethanol (100 %) (for ethanol 50 %) | 2.39 | Ethanol 75 % with polyphenols | 29.7 |
| | Water (for ethanol 50 %) | 8.23 | | |
| | Ethanol (100 %) | 0.000 | | |
| **Evaporation of ethanol fractions** | Extract (ethanol 75 %) | 29.7 | Total polyphenols (measured as GAE[b]) | $0.75 \times 10^{-3}$ |
| | Thermal energy (kJ) | 42.1 | Pure Ethanol to reuse | 20.0 |
| | | | Wastewater | 9.65 |

[a] Electricity consumption was estimated from the power and use-time of each equipment. Electricity (1) (heating and stirring): 1020 W and 90 min considering a capacity of 10 L; Electricity (2) (ultrasound bath and centrifuge): 180 W for 45 min considering a capacity of 24 tubes, and 300 W for 20 min considering 24 tubes, respectively (1 experiment is equivalent to one tube).
[b] GAE: gallic acid equivalent.

**Table 5**
Inventory data to extract TPC from 0.05 g SCG in 45 min using ethanol (20 %) as solvent (adapted from Yoo et al. (Yoo et al., 2018).

| | Inputs | | Outputs | |
|---|---|---|---|---|
| Stage | | Amount/ experiment with solvents reuse (g) | | Amount/ experiment with solvents reuse (g) |
| **Extraction and separation** | Ethanol 20 % | 0.0266 | Wet $SCG_2$ (53 %) | 0.106 |
| | Water | 0.107 | | |
| | $SCG_2$ | 0.05 | Extract (with polyphenols | 0.767 |
| | Electricity[a] (kJ) | 35.3 | | |
| **Evaporation of solvent** | Extract (with total polyphenols) | 0.767 | Water for reuse | 0.552 |
| | | | Acetone for reuse | 0.138 |
| | | | Waste water | 0.0767 |
| | Thermal energy (kJ) | 1.72 | Total polyphenols (measured as GAE[b]) | $0.46 \times 10^{-3}$ |

[a] Electricity consumption was estimated from the power and use-time of each equipment. Ultrasound bath: 180 W and 45 min per experiment, considering a capacity of 24 tubes. Centrifugation: 300 W and 20 min, considering 24 tubes capacity (one tube is one experiment).
[b] GAE: gallic acid equivalent.

#### 3.2.4. Desorption

The desorption process consists of the recovery of the TPC from the resin. Hence, the resin was subjected to three wash cycles: initially with 8 mL of water, followed by 18 mL of 50 % ethanol, and finally with 18 mL of 100 % ethanol to recover the extracted compounds (Yoo et al., 2018). The humidity of this resin after the desorption process was estimated to be approximately 53 %, similar to that of the SCG. The wet resin was assumed to be treated in a municipal solid waste incineration plant. Energy requirements were not considered in the adsorption and desorption processes.

#### 3.2.5. Evaporation of solvent

The evaporation process consisted of the evaporation of the solvent (only ethanolic fractions) to recover the total polyphenols (TPC) obtained. The reference article (Yoo et al., 2018) did not consider any amount of TPC transferred to the water fraction. The mixed ethanolic fractions contained approximately 75 % ethanol, with the remaining 25 % being water. 90 % of the ethanol was considered for reuse, while the remaining 10 % was assumed to be mixed with water and treated in a wastewater treatment facility. The thermal energy needed for solvent evaporation was estimated theoretically, by considering heating to boiling point and evaporation of each solvent.

The system boundaries for ethanol 20 % and water in study B corresponds to the one shown in Fig. 2, because the processes involved are the same. However, the inventory data used in this analysis (study B) was sourced from Yoo et al. (Yoo et al., 2018). The TPC yield using ethanol 20 % and water was 9.2 and 6.5 mg GAE/g SCG (being 0.46 and 0.33 for 0.05 g SCG), respectively, using an extraction time of 45 min.

## 4. Results and discussion

### 4.1. Results for study A: Comparison of different extraction times

#### 4.1.1. Main assumptions and limitations of study A

In study A, several assumptions were made and some of them might be considered also as limitations because they affect the results of the study.

The system boundaries of the study encompass only the process steps from the extraction of SCG to the obtention of TPC. Upstream processes, such as the collection and transportation of the SCG to the processing facility, as well as downstream processes, like the final use of TPC in the production of a commercial product, were excluded.

In the inventory analysis, data come from laboratory scale experiments and might change when the process is scaled-up. Although this was not the case for the laboratory experiments, a 90 % recirculation rate for all solvents after distillation was considered. Thus, when a 20 % acetone/water mixture was used as the extraction solvent, it was assumed that 90 % of both acetone and water separated by distillation would be reused in subsequent extraction cycles, while the remaining 10 % would be sent to a wastewater treatment plant, with the resulting

sludge being incinerated. Additionally, the remaining wet spent coffee grounds (SCG) from the extraction and filtration step, having 53 % humidity, was assumed to be treated at a composting facility. Finally, the electricity consumption during the extraction and filtration step was not measured experimentally; instead, it was overestimated based on the equipment's power rating and usage time. Electricity production was considered from the Spanish grid mix.

Regarding the impact assessment, only sixteen out of twenty-five impact categories from the EF 3.1 method were selected for the study.

However, it was presumed that none of these assumptions would change the main trends in the comparisons, as all systems were compared using the same hypotheses. The most critical assumption might be the exclusion of downstream processes from the study's scope, as the production of the final product, where TPC will serve as a raw input, could be significant and may influence the solvent evaporation step.

#### 4.1.2. Results from comparing different extraction times using water as solvent

The environmental comparison of different extraction times (1, 10, 20, and 40 min) for total polyphenol compounds (TPC) extraction using water as a solvent was conducted. The results, as presented in Fig. 4, illustrate the environmental impacts associated with the functional unit (FU) of extracting 100 mg of TPC (measured as gallic acid equivalent, GAE).

The data reveal that increasing the extraction time from 1 to 10 min not only enhances the extraction yield by 17 % but also maintains or reduces environmental impacts. However, extending the extraction time to 20 or 40 min increases TPC yield by 22 % and 34 %, respectively, compared to 1 min, while significantly raising environmental impacts. This increase is primarily driven by higher electricity consumption during the extraction process, particularly for stirring and centrifugation. Electricity consumption is the dominant factor in most impact categories, except for water eutrophication (Eu-water) and ozone depletion (OD). This is evident in Fig. 6, which visualize the hotspots to each impact category using a 20 % acetone/water mixture as the solvent. Using water as extraction solvent instead of acetone 20 % a similar trend is observed. For the Eu-water and OD impact categories, the main contributing factor is water consumption. Less water is required to obtain 100 mg TPC as extraction time increases, with the least water needed for 40 min, followed by 20 min, 10 min, and finally 1 min.

Consequently, the optimal extraction time for balancing efficiency and environmental considerations is identified as 10 min for TPC extraction from SCG.

#### 4.1.3. Results from comparing different extraction times using 20 % acetone/water mixture as solvent

The environmental assessment of different extraction times (1, 10, and 20 min) for TPC extraction using acetone 20 % as a solvent was investigated. Figs. 1 and 5, respectively, illustrate that increasing the extraction time from 1 to 10 min resulted in a 21 % increase in TPC yield, with a decrease in environmental impacts, as less inputs were required to obtain 100 mg TPC. Only in land use (LU) impact category, a slight impact increase was observed between 1 and 10 min, due to higher electricity consumption, which contributed 128 % to the total impact. However, this was partially offset by a 34 % environmental benefit from the composting of $SCG_1$.

The environmental impacts for acetone 20 % at 10 min were due mainly to electricity, contributing between 63 % and 90 % to the total impacts, and secondly to virgin acetone consumption (see Fig. 6). However, for Eu-water and OD, the impacts were mainly attributed to acetone, contributing over 57 %, and water consumption, which accounted for more than 35 % of the total impacts. It is important to remember that the study assumes 90 % of the solvents are recirculated, and only the 10 % added as virgin material contributes to the environmental impact. Similarly, for RU-mineral, the impacts were predominantly caused by acetone (76 %), with electricity contributing 23 %.

On the other hand, extending the extraction time to 20 min only yielded a 24 % increase in TPC yield compared to the 1 min extraction, with increased impacts across all categories. This increase in environmental impacts is primarily attributed to the higher electricity consumption required for the longer extraction process, with virgin acetone usage also contributing.

#### 4.1.4. Results from comparing conventional solvents in their optimal time conditions

Water and acetone 20 % at their optimum extraction time of 10 min were also compared environmentally. The environmental impacts of both solvents are presented in Fig. 7. The comparison of the results revealed that water is clearly better environmentally in only 4 out of 16 impact categories (Eu-water, HT-cancer, OD, and RU-mineral), while acetone 20 % performs slightly better in 8 out of 16 impact categories, with only the previous four categories being significantly higher compared to water. The impacts for acetone 20 % are mainly due to the

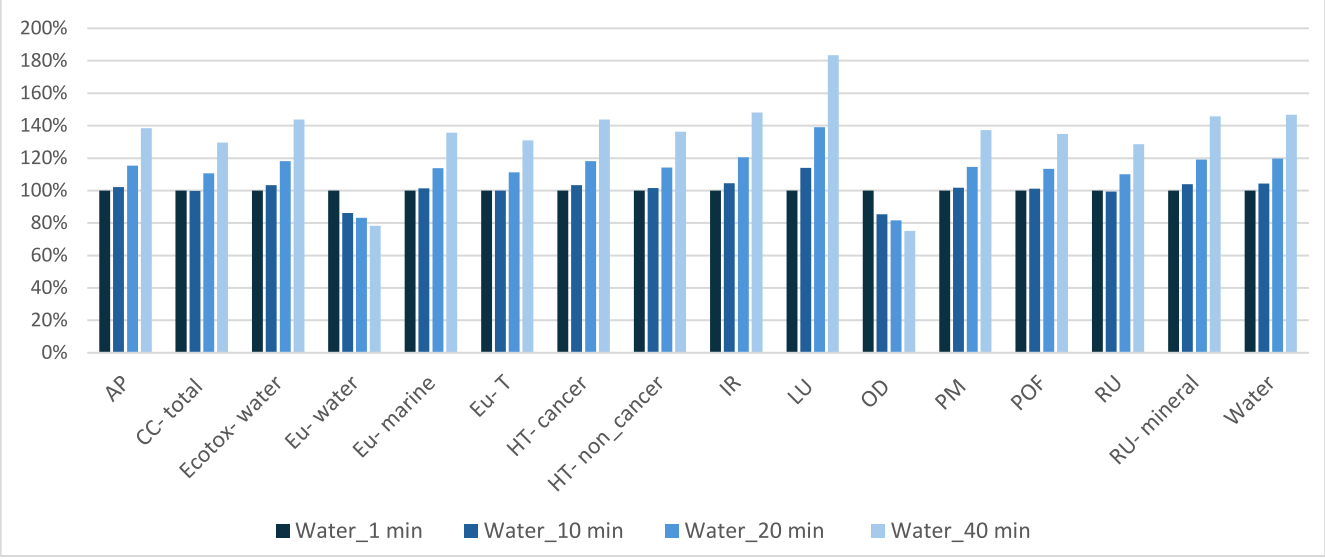


**Fig. 4.** Environmental impacts of TPC extraction using water and different extraction times (water_1 min is the baseline with 100 % impact in all impact categories).

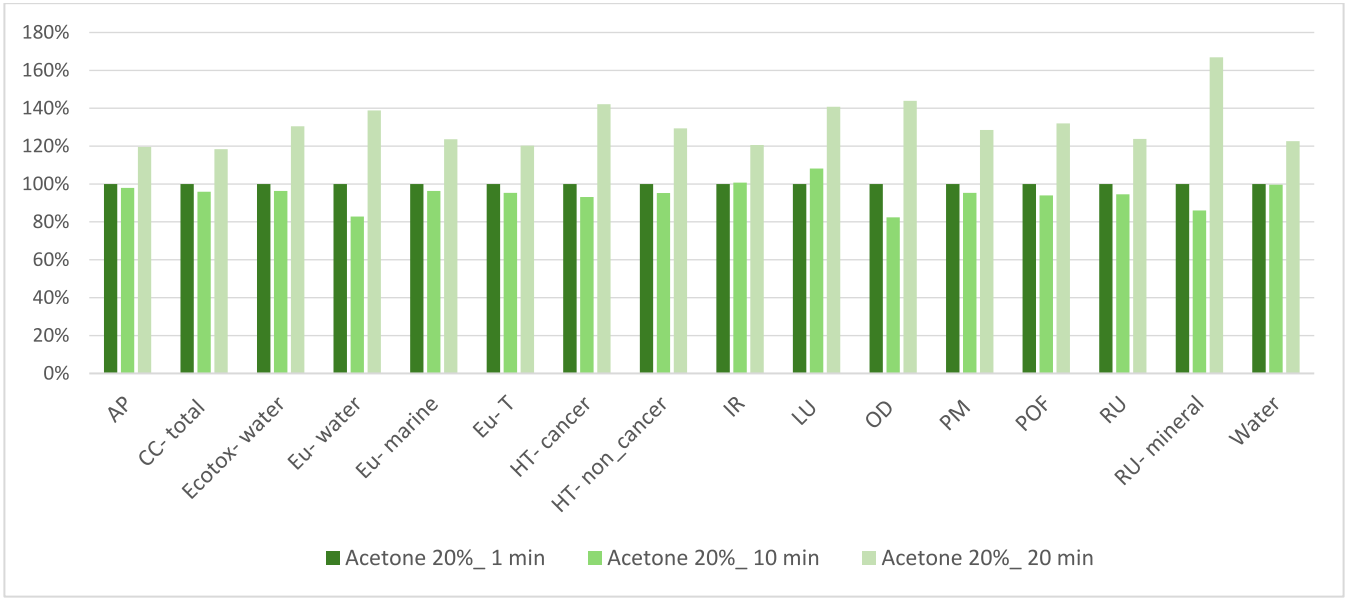


**Fig. 5.** Environmental impacts of TPC extraction using acetone 20 % and different extraction times (acetone 20 %_1 min is the baseline option, with 100 % impact in all impact categories).

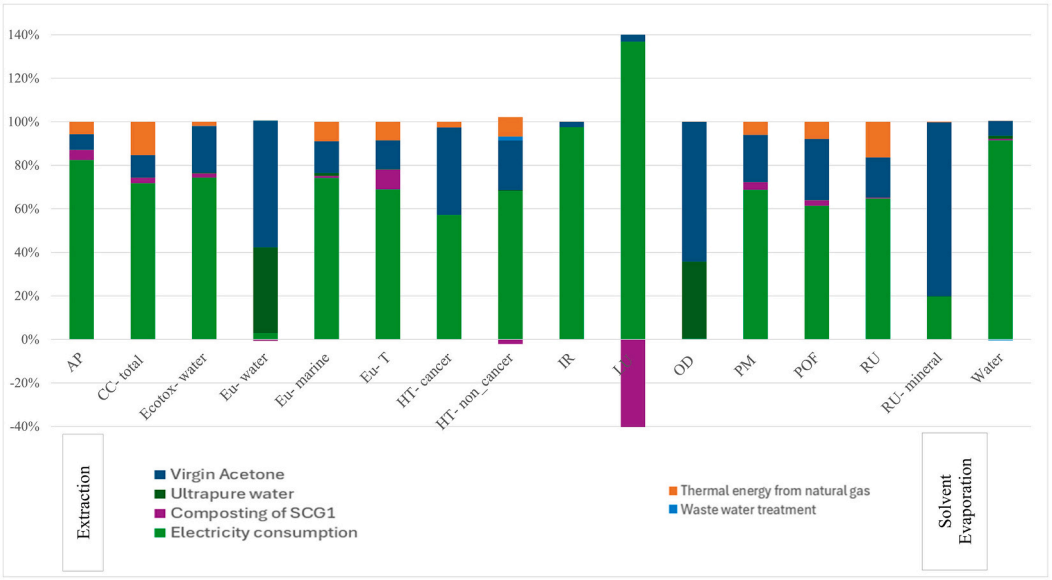


**Fig. 6.** Hotspots in the Environmental impact categories when using a 20 % acetone/water mixture as solvent with 1 min extraction time.

production of virgin acetone and the consumed electricity (see Fig. 6), while the main contributor to water impacts is electricity. Specifically, more electricity is needed to produce 100 mg of GAE, as acetone yields 3.74 mg GAE and water yields 3.15 mg GAE (for 0.7 g SCG). Therefore, the environmental impact of using water is primarily linked to its higher electricity consumption, while for acetone 20 %, the primary contributors are the use of the solvent itself and the energy consumption.

### 4.2. Results for study B: comparison of DES with conventional solvents

#### 4.2.1. Main assumptions and limitations of study B

In study B, which compares DES with conventional solvents, the same assumptions from study A were adopted, including the system boundaries, inventory data from laboratory experiments, a 90 % solvent recirculation rate, over-estimation of electricity consumption, etc. Additionally, in this study, the production of DES was modelled based on its components: choline chloride and 1,6-hexanediol. The production process of choline chloride was modelled using data from the literature (Zaib et al., 2022), while 1,6-hexanediol was substituted with dimethyl hexanediol. Since the reference article did not specify the time required for preparing DES, a duration of 90 min was adopted based on the study by Zahrina et al. (Zahrina et al., 2018).

#### 4.2.2. Environmental results for study B

The environmental impacts of DES, water, and ethanol 20 % extraction solvents are presented in Fig. 8. The results illustrate the environmental impacts associated with extracting 100 mg of TPC (measured as mg GAE), given that the extraction yield of DES, ethanol 20 %, and water were 0.75, 0.46, 0.33 mg GAE (from 0.05 g SCG) respectively.

The comparison of the results reveals that despite its lower yield, ethanol 20 % is clearly environmentally better than DES in 15 out of the

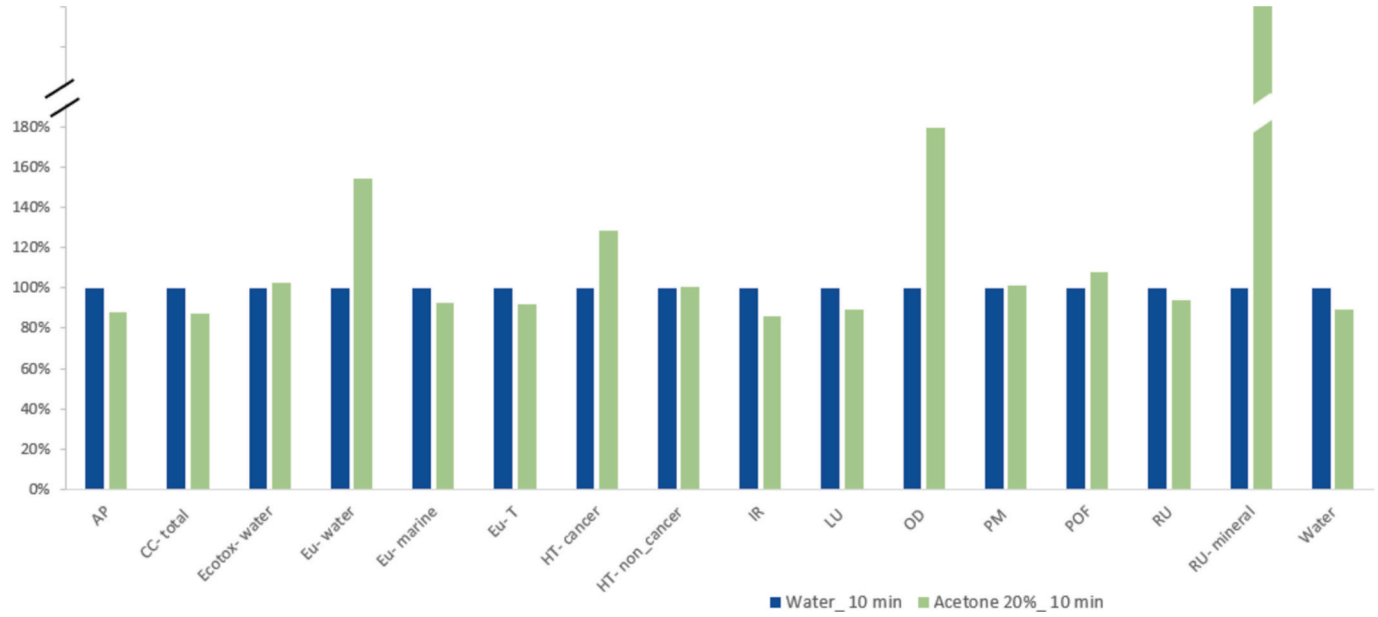


**Fig. 7.** Environmental impacts of TPC extraction using acetone 20 % and water at their optimum extraction time (water is the baseline option, with 100 % impact in all impact categories).

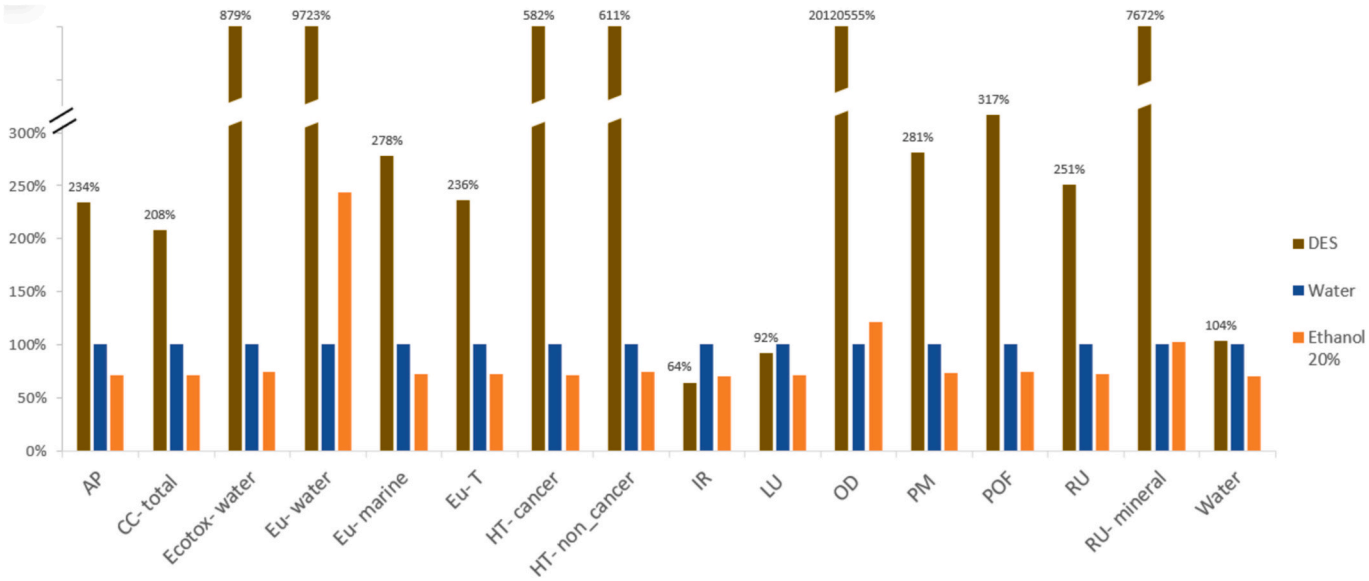


**Fig. 8.** Environmental comparison of DES, water and ethanol 20 % for the extraction of TPC (water is the baseline option, with 100 % impact in all impact categories).

16 studied impact categories. Additionally, ethanol 20 % performs better than water in 13 out of 16 impact categories, due to its higher yield. It is essential to emphasize that the extraction yield of each system significantly influences the environmental results, since the impacts are calculated to obtain a specific amount (100 mg) of the active substance (see Inventory Tables per FU in supplementary materials, SM1).

The environmental impacts associated with DES are mainly attributed to the preparation of DES, and the adsorption stage (see Fig. 9), due to the use of dimethyl hexanediol and resins, respectively. Furthermore, the impacts of the DES system are significantly influenced by the electrical energy consumed during the extraction stage. However, these impacts are lower than those associated with water and ethanol 20 %. Interestingly, the desorption stage presents lower impacts, as approximately 90 % of the ethanol required is considered to be reused.

When comparing the environmental profiles of ethanol 20 % extraction and water extraction, the ethanol extraction method performs worse in two impact categories: eutrophication of water (Eu-water) and ozone depletion (OD).

In the ethanol extraction system, the primary contributor to these impacts is the extraction stage, which involves electricity consumption for stirring and centrifugation. Additionally, for ozone depletion (OD) and freshwater eutrophication (Eu-water), the use of virgin ethanol and water significantly contributes to these environmental impacts, with contributions of 53 % and 41 % in OD, respectively, and 75 % and 14 % in EU-water.

### 4.2.3. *Sensitivity analysis*

As detailed in Section 4.2.2, the DES preparation process (due to DES raw materials) and the adsorption stage (due to the resin used) significantly contribute to the environmental impacts of deep eutectic solvents

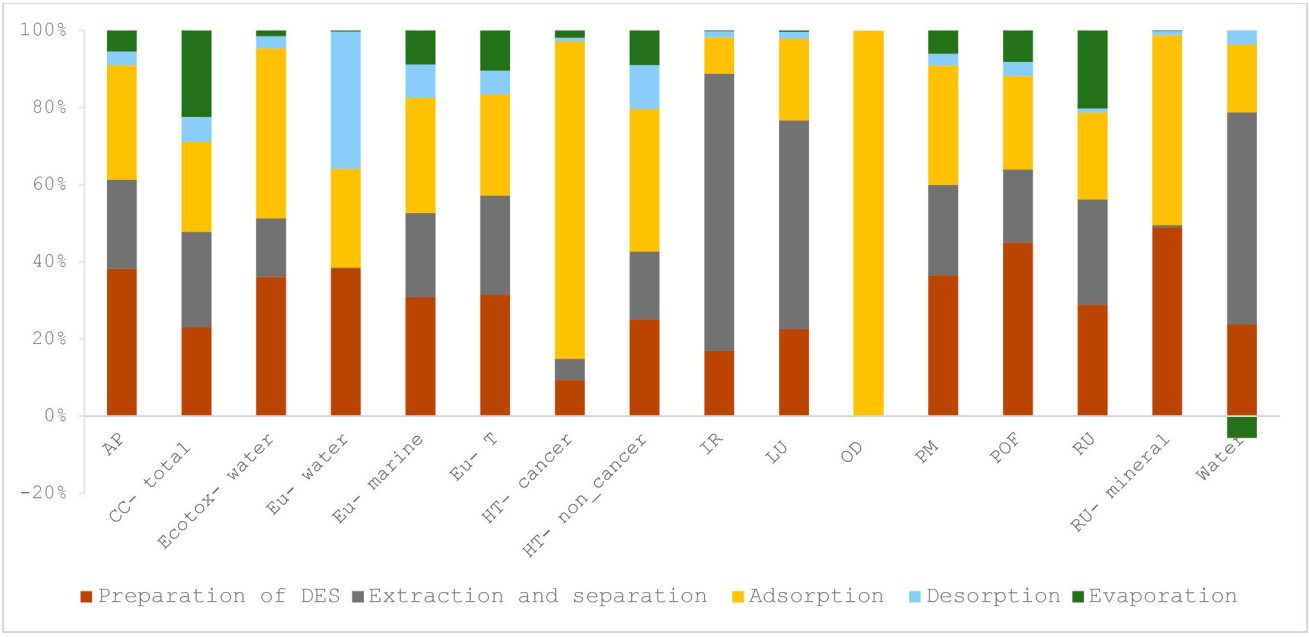


**Fig. 9.** Contribution of different steps in the environmental impacts of DES.

(DES) system. In order to reduce the contribution of DES preparation stage, the recycling of DES was investigated. Kovač's et al. (Kovač et al., 2021) highlights that DES can be recycled up to three times, suggesting that recycling DES in the desorption step, after water evaporation, could further diminish the environmental impacts of the DES preparation step. It was assumed that 90 % of the DES in water will be reused in the extraction process (considering one-time reuse for DES) (see Fig. 10 and Table 6).

Additionally, optimizing the adsorption process, which involves the use of macroporous resin, presents a viable approach. This can be achieved by reducing the quantity of resin used per mL of extract and, secondly, by extending the resin's reuse cycle beyond six. In this study, where the extract-to-resin ratio previously employed was 0.16 mL/g, a significant adjustment was made by searching for ratios described in the literature (see Table S6 in the Supplementary Materials, SM1). The higher ratio of 30 mL/g, used for TPC or chlorogenic acid extraction using DES (Liao et al., 2024), was chosen for the sensitivity analysis. Regarding the number of reuse cycles, the maximum described number of cycles (12 cycles), which was reported for ethanol 60 % as a solvent (see Table S6 in SM1), was considered here for DES. These three new

**Table 6**
Operational Parameters in the Base case scenario and the Improved Scenario for the DES System.

| Parameter | Base Case Scenario | Improved Scenario | Reference |
|---|---|---|---|
| **DES** | Not Recycled | 90 % Recycled | (Kovač et al., 2021) |
| **Extract to Resin Ratio** | 0.16 mL/g | 30 mL/g | (Liao et al., 2024) |
| **Resin Reuse Cycles** | 6 cycles | 12 cycles | (Ma et al., 2009) |

assumptions (Table 6) will significantly reduce the amounts of DES and resin required, which are the main contributors to most of the environmental impact categories.

The environmental results of these adjustments, all together, are illustrated in Fig. 11, revealing a decrease across all impact categories. Despite these improvements, DES continues to exhibit higher impacts in 11 out of the 16 evaluated impact categories compared to water or ethanol 20 % extraction systems.

The main contributors to these impacts are the extraction and

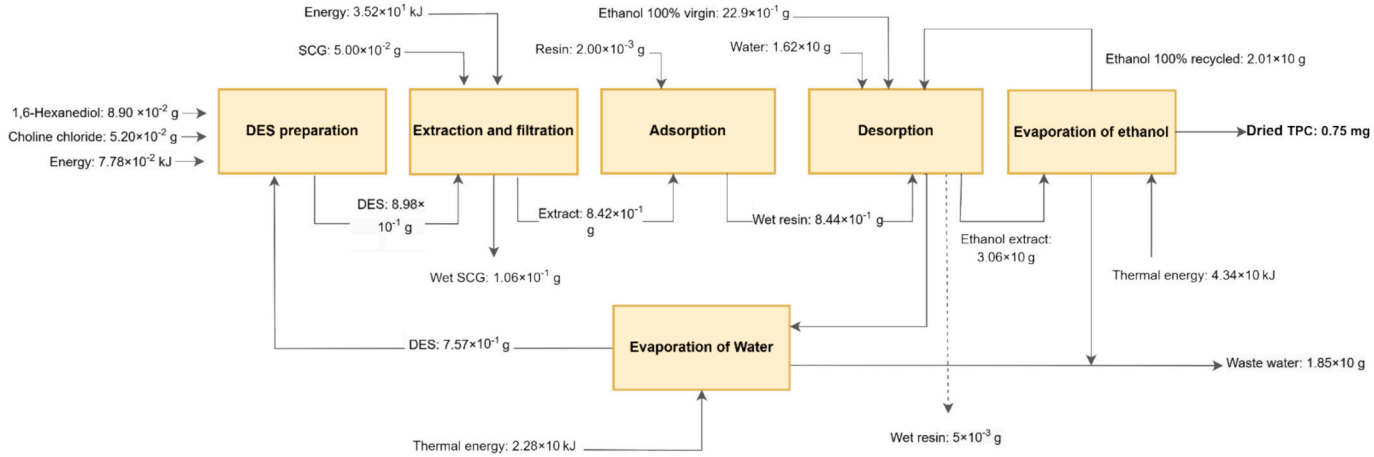


**Fig. 10.** Inventory data for DES-Improved Scenario .

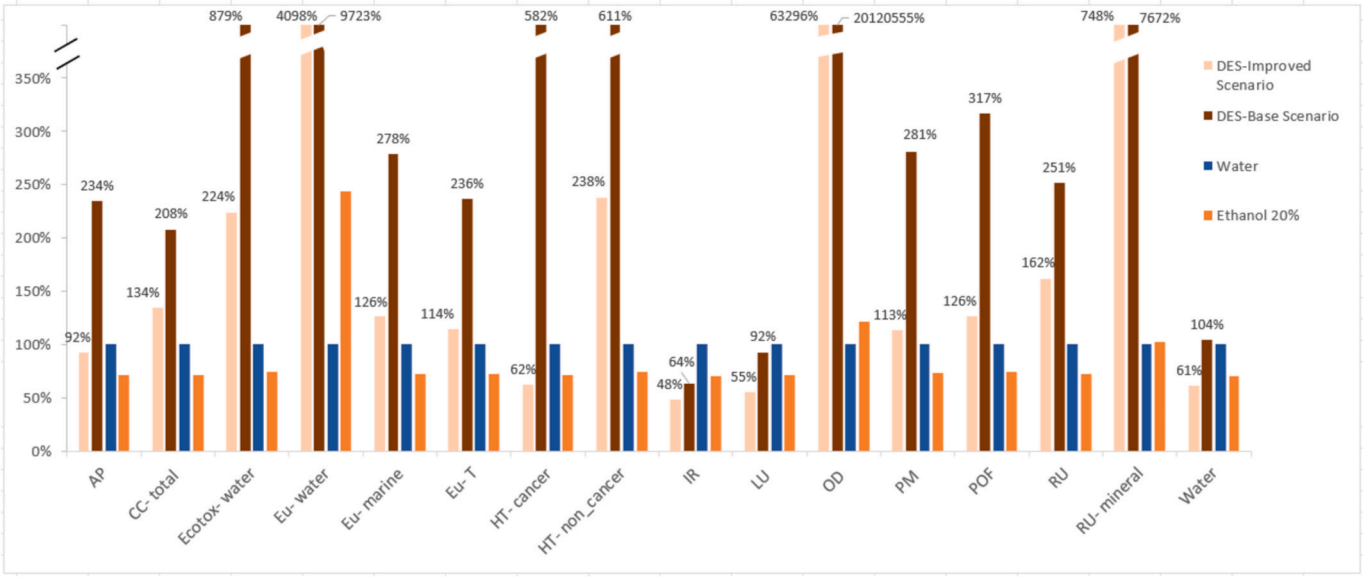


**Fig. 11.** Environmental comparison of DES (Base and Improved Scenarios), water and ethanol 20 % for the extraction of TPC (water is the baseline option, with 100 % impact in all impact categories).

separation stage, due to electricity consumption, followed by the ethanol evaporation process, due to energy consumption (see Fig. 12). However, for freshwater eutrophication (EU-water), the key impact factor is the desorption stage, due to water consumption. Additionally, ozone depletion (OD) is mainly driven by the adsorption process, influenced by the use of macroporous resin, while resource use minerals and metals (RU-mineral) is primarily impacted by DES preparation stage, with dimethyl hexanediol contributing 93 % and choline chloride contributing 7.4 %, respectively, to this impact.

### 4.3. Discussion of the results

In this section, the results from both studies, A and B, will be discussed. As previously explained in section 2, the connection between the two studies stems from the shared approach to optimization, which takes into account both TPC yield and environmental impact. However, the analyses are conducted separately because the yields cannot be directly compared, as different SCG samples were used as raw materials. Additionally, inventory data for study A was obtained by our research team, while for the second study come from Yoo et al. (Yoo et al., 2018). This was the only study found in the literature performing the extraction of TPC from SCG using DES compared to water in the same conditions. Hence, the conventional solvents used in study A (water and 20 % acetone) are not exactly the same than in study B (water and 20 % ethanol).

For study A, which compared different extraction times using the same solvent, the most noteworthy finding is that the optimal time (considering both yield and environmental impact) was neither the one that produced the highest yield nor the shortest duration, but rather an intermediate time. This same conclusion was observed with both

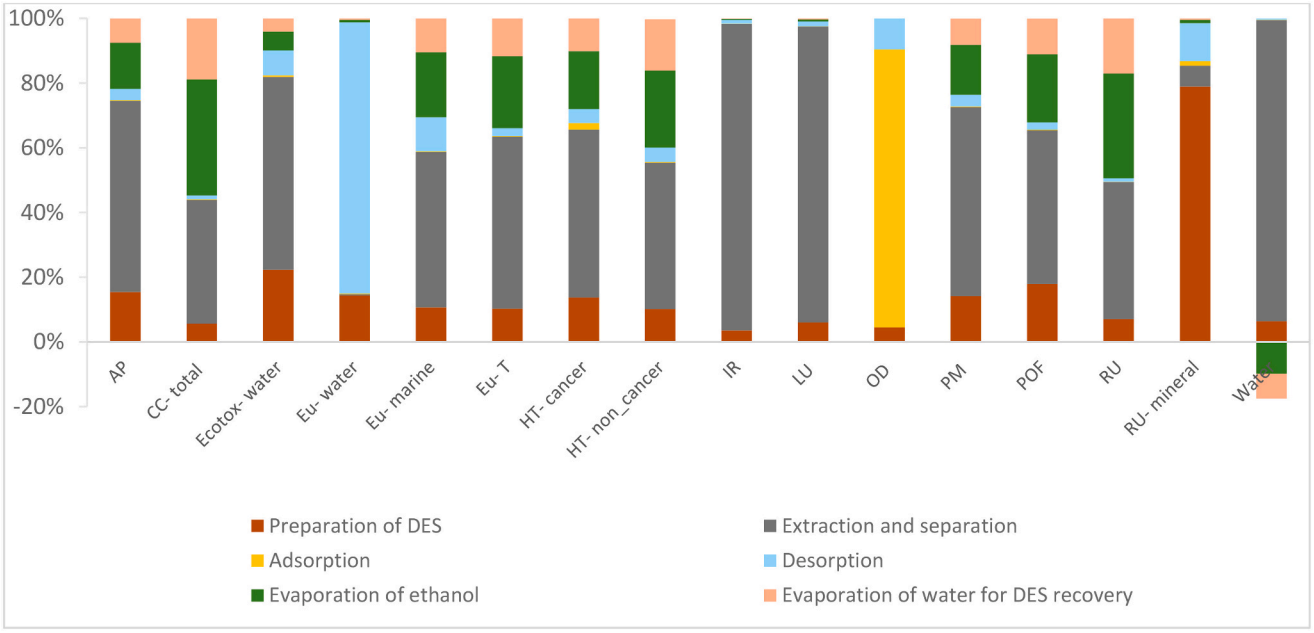


**Fig. 12.** Contribution of different steps in the environmental impacts of DES-Improved Scenario .

solvents tested: water and acetone 20 %. Time influences not only electricity consumption in the extraction process but also the TPC yield obtained. A higher yield, achieved with longer extraction times, increases electricity consumption; however, it reduces the amount of solvent and other resources needed to produce the same quantity of TPC (100 mg, in the present study). Therefore, the optimal time will be the one where the increase in yield offsets the impact of the additional electricity consumption required to achieve it. However, since electricity consumption at the laboratory scale may be more significant than at the industrial level, the optimal extraction time identified here (10 min) may not necessarily apply on a larger scale. Moreover, in this case, only by significantly reducing the impact of this electricity, such as by using renewable energy sources, would make yield the primary factor to consider for optimizing the process. Therefore, it is advisable to consider both yield and environmental impact when optimizing extraction conditions at the laboratory scale before scaling up the process because this approach provides valuable insights for developing more eco-efficient industrial processes.

The objective of study B was to compare newly developed eco-friendly solvents, known as Deep Eutectic Solvents (DES), with conventional solvents, specifically water and a 20 % ethanol/water mixture. DES are emerging as promising solvents in current research due to their potential to enhance extraction yields. The main outcome from this study is that it is difficult for DES to substitute water or other friendly solvents like ethanol, unless the increase of yield achieved with DES compensates his environmental impact. DES increases the number of steps needed for the process: DES preparation, extraction of TPC and filtration of SCG, adsorption of TPC in a resin, desorption of TPC from the resin using ethanol/water mixtures and finally ethanol evaporation. Hence, just looking at the inventory data, one can see that ethanol and water use are not avoided and DES is obtained from the combination of two components (ie., Choline Chloride and 1,6-hexanediol), chemical substances not so friendly as water or ethanol. When looking at the impact results obtained first, the main aspects affecting the environmental impact of DES system were the 1,6-hexanediol and the resin needed. The first in the preparation of DES and the second in the adsorption step. A sensitivity analysis was conducted, assuming that the affected steps could be optimized: by achieving a 90 % reuse of DES (a very optimistic rate, considering it must be recovered from the resin) and reducing the amount of resin required (less resin per mL of extract and doubling the number of cycles for resin reuse). The most significant aspects became the electricity consumption during extraction and the energy required for ethanol evaporation and reuse. Under these new conditions, the DES system still performed worse than 20 % ethanol and water systems (in 11 out of 16), despite TPC yields of 15 mg, 9.2 mg, and 6.6 mg TPC/g SCG for DES, ethanol, and water, respectively. Therefore, if DES is intended to replace widely used conventional solvents like water and ethanol in extraction processes, the extraction yield must be significantly higher, and further research is needed to really optimize all the process steps.

The aim of this paper was to test the hypothesis that optimal extraction conditions are not those that maximize yield but rather those that balance resource use to achieve a satisfactory yield. This hypothesis has been supported by the results from both case studies.

## 5. Conclusions and recommendations

The present study aimed to highlight the importance of considering the environmental impact in addition to yield for the optimization of extraction processes. This was visualized using the extraction of total polyphenols (TPC) from spent coffee ground (SCG) at a laboratory scale. Two specific comparisons were performed: i) the optimization of extraction time using water or a mixture of acetone/water (20:80 *w*/w) (study A); and ii) the comparison of newly developed eco-friendly solvents, deep eutectic solvents (DES), with the most simple and conventional ones, water and ethanol/water mixtures (study B).

Life Cycle Assessment (LCA) was used to evaluate the environmental impact of both comparisons, using the production of 100 mg of TPC as the reference unit. For the first comparison, the results showed that both water and acetone 20 % reached their optimal extraction time at 10 min, although 20 or even 40 min time gave higher extraction yields. When comparing the best conditions for both solvents, Water was found to be clearly environmentally better in four out of sixteen evaluated impact categories, while acetone 20 % showed a slight advantage in eight other categories.

Regarding the second comparison (DES, water, and 20 % ethanol/water mixture), although DES yielded higher extraction results (15, 9.2 and 6.5 mg GAE/g SCG respectively), the processes involved with DES, including solvent preparation and adsorption, led to greater environmental impacts than those associated with water or ethanol 20 %. This was true even when considering the best conditions for DES in a sensitivity analysis (such as the recovery and recycling of 90 % DES and the use of the minimum amount of resin possible for the adsorption process together with its reuse). In this comparison, among the solvents studied, ethanol 20 % was the most eco-friendly option. The conclusion is that DES may be an option to avoid other more harmful solvents but should not substitute abundant and non-dangerous ones like water or ethanol-water mixtures, which are also easier to use at an industrial scale.

Despite the main limitation of this study being its reliance on laboratory-scale experiments, it provides crucial insights that can inform future work as the process is scaled up. Additionally, while the results rely on certain assumptions, such as a 90 % solvent recovery rate, which influence the overall environmental impact, the comparison remains robust as all options are evaluated using the same criteria. This ensures that the key findings are valid and can guide decision-makers in avoiding the scale-up of less eco-efficient processes.

The study highlight the significance of incorporating environmental considerations into the selection of green solvents and the optimization of experimental conditions, particularly at the laboratory scale. Relying solely on extraction yield is insufficient. By integrating both yield and environmental impact, Life Cycle Assessment (LCA) emerges as an essential tool for optimizing processes, ensuring that environmental sustainability is considered alongside efficiency. This study demonstrates the value of LCA in making informed decisions about greener technologies.

## Funding

This work was supported by the Spanish Ministry of Science and Innovation to the project KAIROS-BIOCIR (PID2019-104925RB-C32). The first author also appreciates the support (2021FI SDUR 00130) from the Secretariat for Universities and Research of the Ministry of Business and Knowledge of the Government of Catalonia and the European Social Fund.

## CRediT authorship contribution statement

**Ibtissam Bouhzam:** Writing – review & editing, Writing – original draft, Visualization, Software, Investigation, Formal analysis. **Rosa Cantero:** Writing – review & editing, Visualization, Validation, Supervision, Methodology, Formal analysis. **María Margallo:** Resources, Data curation. **Rubén Aldaco:** Project administration, Funding acquisition. **Alba Bala:** Visualization, Data curation. **Pere Fullana-i-Palmer:** Project administration, Funding acquisition, Conceptualization. **Rita Puig:** Writing – review & editing, Validation, Supervision, Project administration, Methodology, Funding acquisition, Conceptualization.

## 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.

## Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.scitotenv.2024.177038.

## Data availability

Data will be made available on request.

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