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# **Life cycle assessment (LCA) Of Coffee Bags Recycling with Green Surfactant and Their Aqueous Solutions**

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## **Abstract**

The growing demand for multilayer packaging, especially in industries like food and beverage, poses significant challenges for recycling due to the complex combination of materials such as polyethylene (PE), aluminum (AL), and polyethylene terephthalate (PET). These materials provide excellent protective properties but are difficult to separate and recycle, leading to high landfill rates and environmental concerns. This thesis explores the use of Switchable Anionic Surfactants (SAS), particularly Triethanolamine (TEA) and Lauric Acid, as an innovative solution for recycling multilayer coffee bags.

Through a detailed Life Cycle Assessment (LCA), four distinct recycling scenarios were evaluated, ranging from basic delamination to a fully optimized closed-loop system. The study utilized GaBi software and the EF 3.1 methodology to quantify environmental impacts across categories such as climate change, resource depletion, and water use. The results indicated that while SAS technology shows promise in improving material recovery, significant trade-offs exist, particularly in the areas of energy consumption and toxic emissions.

In the early scenarios, surfactant preparation and delamination were the most impactful stages, contributing heavily to climate change and resource depletion. However, as the system progressed to more advanced stages—particularly in Scenario 4, where Lauric Acid and CO<sub>2</sub> were fully recovered—the focus shifted towards improving resource efficiency and minimizing waste generation. Despite these improvements, delamination remained a key environmental hotspot, indicating the need for further optimization of the recycling process.

The findings of this thesis suggest that while SAS-based recycling systems have the potential to align with circular economy principles, ongoing technological advancements are required to reduce energy demands and toxic emissions. This research provides valuable insights for developing more sustainable recycling processes for multilayer packaging and highlights the critical role of LCA in guiding environmental decision-making.

# 1. Chapter 1: Introduction

## 1.1. Food packaging and multilayer materials

Food packaging is an essential part of the modern food supply chain, designed to maintain food quality, safety, and freshness during transportation and storage, it plays a significant role in determining the shelf life of a food product. (Marsh & Bugusu, 2007). To meet these demands, the packaging often employs multilayer materials, combining different types of polymers and materials such as polyethylene (PE), polyethylene terephthalate (PET), aluminium, and paper (Licciardello, 2017). These materials are engineered to provide excellent barrier properties, shielding food from environmental factors like oxygen, moisture, light, and microorganisms, all of which can degrade the food's quality (Licciardello, 2017).

Each layer in multilayer packaging serves a specific function. For example, the outer layer, typically made of polyethylene, provides mechanical strength and moisture resistance (Robertson, 2021), while an aluminium layer acts as a barrier to oxygen and light, maintaining the product's aroma and flavour. Additional layers like PET protect the product, while adhesives and tie layers bond the materials together and enhance the packaging's overall performance (Robertson, 2021). These composite materials are made of several laminated layers, including paper (75% by weight, composed of long fibres that provide stiffness), aluminium (5%, which prevents the penetration of air and light, thus assuring the preservation of food contents) and LDPE (20%, for making the packaging impermeable and for preventing the contact of food with the aluminium layer). ( Chiara Samorì, Daniele Cespi 2017)

However, the complexity of these multilayer materials creates significant challenges in recycling. The bonding of different materials during manufacturing makes it difficult for traditional recycling processes to handle, as these processes typically require homogeneous material streams (Schyns & Shaver, 2021). As a result, recycling rates are low, with a significant proportion of multilayer packaging ending up in landfills or being incinerated. This issue is compounded by the growing demand for flexible packaging in the food industry due to its lightweight nature, durability, and space-saving benefits (Brody et al., 2008).

## Global and EU Waste Management of Packaging Plastics

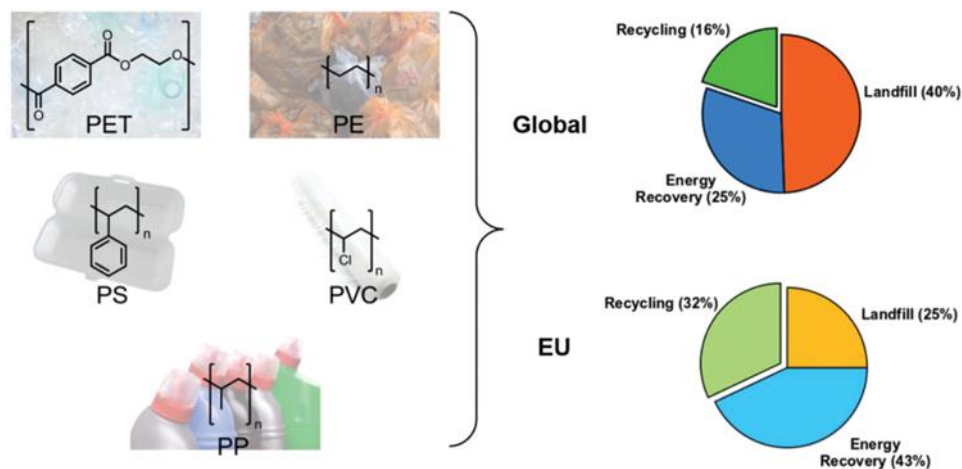


Figure 1 The main packaging polymers: poly(ethylene terephthalate) (PET), polystyrene (PS), polyethylene (PE), polypropylene (PP), and poly(vinyl chloride) (PVC) and current global and EU plastic waste management rates.

A graphical representation of global and European Union (EU) waste management practices highlights the disposal challenges associated with multilayer packaging. Globally, only 16% of plastic waste is recycled, while 40% ends up in landfills, and 25% is incinerated for energy recovery. In contrast, the EU demonstrates higher recycling rates, with 32% of plastic packaging being recycled, 25% sent to landfills, and 43% undergoing energy recovery (Schyns & Shaver, 2021).

These statistics underscore the recyclability challenges of materials like PET, PS, and PE, which are often used in multilayer packaging. The low global recycling rates reflect the difficulty in processing multilayer packaging due to the inseparability of the different layers, leading to poor recycling outcomes and high landfill rates (Schyns & Shaver, 2021). Even in the EU, where recycling infrastructure is more advanced, the recycling rates remain modest due to the technical limitations of recycling complex packaging materials.

Globally, multilayer packaging is frequently used for products that require high levels of protection, such as beverages, snacks, coffee, and perishable goods. For instance, coffee packaging typically contains multiple layers to protect against moisture and oxygen, ensuring that the coffee remains fresh and flavorful over time. However, these multilayer structures are difficult to recycle because of the combination of materials such as plastic, metal, and adhesives.

The graph also highlights that in both global and EU contexts, energy recovery is a significant component of waste management, accounting for 25% and 43% of plastic waste management practices respectively. While energy recovery reduces the waste burden, it does not align with the goals of a circular economy, which aims for higher recycling rates and less reliance on incineration (Schyns & Shaver, 2021).

The environmental impact of multilayer packaging, due to its low recyclability and high carbon footprint, remains a critical issue for the food packaging industry (Hahladakis & Iacovidou, 2019).

Efforts to improve the sustainability of multilayer packaging have led to the exploration of advanced recycling technologies. Chemical recycling techniques such as the use of Switchable solvents have also been used in the delamination of complex multilayer materials like pharmaceutical blisters and food and beverage cartons exploiting the solubilization of the adhesives present between the polymeric layer (Mumladze et al., 2018; Yousef et al., 2018). These technologies are essential for achieving a circular economy for food packaging, where materials can be efficiently reused and recycled instead of being discarded after a single use (Geueke et al., 2018).

Despite these technological advances, the recyclability of multilayer packaging remains a major challenge. Traditional mechanical recycling methods are not equipped to handle the complex composition of multilayer materials, contributing to the large volumes of packaging that end up in landfills or incinerators (Schyns & Shaver, 2021). Plastic packaging is mainly made of fossil-fuel based raw materials. The use of renewable raw materials has steadily increased over the last years (European Bioplastics, 2017), but is still of considerably small market share. Recyclability is not influenced by the source of the raw materials, but by the type of plastic. (Geueke et al., 2018).

In the future, a combination of improved recycling technologies and a shift toward more sustainable packaging materials will be crucial in reducing the environmental impact of food packaging.

While multilayer packaging offers significant benefits for food preservation and distribution, its environmental impact remains a considerable challenge. The low recyclability of these materials contributes to high landfill rates, as shown in both global and EU waste management statistics. Innovations in recycling technologies and a shift towards more sustainable packaging materials are essential to reducing waste and improving the lifecycle management of these complex materials (Licciardello, 2017).



### **1.3. Coffee bags**

Coffee packaging has undergone significant advancements from its humble beginnings to the sophisticated multilayer materials used today. Initially, coffee was stored in basic containers like jute sacks and metal cans, which offered minimal protection against environmental factors. As global coffee consumption expanded and consumer demand for quality increased, the need for improved packaging became evident (Samorì & Pitacco, 2023). Innovations such as vacuum sealing in the early 20th century, which removed oxygen from packaging, and the introduction of degassing valves in the 1960s, which allowed carbon dioxide to escape without letting oxygen in, marked major milestones in the evolution of coffee packaging (MTPak Coffee, 2021; Coffee Bean Tree, 2023).

Today, modern coffee bags typically consist of multilayer materials that include plastic, aluminum, and paper. These materials serve different functions: plastic provides flexibility and durability, aluminum acts as a moisture and oxygen barrier, and paper offers structural support and branding opportunities (Dataintel, 2023). This combination ensures that the coffee remains fresh and protected from moisture, light, and external contaminants for extended periods, a crucial aspect of maintaining quality in global supply chains.

#### **1.3.1. History and Background**

The history of coffee packaging reveals a consistent focus on improving product preservation. In the 1800s, coffee was initially stored in airtight paper bags or metal cans, which did little to maintain freshness over time. A significant leap forward came with the invention of vacuum-sealed packaging by R.W. Hills in 1900, which greatly extended the shelf life of coffee by removing air from the container.

Later, Francesco Illy introduced pressurized packaging, replacing air with inert gases to further enhance coffee preservation. The mid-20th century saw the widespread adoption of multilayer flexible packaging, combining plastic and aluminum to protect coffee from oxygen and moisture. One of the most important innovations during this period was the invention of the one-way degassing valve by Goglio, which allowed roasted coffee beans to release carbon dioxide without letting in oxygen, preserving the coffee's flavor (MTPak Coffee, 2021).

Today, the global coffee market continues to grow, with over 169.6 million 60 kg bags of coffee produced in 2020 (Craft Coffee Spot, 2023). Packaging plays a critical role in maintaining product quality throughout the supply chain, especially in major coffee-consuming regions like Europe and Italy. Italian companies, in particular, have become pioneers in coffee packaging innovations, focusing on developing sustainable and high-performance materials (Dataintel, 2023).

In response to growing environmental concerns, many manufacturers are now exploring biodegradable and recyclable options, such as compostable bags made from kraft paper, low-density polyethylene (LDPE), and polylactic acid (PLA) (Xianhui Zhao, Ying Wang, 2023).

### **1.3.2. Composition and uses**

Packaging solutions for coffee are based on PET, aluminum foil, and polyethylene. Every composite serves its dedicated function: PET protects against oxygen, the foil provides great protection from many environmental factors, PE film serves as a sealing layer and guarantees your package is airtight and moisture-proof. This combination is optimal for conserving the aroma and taste of premium coffee. (uniflexpackaging.eu 2024)

These layers work together to maintain the quality and shelf life of the coffee, ensuring it reaches consumers in optimal condition.

However, the multilayer structure presents significant challenges for recycling. They often require the use of adhesives to bond different materials which have different properties. These adhesive layers are called “tie-layers” in a multilayer structure. Commonly used adhesives include acrylics and polyurethanes (PU), which complicate the separation of materials during recycling. Conventional mechanical recycling methods struggle to separate these tightly bonded layers, particularly the plastic and aluminum components (Li & Theodosopoulos, 2024, Loukodi & Lovell)

This has led to low recycling rates for multilayer coffee bags, with most of them being incinerated or sent to landfills, contributing to environmental pollution (Kaiser & Schmid, 2018).

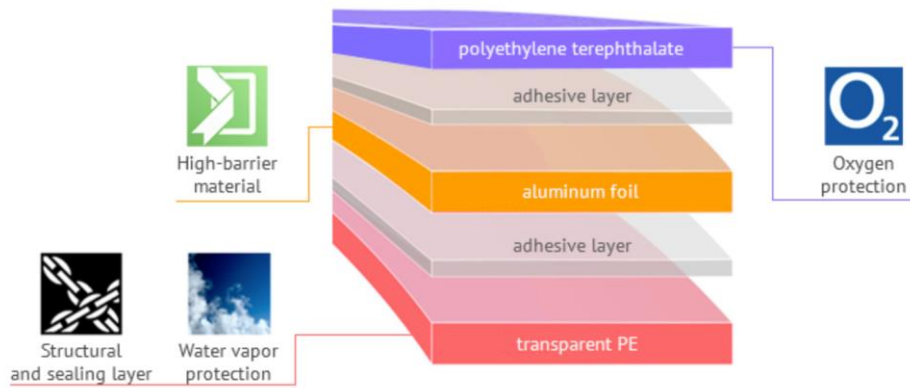


Figure 3 multilayer coffee bag (uniflexpackaging.eu 2024)

### 1.3.3. Problem Statement

The recycling of coffee bags, like other forms of multilayer flexible packaging, poses both environmental and technical challenges. The combination of polyethylene (PE), aluminum, and polyethylene terephthalate (PET) provides excellent barrier properties but creates a complex material that is difficult to recycle. Adhesives used in the packaging exacerbate this problem, as they do not respond well to traditional separation techniques, making it nearly impossible to efficiently separate the layers for recycling (Bauer & Tacker 2021). Even if the combination of several polymeric layers is essential to attain the technical performances of the packaging, the uncertainty about the variable number of layers, their thickness and composition, the presence of glues or additives, and the presence of aluminum, in turn, variable in the mode of deposition and amount, decrease the rate of success of layers separation and recycling. (Vollmer et al,2020)

Mechanical recycling, which is the most widely used process, requires the different materials to be separated before they can be reprocessed. However, the strong adhesion between layers in coffee bags makes this process inefficient and costly. As a result, most multilayer packaging is either incinerated for energy recovery or sent to landfills, contributing to waste accumulation and environmental degradation (Kaiser & Schmid, 2018).

Efforts to improve the recyclability of coffee bags have led to the exploration of chemical recycling technologies. One promising method involves the use of Switchable Anionic Surfactants (SAS), which can break down adhesives and enable the separation of the different material layers (Varzakas & Krauter, 2021). While these

technologies show potential, they are still in the early stages of development, and their large-scale implementation remains a challenge. Until more efficient recycling technologies are adopted on a wider scale, the majority of coffee bags will continue to contribute to landfill waste, posing a significant barrier to sustainability and the circular economy (Kaiser & Schmid, 2018).

## **1.4. Switchable anionic surfactant (SAS)**

Switchable Anionic Surfactants (SAS) represent a groundbreaking solution for the recycling of complex multilayer packaging materials. Coffee bags, often constructed from layers of polyethylene (PE), aluminum, and polyethylene terephthalate (PET), present significant challenges for traditional recycling methods due to the strong adhesives binding these layers together. The use of SAS, in my case study particularly a combination of triethanolamine (TEA) and lauric acid, offers an efficient chemical process to break these bonds, making it possible to separate and recover the individual materials.

SAS work by changing their hydrophilicity in response to external stimuli like CO<sub>2</sub>. It is worth mentioning that the delamination performance of TEA-Laurate is a peculiarity of this surfactant, other commercial surfactants as well as other combinations of carboxylic acids and bases tested were poorly performing in comparison to C12-TEA; moreover, it proved to be the only SAS recoverable from the aqueous solutions simply by adding CO<sub>2</sub> at ambient pressure. additionally, TEA- Laurate is safer for human health and the environment than the majority of other switchable systems developed so far, and its application as a diluted aqueous solution largely reduces the usage risk. (martina vagnoni,walter pitacco,2023)

In this context, the TEA-lauric acid combination has been shown to effectively delaminate multilayer materials, making them easier to recycle. The unique chemical properties of SAS enable a more efficient and environmentally friendly recycling process compared to conventional methods. (Vagnoni et al., 2023; Mumladze, Tamaria;Yousef, Samyb2018).

### **1.4.1.SAS component, how used of SAS for delamination**

The SAS system in this case study primarily involves TEA-Laurate, a mixture of **lauric acid** and **triethanolamine (TEA)**. This system is effective at breaking the adhesive bonds in multilayer packaging, such as the aluminum and polyethylene

layers found in coffee bags. When CO<sub>2</sub> is introduced to the system, the surfactant undergoes a change in hydrophilicity, switching from hydrophilic to hydrophobic, which enables the breakdown of adhesives and facilitates the separation of layers (Vagnoni et al., 2023).

In studies, the TEA-Laurate combination has shown superior efficiency in recovering materials like PE from complex structures. It works by swelling the layers and dissolving the adhesives, allowing for easy mechanical separation without significant damage to the materials. This approach has been particularly successful in packaging systems where traditional recycling methods fall short (Mumladze et al., 2018).

### **1.4.2. Problem Statement for SAS in Recycling**

Despite the promising potential of SAS for recycling, several challenges remain in implementing this technology at scale. One key issue is the recovery of the surfactant itself. Although the CO<sub>2</sub>-switching mechanism allows for some level of recovery, inefficiencies in the process can result in the loss of surfactant materials, reducing the overall economic viability of the recycling system (Vagnoni et al., 2023).

Additionally, the performance of SAS can vary depending on the specific adhesives used in different types of multilayer packaging. While the TEA-lauric acid system works effectively for some materials, further optimization is needed to ensure broad applicability across different packaging compositions. Furthermore, scaling up this technology to industrial levels presents challenges in terms of cost, environmental impact, and ensuring consistent recovery rates (Mumladze et al., 2018).

## **1.5. LCA methodology**

Life Cycle Assessment (LCA) is an international methodology standardized since 1996 by ISO 14040 series. ISO 14040 define LCA as an established methodological approach to environmental impact analysis of products and services, which consists of the compilation and assessment across the entire life cycle of the input and output flows, as well as the potential environmental impacts, of a product system.

There are other definitions of what LCA methodology is, for example SETAC (Society of Environmental Toxicology and Chemistry) defined it as a process to evaluate the environmental burdens associated with a product, process, or activity by identifying and quantifying energy and materials used and wastes released to the environment; to assess

the impact of those energy and materials used and releases to the environment; and to identify and evaluate opportunities to affect environmental improvements.

The assessment includes the entire life cycle of the product, process, or activity, encompassing, extracting, and processing raw materials; manufacturing, transportation, and distribution; use, re-use, maintenance; recycling, and final disposal (SETAC, 1993). According to the Integrated Product Policy (IPP), the LCA is currently the best framework available for assessing the potential environmental impacts associated with a product's life cycle (EC, 2003).

As reported in the ISO website, ISO 14040:2006 (ISO, 2006a) describes the principles and framework for all life cycle assessment (LCA) phases, reporting and critical review of the LCA, limitations of the LCA, the relationship between the LCA phases, and conditions for use of value choices and optional elements, while ISO 14044:2006 specifies requirements and provides guidelines (ISO, 2006b).

At the European level, on the other hand, the Joint Research Centre of the European Commission has published the ILCD - International Reference Life Cycle Data System handbook with the aim of providing detailed guidance to operate life cycle assessment in order to quantify the emissions, resource consumption and environmental impact of products (EC-JRC-IE, 2010).

LCA methodology consists of 4 phases, illustrated in figure 4 below:

1. Goal and scope definition (ILCD handbook split this phase in two)
2. Inventory analysis (LCI)
3. Impact assessment (LCIA)
4. Interpretation

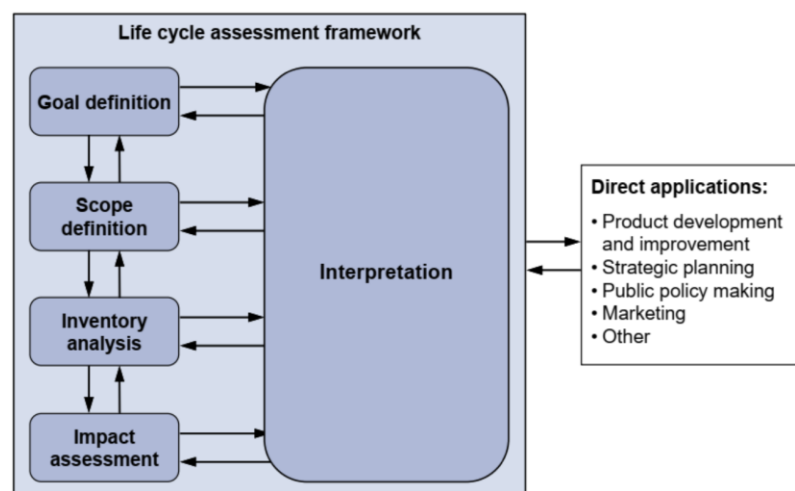


Figure 4 LCA phases by ILCD Handbook

### **1.5.1. Goal and scope definition**

The goal definition phase is arguably the most critical, as it shapes all subsequent decisions made throughout the methodology. It directly influences the scope of the study, which in turn determines the framework for both the Life Cycle Inventory (LCI) and Life Cycle Impact Assessment (LCIA). Moreover, the quality control process is guided by the requirements set out in the scope. Interpretation, the final step in the methodology, must align closely with the defined objectives, making a clear goal definition crucial for an accurate interpretation of results. At this stage, key elements such as the decision-making context, the study's intended application, and its target audience are identified.

Examples of LCA applications include:

- Identifying weak points in a product
- Comparing goods or services
- Designing for recyclability
- Policy development: such as forecasting and analyzing the environmental impacts of new technologies or raw material strategies (EC-JRC-IES, 2010).

It is also important to acknowledge any limitations in the usability of the results, arising from the methodology or assumptions specific to the case study. The goal definition must also clarify who commissioned the LCI/LCA study and any organizations that have financial or influential involvement in the study.

During the scope definition phase, the study's subject is further detailed in alignment with the goals. The system's function, the functional unit, and the reference flows must also be specified. The functional unit serves to quantify the system's functions, providing a standard unit of measurement to which environmental impacts are referenced, allowing for meaningful comparisons.

The reference flow refers to the specific flow of materials and energy against which all other flows are measured.

The final task in this phase is defining the system boundaries, which determine which process units are included in the system. The process unit is the smallest part of the system for which input, and output flows can be measured. There are three key system boundaries: cradle-to-grave (the most comprehensive, covering all life cycle stages), cradle-to-gate, and gate-to-gate.

## **1.5.2. Inventory analysis**

In this second phase, guidance can be taken from the ILCD-Handbook, Specific guide for Life Cycle Inventory data sets (EC-JRC-IES, 2010). During the inventory analysis, data collection and system modeling are performed, always aligned with the objectives and scope defined in the first phase. The outcomes of this analysis provide the foundation for the following LCIA phase.

Data collection and modeling are often iterative processes. As the understanding of the system deepens, the necessary data become clearer, and irrelevant data can be identified and excluded from further analysis. Typically, this phase demands the most resources and effort within an LCA, especially for the gathering, acquiring, and modeling of data.

The data gathered can pertain to foreground or background processes and may either be primary or secondary data. Primary data are obtained directly from the commissioner of the study or the producer, developer, or operator responsible for the product or technology being evaluated. Secondary data are retrieved from external databases, usually integrated into specialized LCA software.

For key processes, or foreground processes which are under the direct control of the decision-maker commissioning the LCA, it is preferred that primary, specific data be used. For background processes, where the decision-maker has limited or no direct control, secondary, generic data may be sufficient.

After collecting the necessary data, the next step is system modeling.

This can sometimes present challenges related to multifunctionality, which occurs when a process generates more than one product or by-product. In such cases, energy and material consumption must be distributed across the different outputs.

Allocation criteria are used to solve this, and ISO 14044: 2006 outlines the hierarchy of methods for addressing multifunctionality:

- 1. System breakdown:** Breaking down the multifunctional process into single-function units.
- 2. System expansion:** If breakdown isn't feasible, the system can be expanded to account for additional co-product functions.
- 3. System allocation:** Flows can be attributed based on either a physical causal relationship, economic factors, or energy content.

The final results of the inventory analysis must align with the chosen functional unit and focus only on elementary flows. These are materials or energy taken from the environment that have not undergone any human transformation or materials/energy released back into the environment without further modification (ISO, 2006a).

### **1.5.3. Impact assessment**

The Life Cycle Impact Assessment (LCIA) is the phase where the inputs and outputs gathered during the inventory stage are translated into impact indicators relevant to human health, the environment, and resource depletion (EC-JRC-IES, 2010). This stage enables the environmental consequences of a system's operations to be quantified in relation to these categories. More detailed guidance for this phase is available in the ILCD handbook specifically focused on existing Environmental Impact Assessment methodologies applicable for LCAs.

The LCIA phase is comprised of mandatory and optional steps:

- **Classification:** This mandatory step involves identifying the environmental impact categories that the system affects, such as climate change or acidification. The selection of impact categories depends on the specific LCA method used.

- **Characterization:** Another mandatory step, characterization quantifies the contribution of each flow to the various impact categories. This is essential since different substances and flows impact the same environmental category in varying degrees. Characterization factors, provided by the chosen model, are applied to each elementary flow, bringing them to a common unit of measurement for the relevant impact category. After this step, each impact category will have a quantified score.

In addition to the mandatory steps, there are optional steps:

- **Normalization:** During this process, each impact category score is compared to a reference value, enabling the relative significance of each impact category to be assessed and compared.

- **Weighting:** This step involves assigning a weight to each impact category based on its perceived importance. The weighted value of each category is multiplied by its normalized score, and the resulting values are summed to provide an overall measure of the environmental impact of the system or product under study. (European Commission, 2023)

#### **1.5.4. Interpretation**

The interpretation phase of Life Cycle Assessment (LCA) is critical for both refining the life cycle inventory model and drawing final conclusions and recommendations from the study. This phase serves as a bridge between the results generated from the LCIA and the study's goals, ensuring that the findings align with the study's objectives.

The first step in this phase involves identifying the most significant processes, parameters, assumptions, and elementary flows that contribute heavily to the overall environmental impact. These significant contributors, also known as "hotspots," are key to understanding where the largest environmental burdens occur within the system.

Next, these significant aspects are evaluated based on their sensitivity, meaning their influence on the overall LCA results is analyzed. This sensitivity analysis helps to determine how variations in data, assumptions, or methodology might affect the final outcomes, providing a deeper understanding of the reliability of the results.

Finally, the insights gained from this analysis are used to formulate the conclusions and recommendations of the LCA study. This may involve suggesting improvements to the system, identifying potential environmental benefits of certain practices, or advising on strategies for reducing the environmental impacts associated with the product or process under review. These recommendations should be practical and actionable, ensuring the LCA delivers value to decision-makers and stakeholders.

( Pant & Zampori,2022)

## **2. Chapter 2: Literature Review and Research Purpose**

The primary aim of this study is to explore the environmental impacts and effectiveness of recycling multilayer coffee bags using Switchable Anionic Surfactants (SAS) through a Life Cycle Assessment (LCA). Coffee bags are widely used, and their multilayer structure, often composed of polyethylene (PE) and aluminum (AL), presents significant recycling challenges. Traditional recycling methods often lead to insufficient recovery rates or environmental burdens due to the complexity of separating these materials. This study evaluates alternative recycling methods by incorporating SAS and compares the environmental impact across multiple scenarios.

### **2.1. Objectives of the Coffee Bag Recycling Study**

The core objective of this study is to assess the environmental viability of using SAS for the delamination and recycling of multilayer coffee bags.

The study aims to:

- Evaluate the environmental impacts associated with the use of SAS, specifically Triethanolamine (TEA) and Lauric Acid, in recycling processes.
- Quantify resource efficiency through a detailed LCA, focusing on energy consumption, material recovery, and emission reductions.
- Compare different recycling scenarios to identify the most sustainable and efficient method for recycling coffee bags. This will involve modeling the entire process using GaBi software and assessing impacts using the EF 3.1 methodology.
- Provide recommendations for improving recycling methods in line with the principles of the circular economy and reducing the environmental footprint of coffee packaging waste.

### **2.2. Application of Switchable Anionic Surfactants (SAS)**

The study focuses on SAS's efficiency in breaking down the multilayer structure of coffee bags, which consists of PE and AL and PET layers, without causing significant environmental harm.

The use of SAS in recycling is part of an effort to employ green chemistry solutions that minimize hazardous chemical use while enhancing the recovery of reusable materials. In this study, SAS application is tested under four distinct scenarios, each exploring

different combinations of surfactants, washing methods, and recovery processes. These scenarios help to demonstrate how the flexibility of SAS can be harnessed to improve recycling outcomes and reduce waste generation.

### **2.3. Comparison of LCA Across Different Scenarios**

The study involves the comparison of four recycling scenarios, each varying in terms of process structure and environmental impact. The LCA for each scenario is modeled using GaBi software, with the EF 3.1 method employed to assess the environmental performance of the recycling processes. The key areas of focus for comparison include:

- Energy Consumption: Each scenario will be evaluated based on its energy usage during delamination and material recovery, highlighting opportunities for energy savings.
- Material Recovery: The efficiency of recovering key materials like PE and AL will be measured, with a focus on maximizing the reuse of surfactants, water, and CO<sub>2</sub>.
- Environmental Impact: Each scenario's contribution to climate change, resource depletion, and other environmental indicators will be analyzed using EF 3.1's impact categories such as greenhouse gas emissions, water use, and resource extraction.
- Scenario Outcomes: The results will provide a comparative analysis of the four scenarios, determining which one offers the lowest environmental burden while maintaining effective material recovery.

### **3. Chapter 3: Materials and Methods**

This chapter provides a detailed explanation of the materials, methods, and processes used in the experimental study of recycling multilayer coffee bags. The study involves four distinct recycling scenarios, each employing different approaches to delaminate and recover materials from multilayer coffee bags, using Switchable Anionic Surfactants (SAS). The materials used, experimental setups, and the tools employed for data collection and analysis are described in this section.

#### **3.1. Materials Used in Coffee Bag Recycling**

The recycling process for coffee bags in this study focuses on using green surfactants to delaminate the multilayer structure of the bags. These materials, including Triethanolamine (TEA), Lauric Acid, and Ammonium Hydroxide (NH<sub>4</sub>OH), were selected for their effectiveness in separating polyethylene (PE), aluminum (AL) and Poly terephthalic acid(PET) layers, and for their relatively low environmental impact.

##### **3.1.1. Triethanolamine (TEA) reference**

Triethanolamine (TEA) is an organic compound used as a switchable surfactant in the delamination process. TEA acts by breaking the chemical bonds between the layers of the coffee bags, aiding in the separation of PE and AL plus PET together. The switchable nature of TEA allows it to alternate between ionic and non-ionic states, depending on the environmental conditions (e.g., pH levels). This flexibility makes TEA a valuable surfactant in recycling processes, as it can be reused after being recovered from the system.

##### **3.1.2. Lauric Acid and Ammonium Hydroxide reference**

Lauric Acid is a fatty acid that works in conjunction with TEA to enhance the delamination process. It forms part of the switchable anionic surfactant system, aiding in breaking down the multilayer structure. Ammonium Hydroxide (NH<sub>4</sub>OH), on the other hand, is used as a basic washing solution in certain scenarios to further separate the materials and ensure effective cleaning of the residues. NH<sub>4</sub>OH also facilitates the recovery of Lauric Acid from the waste materials, making it a critical component for maximizing surfactant reuse.

## 3.2. Experimental Setup and Procedures

### 3.2.1. Overview of the Experimental Work

The recycling process of multilayer coffee bags in this study is conducted twice per day, with a total of 10 cycles per week. Each experimental cycle includes specific amounts of materials, and for ease of understanding and calculation, the quantities described correspond to a single experimental run. Given the relatively small amounts involved—both in terms of coffee bag weight and surfactant (SAS) usage—all calculations for mass balance and energy consumption are based on cumulative weekly data. This approach ensures accurate scaling and reflects real-world lab conditions.

### 3.2.2. General Process

**Step 1: Delamination Process** The delamination process is the first crucial step in separating the multilayer structure of coffee bags. In this step, 9 grams of coffee bags are placed in a container filled with 4 liters of water.

To initiate the delamination, 14 mM (11.46 grams) of Lauric Acid and 18 mM (12.80 grams) of Triethanolamine (TEA) are added to the mixture. These chemicals form part of the Switchable Anionic Surfactant (SAS) system, which plays a vital role in breaking down the bonds between the layers of the coffee bag. The mixture is stirred at 250 rpm, ensuring adequate mixing, and heated to 90°C for 3 hours using an electronic heater. The heat facilitates the chemical reactions needed for delamination, while the stirring ensures that the surfactants effectively penetrate the multilayer structure. After 3 hours, the coffee bag residuals are ready for transfer to the next phase of the process. This step creates a contaminated solution, referred to as Contaminated Solution 1, which will be dealt with in later stages.

**Step 2: Basic Washing Solution** In the second step, the delaminated coffee bag residues are transferred into a new container. At this point, an additional 4 liters of tap water is introduced to replace the contaminated water left from the previous step. This step is critical for ensuring that the chemical residues from the delamination process do not interfere with subsequent washing. To this new solution, 20 mM (3.1 grams) of Ammonium Hydroxide (NH<sub>4</sub>OH) is added. NH<sub>4</sub>OH acts as a basic washing agent, assisting in the further separation of surfactants like TEA-Laurate from the solution. The mixture is stirred again at 250 rpm for 1 hour to allow sufficient time for

separation, and the result is a new contaminated solution referred to as Contaminated Solution 2. This step is essential to clean the residuals and prepare them for final washing.

**Step 3: Water Washing** The third step involves a basic water wash to further cleanse the residual coffee bag material. 4 liters of tap water are added, but unlike previous steps, this stage does not require stirring or any form of energy input. The solution sits for 1 hour, allowing any remaining surfactants or contaminants to dissolve passively in the water. At the end of this step, the remaining solution, known as Contaminated Solution 3, contains the residual surfactants and  $\text{NH}_4\text{OH}$  from the previous phases. This step ensures that the coffee bag material is adequately washed and prepared for final separation.

**Step 4: Final Washing** In the final step, the washed coffee bag residues are placed in a new container for a final rinse. 10 liters of tap water are added, and the mixture is stirred at 30 rpm for 1 hour. This gentle stirring is sufficient to remove any remaining surfactants from the coffee bags while minimizing energy consumption. The result is wastewater containing only trace amounts of chemicals, which are negligible and can be recycled as clean water in the system. At the end of this stage, the delaminated coffee bags are fully separated into 71% Polyethylene (PE), which floats on the surface, and 29% Aluminum/Polyethylene Terephthalate (AL/PET), which settles at the bottom of the container. The successful separation of these materials demonstrates the effectiveness of the delamination process. The focus of this study is on developing four different recycling scenarios that vary in terms of surfactant and water reuse, aiming to minimize waste and environmental impact.

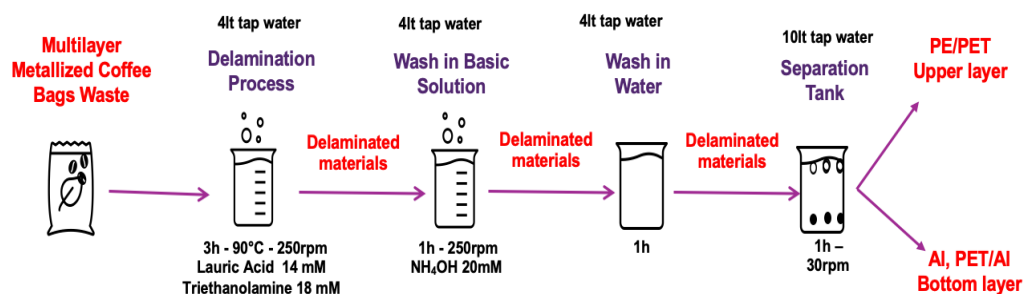


Figure 5 overview diagrams of the basic delamination scenario.

All these processes take place in chemistry laboratory at the university of Bologna and the figure 6. shown the delamination laboratory equipment:

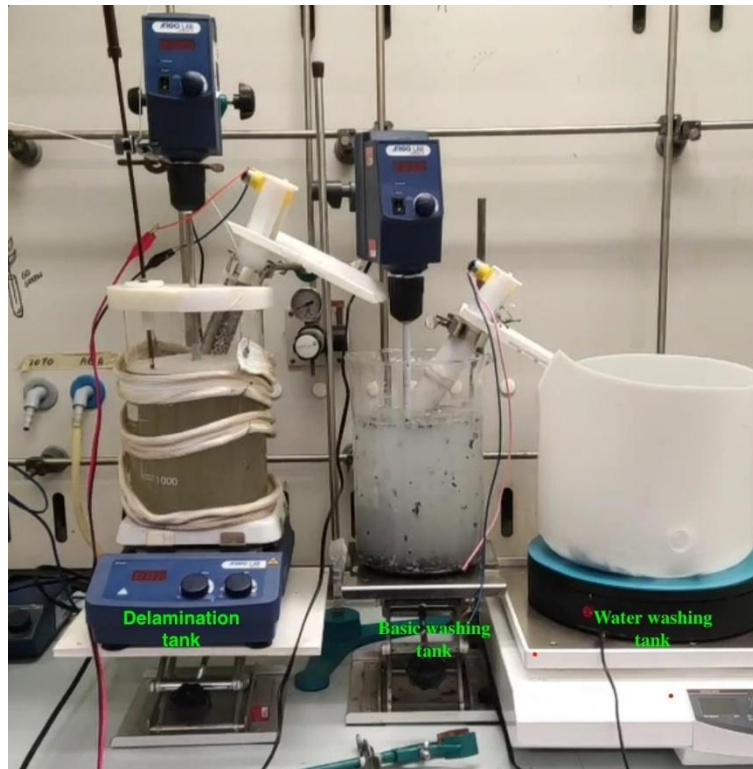


Figure 6 Delamination laboratory equipment.

The delaminated materials obtained at the end of process are shown in figure 7. Including PE and AL+PET.



Figure 7 The Delaminated materials.

### 3.2.3.Scenario Descriptions

#### 3.2.3.1. Scenario 1: Disposal of Contaminated Solutions

In Scenario 1, the process is straightforward: all three contaminated solutions (from the delamination, basic washing, and water washing steps) are disposed of by sending them to a wastewater treatment plant. This scenario represents a

baseline where no recovery of surfactants or materials is attempted. While the same amount of materials and chemicals are used as described in the general process, the focus is on exploring the environmental impact of simply discarding the contaminated solutions. This scenario does not involve any further treatment or recycling of materials and thus reflects a traditional approach to waste management, where resources are consumed and then discarded.

### **3.2.3.2. Scenario 2: Recovery of Lauric Acid via Precipitation**

In Scenario 2, the primary goal is the recovery of Lauric Acid from the contaminated solutions. After the three contaminated streams from the delamination, basic washing, and water washing steps are collected, they are directed to a precipitation tank. In this tank, dried ice (CO<sub>2</sub>) is introduced, causing the Lauric Acid to precipitate out of the solution without requiring additional energy input. This recovered Lauric Acid can then be reused in subsequent cycles, reducing the need for fresh inputs.

After Lauric Acid recovery, the remaining contaminated solution is sent to the wastewater treatment plant, like Scenario 1. This scenario illustrates the potential for recovering valuable surfactants through a simple, energy-efficient process, contributing to a more sustainable recycling loop.

### **3.2.3.3. Scenario 3: Recovery of Lauric Acid and CO<sub>2</sub>**

Scenario 3 builds upon Scenario 2 by recovering both Lauric Acid and CO<sub>2</sub>. After Lauric Acid is precipitated from the contaminated solutions, CO<sub>2</sub> recovery is implemented for Contaminated Solution 1. This step involves using thermal energy and electricity to heat the solution to 90°C, while stirring at 350 rpm for 100 minutes. This process allows the CO<sub>2</sub> to be captured and reused in subsequent cycles, reducing the overall consumption of this gas. The remaining two contaminated solutions, after Lauric Acid and CO<sub>2</sub> recovery, are sent to the wastewater treatment plant. This scenario adds a layer of complexity to the process but demonstrates the potential for multiple resource recoveries, increasing the sustainability of the system.

### **3.2.3.4. Scenario 4: Complete Cycle with Surfactant recovery and Water Reuse**

Scenario 4 is the most complex, aiming to create a closed-loop system with minimal waste. In this scenario, Lauric Acid recovered from all three contaminated streams using CO<sub>2</sub>, like Scenario 2. After this step, the focus shifts to recovering CO<sub>2</sub> and other materials from the remaining contaminated solutions. Three flows emerge from this process:

- Flow 1: HCO<sub>3</sub>-TEA<sup>+</sup> is processed by heating to 90°C and stirring at 350 rpm for 100 minutes. After CO<sub>2</sub> extraction, the remaining solution is wastewater that must be sent to a municipal wastewater treatment plant.
- Flow 2: HCO<sub>3</sub>-NH<sub>4</sub>OH is processed for 78 minutes under the same conditions. After CO<sub>2</sub> is extracted, the resulting solution contains NH<sub>4</sub>OH and water, which can be returned to the cycle for reuse.
- Flow 3: This flow is processed for 60 minutes at 90°C and 350 rpm to extract CO<sub>2</sub>, resulting in clean water that can also be reused in the process.

This scenario demonstrates the potential for maximum resource recovery, minimizing the need for fresh water and chemicals while reducing the environmental impact. By closing the loop, Scenario 4 aligns with the principles of a circular economy, making it the most sustainable approach explored in this study.

The description and specific data for each scenario were provided by the Green Chemistry Laboratory.

## **3.3. Application of LCA methodology in case study**

To evaluate the environmental performance of the separation methods outlined earlier, the LCA methodology, as governed by ISO 14040 and 14044 standards and the European Commission's ILCD Handbook, was applied and tailored to fit the specifics of this case study.

### **3.3.1. Goal and Scope Definition**

The goal of this Life Cycle Assessment (LCA) is to evaluate the environmental performance of four different recycling scenarios for multilayer coffee bags, focusing

on the use of Switchable Anionic Surfactants (SAS) for delamination. The primary objective is to quantify the environmental impacts of each scenario and perform a comparative analysis to identify the most sustainable approach. The study aims to pinpoint environmental hotspots within each scenario, focusing on the processes and steps that contribute most significantly to the overall environmental burden. Based on the analysis, recommendations will be made to mitigate these impacts, optimize efficiency, and propose more sustainable recycling practices.

The motivation behind this research is to provide a detailed environmental assessment of the delamination and recycling methods for multilayer coffee bags, which will help chemists and engineers develop more sustainable chemical processes. Additionally, the study aims to offer practical insights for scaling up the recycling processes while maintaining a low environmental footprint in the future.

### Scope Definition

The scope of this study is defined by the system boundaries, functional unit, and the specific processes involved in the recycling of multilayer coffee bags. The study adopts a cradle-to-gate approach, covering the delamination, washing, material recovery, and wastewater treatment phases of the recycling process. All upstream processes, such as raw material extraction, coffee bag production, and consumer use, are excluded from the scope. The focus is exclusively on the recycling phase, as this is the core of the environmental impact evaluation.

### System Boundaries

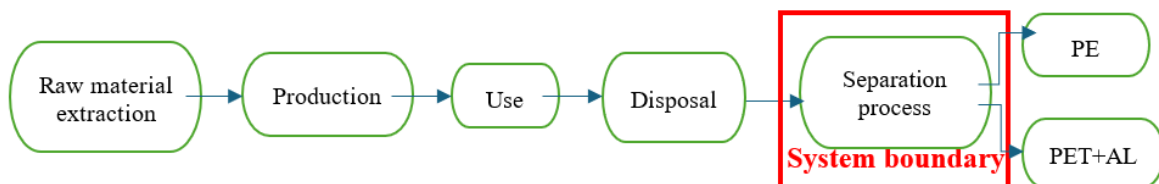


Figure 8 Gate-to-gate system boundaries.

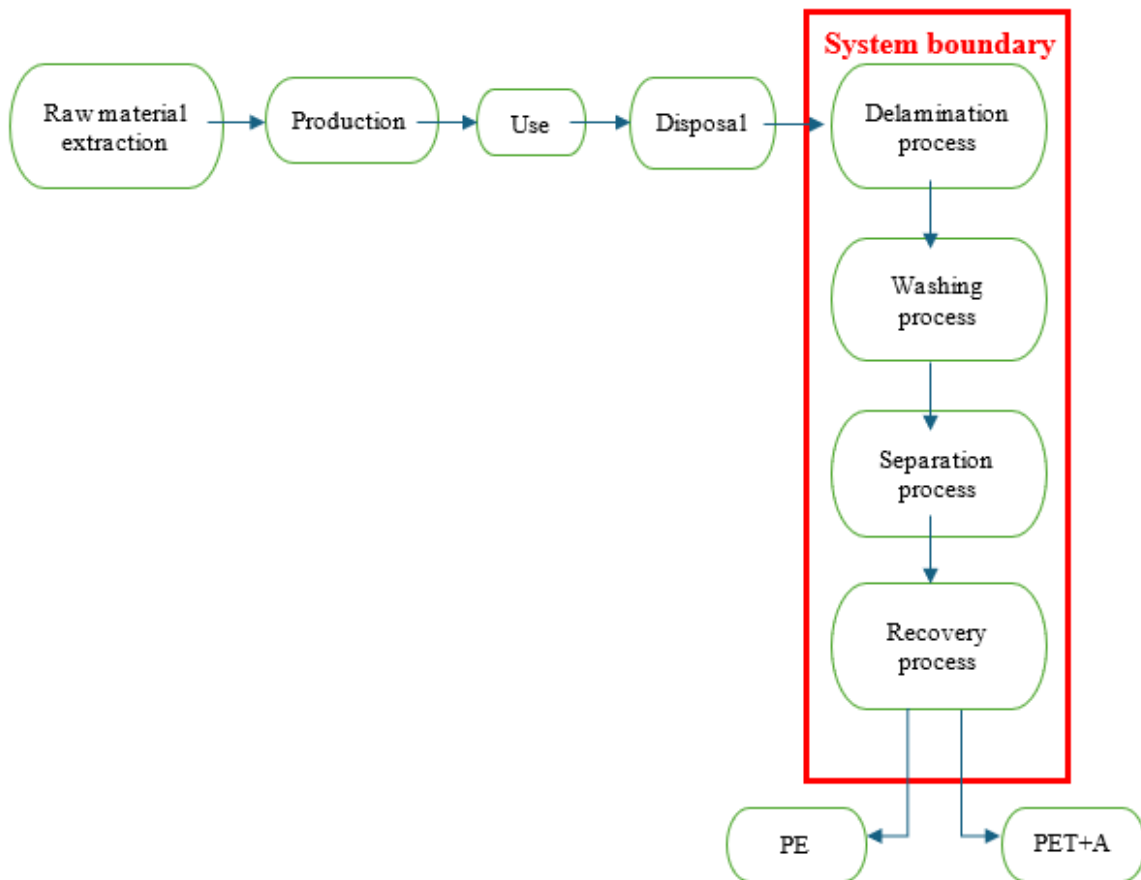


Figure 9. Flow chart of the main scenario.

The system boundaries overall encompass the following processes:

- Delamination Process: Involving Lauric Acid and Triethanolamine (TEA) to separate the layers of the coffee bags.
- Basic Washing Solution: Using Ammonium Hydroxide (NH<sub>4</sub>OH) to further clean the material and assist in separating surfactants.
- Water Washing: Rinsing the residual coffee bag material with water to remove contaminants.
- Final Washing or separation tank: A final rinse to ensure complete separation of the materials.
- Recovery and Treatment: Including the recovery of Lauric Acid and CO<sub>2</sub> in scenarios 2, 3, and 4, and the disposal or reuse of wastewater.

No CO<sub>2</sub> emissions are released into the atmosphere in any of the scenarios, as the CO<sub>2</sub> used in the recycling process is fully captured or reused. All energy and material

flows, such as water, chemicals, and electricity used during the recycling processes, are accounted for within the system boundaries.

### **Functional Unit**

The functional unit of the LCA is defined as the recycling of 1 kilogram of multilayer coffee bags. With the delamination of a 9g coffee bag waste into 71% plastic (PE) and 29% aluminum plus PET, respectively.

This provides a consistent basis for comparing the environmental impacts of the four recycling scenarios.

### **Assumptions and Simplifications**

Several assumptions and simplifications were made to streamline the modeling process:

- a. Zero burden boundary: The waste material input (coffee bags) is considered to have no environmental burden, meaning that the upstream processes (e.g., material extraction, coffee bag production) are excluded from the scope (ISO 14044, 2006).
- b. Energy considerations: Only the energy required to heat the solutions from room temperature to the desired level is included. Energy needed to maintain the temperature is not considered, simplifying the energy calculations.
- c. Process simplification: Multiple washing or delamination steps are consolidated into a single step to streamline the analysis, without affecting the integrity of the process.
- d. Localized datasets: The study relies exclusively on Italian geographic datasets, ensuring that the environmental impacts reflect local context accurately.
- e. No CO<sub>2</sub> emissions: There are no atmospheric CO<sub>2</sub> emissions, as the CO<sub>2</sub> used in the recovery process is fully captured and reused within the system.

### **EF 3.1 PEF method**

The Product Environmental Footprint (PEF) method was developed to standardize the calculation of the environmental footprint of a product or service and to obtain studies that are as reproducible and comparable as possible (Zampori & Pant, 2020). The idea of creating this common methodology was born in 2010, when the Council of the European Union invited the Commission to develop a common method for assessing the environmental impacts of products (Council of the European Union, 2010).

The PEF method has been in use since 2013. To enhance its reliability, a pilot phase was carried out between 2013 and 2018, where the method was tested across various

product categories. I opted to use the EF 3.1 method because it is a recent and reliable approach, widely recognized at the European level and endorsed by the European Commission. Additionally, this method supports normalization and weighting of results, enabling a direct comparison of the environmental performance of different products and services.

The EF 3.1 method includes the 16 impact categories, as reported in figure 10 (Understanding Product Environmental Footprint and Organization Environmental Footprint methods 2021) .

Impact category	Impact category Indicator (unit of measure)	Description
 Climate change, total	Radiative forcing as global warming potential – GWP100 (kg CO <sub>2</sub> eq)	Increase in the average global temperature resulting from greenhouse gas emissions (GHG)
 Ozone depletion	Ozone Depletion Potential – ODP (kg CFC-11 eq)	Depletion of the stratospheric ozone layer protecting from hazardous ultraviolet radiation
 Human toxicity, cancer	Comparative Toxic Unit for humans (CTUh)	Impact on human health caused by absorbing substances through the air, water, and soil. Direct effects of products on humans are not measured
 Human toxicity, non-cancer	Comparative Toxic Unit for humans (CTUh)	
 Particulate matter	Impact on human health (disease incidence)	Impact on human health caused by particulate matter emissions and its precursors (e.g. sulfur and nitrogen oxides)
 Ionising radiation, human health	Human exposure efficiency relative to U-235 (kBq U-235 eq)	Impact of exposure to ionising radiations on human health
 Photochemical ozone formation, human health	Tropospheric ozone concentration increase (kg NMVOC eq)	Potential of harmful tropospheric ozone formation ("summer smog") from air emissions
 Acidification	Accumulated Exceedance – AE (mol H <sup>+</sup> eq)	Acidification from air, water, and soil emissions (primarily sulfur compounds) mainly due to combustion processes in electricity generation, heating, and transport
 Eutrophication, terrestrial	Accumulated Exceedance – AE (mol N eq)	Eutrophication and potential impact on ecosystems caused by nitrogen and phosphorous emissions mainly due to fertilizers, combustion, sewage systems
 Eutrophication, freshwater	Fraction of nutrients reaching freshwater end compartment (kg P eq)	
 Eutrophication, marine	Fraction of nutrients reaching marine end compartment (kg N eq)	
 Ecotoxicity, freshwater	Comparative Toxic Unit for ecosystems (CTUe)	Impact of toxic substances on freshwater ecosystems
 Land use	Soil quality index, representing the aggregated impact of land use on: Biotic production; Erosion resistance; Mechanical filtration; Groundwater replenishment (Dimensionless – pt)	Transformation and use of land for agriculture, roads, housing, mining or other purposes. The impact can include loss of species, organic matter, soil, filtration capacity, permeability
 Water use	Weighted user deprivation potential (m <sup>3</sup> world eq)	Depletion of available water depending on local water scarcity and water needs for human activities and ecosystem integrity
 Resource use, minerals and metals	Abiotic resource depletion – ADP ultimate reserves (kg Sb eq)	Depletion of non-renewable resources and deprivation for future generations
 Resource use, fossils	Abiotic resource depletion, fossil fuels – ADP-fossil (MJ)	

Figure 10 Impact categories included in PEF details of the methods and indicators.

### **3.3.2. Description of characterization model for each impact category**

it is important to understand that these categories can be classified into two types: midpoint and endpoint. This distinction depends on whether the effects from the emission or extraction of a substance impact a final target (endpoint) or an intermediate stage (midpoint) before reaching the final target (EC-JRC-IES, 2010). At the midpoint level, characterization factors are calculated to reflect the relative significance of an emission or extraction. Examples of endpoint targets include human health, the natural environment, and natural resources.

Each characterization model includes specific **characterization factors (CFs)**, which indicate the impact intensity of a substance relative to a reference substance within a particular impact category (impact category indicator) (EC-JRC-IES, 2010).

These CFs are tailored to each substance or resource, reflecting its unique environmental impact.

These categories provide a comprehensive assessment of how each recycling scenario impacts different environmental dimensions, such as resource use, human health, and climate change.

## **3.4. Software and Tools**

### **3.4.1. GaBi Software for LCA Modeling**

To assess the environmental sustainability of the analyzed protocols, GaBi software version 10.6.2.9 was employed in my case study.

GaBi software is a leading tool used for conducting environmental assessments, particularly for Life Cycle Assessment (LCA). It enables users to model and analyze complex processes by quantifying the inputs and outputs of materials, energy, and emissions associated with a particular system. GaBi helps users understand the environmental impacts of products, services, or processes by mapping out all relevant data across their life cycle stages.

The software is structured into plans, which contain individual processes. Each process includes various flows of materials and energy, categorized into elementary flows, waste flows, and tracked flows. Elementary flows are those that directly impact the environment, while waste flows represent materials that require further processing

or disposal. Tracked flows act as connectors between processes but do not directly affect the environment.

(Sphera, 2022).

GaBi also offers an extensive database of datasets covering numerous industries and sectors, allowing users to simulate real-world conditions and environmental impacts based on accurate, up-to-date data. With this database, users can input data specific to their project and set a functional unit, which acts as a reference point for measuring the overall environmental impact of the system.

A key feature of GaBi is its ability to run scenarios, enabling users to test how changes in certain parameters—such as materials used, or energy consumed—can alter the environmental outcomes. This flexibility makes it ideal for assessing different strategies or optimizing systems for lower environmental impact.

Once the model and scenarios are built, GaBi provides detailed Life Cycle Impact Assessment (LCIA) results, which are visualized through graphs and charts. This makes it easy to interpret which processes contribute the most to environmental burdens and where improvements can be made. Overall, GaBi is an essential tool for anyone looking to conduct comprehensive and reliable LCA studies.

I will be describing every Gabis model regarding each scenario in Result chapter.

### **3.4.2. Data Collection Using Excel for Mass Balance and Energy**

Data for the mass balance and energy consumption of each scenario were collected using Excel spreadsheets. This involved tracking the inputs and outputs of materials such as TEA, Lauric Acid, NH<sub>4</sub>OH, and CO<sub>2</sub>, as well as measuring the energy required for each process step. The mass balance calculations allowed for the accurate quantification of recovered materials, while energy data was used to assess the overall efficiency of each scenario.

## 4. Chapter4: Results

### 4.1. Life Cycle Inventory

This section presents the results of the inventory data collection in the form of tables, detailing the inputs and outputs for each stage of the four recycling scenarios. The data included are primarily derived from laboratory experiments or calculated based on specific guidelines provided by the chemistry researchers involved in the project.

Each scenario has been modeled separately, and the data for each are organized into individual tables. These tables capture all relevant inputs—such as chemicals, energy consumption, and water use—and outputs, including recovered materials and waste. The calculations for mass balance and energy usage for each scenario are documented in an Excel file, which served as the primary tool for organizing and computing the inventory data.

Each inventory table corresponds to a model implemented with the GaBi software.

#### 4.1.1. Material and Energy Flow calculation

Before presenting the data inventory tables for each scenario, it is important to provide a brief explanation of the calculations in each scenario. In my experimental case study, mass balance calculations account for the material losses at each step. This means that during the transfer of delaminated coffee bags to the next tank, an approximate amount of surfactant and water flows into the next tank, resulting in a reduced volume of solution left in the previous tank. The amount of solution loss has been calculated by the chemistry laboratory responsible for conducting this experimental project, and the results are summarized in the following steps:

##### Step 1: Delamination Process

To begin the delamination process, we add water, TEA (Triethanolamine), and Lauric acid, which break down the multilayer structure of the coffee bags, separating the plastic and aluminum layers.

After completing the delamination process, 100 ml of the solution (comprising water and surfactant) is lost. The initial concentrations of the solution are as follows:

- Water: 4000 ml (where 1 ml  $\approx$  1 g)
- TEA: 12.80 g
- Lauric acid: 11.46 g

- TEA-Laurate: 24 g (formed by TEA and Lauric acid)

The initial concentration of TEA-Laurate is:

$$\text{Concentration} = 24 \text{ g}/4000 \text{ ml} = 0.006 \text{ g/ml}$$

At this point, we have two flows:

1. One flow moving to the next tank.
2. One flow remaining in the current tank for 10 cycles.

The concentration of TEA-Laurate in 100 ml of the solution, over 10 cycles, is calculated as:

$$10 \times 100 \text{ ml} \times 0.006 \text{ g/ml} = 6 \text{ g}$$

This means 6 grams of TEA-Laurate is lost over 10 cycles, and the remaining water after the loss is:

$$1000 \text{ ml} - 6 \text{ g} = 994 \text{ ml (or grams)}$$

Thus, the remaining amounts are:

- Water:  $4000 \text{ ml} - 994 \text{ ml} = 3006 \text{ ml}$
- TEA-Laurate:  $24 \text{ g} - 6 \text{ g} = 18 \text{ g}$

This results in Contaminated Solution 1:

$$3006 \text{ ml water} + 18 \text{ g TEA - Laurate}$$

For Lauric acid recovery, we use CO<sub>2</sub> at a concentration of 525.15 g/L, leading to the recovery of 0.52 g/L of Lauric acid.

### Step 2: Transfer to Second Tank

As the remaining solution moves to the second tank, 4 L of water and 3.1 g of NH<sub>4</sub>OH (Ammonium Hydroxide) are added. Thus, the total water in the tank becomes:

$$994 \text{ ml} + 4000 \text{ ml} = 4994 \text{ ml of water}$$

The total concentration of TEA-Laurate is:

$$6 \text{ g}/4994 \text{ ml} \approx 0.00120 \text{ g/ml}$$

Based on the laboratory report, we lose 50 ml of solution with the coffee bag residues, so the loss for 10 cycles is calculated as:

$$10 \times 50 \text{ ml} \times 0.00120 \text{ g/ml} \approx 0.6 \text{ g TEA\_Laurate lost over 10 cycles}$$

Thus, the remaining water is:

$$499.4 \text{ ml} - 0.6 \text{ g} = 499.4 \text{ ml water}$$

And the remaining solution in the second tank is:

4494.60 ml water

5.4 g TEA-Laurate (remaining)

For Lauric acid recovery, we use CO<sub>2</sub> at a concentration of 211.13 g/L, leading to the recovery of 1.07 g/L of Lauric acid.

### Step 3: Washing with Water

In this step, 50 ml of solution, along with coffee bag residues, is lost when transferred to the third tank. Additionally, 4 L of water is added, making the total volume:

$$499.4 \text{ ml} + 4000 \text{ ml} = 4499.4 \text{ ml of water}$$

The concentration of TEA-Laurate becomes:

$$0.6 \text{ g} / 4499.4 \text{ ml} = 0.000133 \text{ g/ml}$$

loss for 10 cycles is calculated as:

$$10 \times 50 \text{ ml} \times 0.000133 \text{ g/ml} = 0.0667 \text{ g/ml TEA\_Laurate lost over 10 cycles}$$

So amount of water transferred is:

$$500 \text{ ml} - 0.0667 \text{ g/ml} = 499.93$$

The remaining water in the third tank is:

$$3999.40 \text{ ml water}$$

$$0.00729 \text{ g TEA - Laurate}$$

This results in Contaminated Solution 3:

$$3999.40 \text{ ml water} + 0.00729 \text{ gr TEA\_La}$$

### Step 4: Final Tank

In the final tank, we assume there is no further loss of solution with transferred coffee bag delaminated. All the solution remains in the tank for 10 cycles, with an additional 10 L of water added.

The concentration of TEA-Laurate is reduced to nearly zero due to dilution:  
 $0.0000901210050 \text{ ml} = 8.9671 \times 10^{-9} \approx 0$

Thus, the final solution is primarily clean water, with negligible amounts of TEA-Laurate.

### Energy Calculation

In this study, the energy consumption for both **electricity** (used for stirring) and **thermal energy** (used for heating) was calculated for each stage of the coffee bag delamination and recycling process across all four scenarios. The energy demand is critical for assessing the environmental impact of the process, as it contributes directly to the overall resource use and carbon footprint.

The energy calculations for each step are presented, categorized into Energy Demand for Stirring and Energy Demand for Heating, measured in megajoules (MJ).

### 1. Energy Demand for Stirring:

The energy consumed by the stirring device is calculated using the formula:

$$\begin{aligned} \text{Energy (kWh)} &= \text{Power (kW)} \times \text{Time (hours)} \\ &= \text{Power (kW)} \times \text{Time (hours)} \end{aligned}$$

Where:

**Power (kW)** is the power rating of the stirring device (in kilowatts).

**Time (hours)** is the total time the stirring device is running.

#### Example Calculation:

Based on the guidelines on the factory label of the stirring device. (Mechanical stirrer rod display, Stirring speed adjustable from 50 to 2200 rpm with a power of 70 W), it has a power rating of 0.07 kWh and it is used for 3 hours in the delamination process. The energy consumption for this process would be:

$$\text{Energy} = 0.07 \text{ kW} \times 3 \text{ hours} = 0.210 \text{ kWh}$$

This calculation can be repeated for each stage where stirring occurs, based on the power rating of the equipment and the duration of the operation.

### 2. Energy Demand for Heating

The energy required to heat the solution is calculated using the **specific heat capacity formula**:

$$Q = mc\Delta T$$

Where:

- **Q** = heat energy (in joules, J)
- **m** = mass of the solution (in kilograms, kg)
- **c** = specific heat capacity of water (approximately 4180 J/kg°C)
- **ΔT** = change in temperature (in °C), which is the difference between the initial temperature (room temperature, 20°C) and the target temperature.

Example Calculation:

Suppose we are heating 4 kg (4 liters) of water from room temperature (20°C) to 90°C. The change in temperature (ΔT) is:

$$\Delta T = 90^{\circ}\text{C} - 20^{\circ}\text{C} = 70^{\circ}\text{C} \quad \Delta T = 90^{\circ}\text{C} - 20^{\circ}\text{C} = 70^{\circ}\text{C}$$

The mass of the solution is 4 kg (since 1 liter of water is approximately 1 kg), and the specific heat capacity of water is 4180 J/kg°C.

Now, the heat energy required (Q) is:

$$Q = 4 \text{ kg} \times 4180 \text{ J/kg}^{\circ}\text{C} \times 70^{\circ}\text{C} = 1,170,400 \text{ J}$$

To convert this to kilowatt-hours (kWh), we use the conversion factor 1 kWh=3,600,000 J | kWh = 3,600,000J:

$$Q = 1,170,400 \text{ J} / 3,600,000 \text{ J/kWh} \approx 0.325 \text{ kWh}$$

Thus, 0.325 kWh of energy is required to heat 4 liters of water from 20°C to 90°C.

## 4.1.2. scenario data Inventory

Table 1 inventory data collected for scenario 1

process	flows	Input / output	amount	measurement
TEA laurate preparation	Lauric acid	input	1.15E-02	kg
	Triethanolamine.	input	1.28E-02	kg
	Thermal energy	input	6.69E-01	MJ
	Water	input	4.00E+00	kg
	Triethanolamine laurate-TEA-laurate	output	4.02E+00	kg
Delamination	Coffee bags	input	9.00E-01	kg
	TEA-laurate	input	4.02E+00	kg
	Electricity	input	7.56E-01	MJ
	Thermal energy	input	1.18E+00	MJ
	<i>Multilayer Al + PET/PE scrap + TEA - laurate % + water%</i>	output	1.90E+00	kg
	<i>TEA - laurate % + water% (contaminated solution 1)</i>	output	3.02E+00	kg
NH4OH preparation	NH3/Ammonia	input	1.51E-03	kg
	Water	input	1.59E-03	kg
	<i>Ammonium hydroxide/NH4OH</i>	output	3.10E-03	kg
washing with basic solution	<i>Al/PET + PE + TEA - laurate % + water%</i>	input	1.90E+00	kg
	NH4OH	input	3.10E-03	kg
	Electricity	input	2.52E-01	MJ
	Water	input	4.00E+00	kg
	<i>TEA - laurate % + water% + NH4OH (contaminated solution 2)</i>	output	4.50E+00	kg

	<i>Multilayer Al + PET/PE scrap + TEA – laurate % + water%</i>	output	1.40E+00	kg
<b>washing with water</b>	<i>Multilayer Al + PET/PE scrap + TEA – laurate % + water%</i>	input	1.40E+00	kg
	<i>Water</i>	input	4.00E+00	kg
	<i>TEA – laurate % + water% (contaminated solution 3)</i>	output	4.00E+00	kg
	<i>PE/AL + PET + water%</i>	output	1.40E+00	kg
<b>separation tank</b>	<i>PE/AL+PET</i>	input	1.40E+00	kg
	<i>Water</i>	input	1.00E+01	kg
	<i>Electricity</i>	input	2.52E-01	MJ
	<i>Clean water</i>	output	1.05E+01	kg
	<i>PE</i>	output	6.39E-01	kg
	<i>Al + PET</i>	output	2.61E-01	kg
<b>WWTP</b>	<i>contaminated solution 1</i>	input	3.02E+00	kg
	<i>contaminated solution 2</i>	input	4.50E+00	kg
	<i>contaminated solution 3</i>	input	4.00E+00	kg
	<i>treated water</i>	output	1.15E+01	kg

Table 2 inventory data collected for scenario 2

<b>process</b>	<b>flows</b>	<b>Input / output</b>	<b>amount</b>	<b>measurement</b>
<b>TEA laurate preparation</b>	<i>Lauric acid</i>	input	1.15E-02	kg
	<i>Triethanolamine.</i>	input	1.28E-02	kg
	<i>Thermal energy</i>	input	6.69E-01	MJ
	<i>Water</i>	input	4.00E+00	kg
	<i>Triethanolamine laurate – TEA – laurate</i>	output	4.02E+00	kg
<b>Delamination</b>	<i>Coffee bags</i>	input	9.00E-01	kg
	<i>TEA-laurate</i>	input	4.02E+00	kg
	<i>Electricity</i>	input	7.56E-01	MJ
	<i>Thermal energy</i>	input	1.18E+00	MJ
	<i>Multilayer Al + PET/PE scrap + TEA – laurate % + water%</i>	output	1.90E+00	kg
	<i>TEA – laurate % + water% (contaminated solution 1)</i>	output	3.02E+00	kg
<b>NH4OH preparation</b>	<i>NH3/Ammonia</i>	input	1.51E-03	kg
	<i>Water</i>	input	1.59E-03	kg
	<i>Ammonium hydroxide/NH4OH</i>	output	3.10E-03	kg
<b>washing with basic solution</b>	<i>Al/PET + PE + TEA – laurate % + water%</i>	input	1.90E+00	kg
	<i>NH4OH</i>	input	3.10E-03	kg

	Electricity	input	2.52E-01	MJ
	Water	input	4.00E+00	kg
	<i>TEA – laurate % + water% + NH4OH (contaminated solution 2)</i>	output	4.50E+00	kg
	<i>Multilayer Al + PET/PE scrap + TEA – laurate % + water%</i>	output	1.40E+00	kg
<b>washing with water</b>	<i>Multilayer Al + PET/PE scrap + TEA – laurate % + water%</i>	input	1.40E+00	kg
	Water	input	4.00E+00	kg
	<i>TEA – laurate % + water% (contaminated solution 3)</i>	output	4.00E+00	kg
	<i>PE/AL + PET + water%</i>	output	1.40E+00	kg
<b>separation tank</b>	<i>PE/AL + PET</i>	input	1.40E+00	kg
	Water	input	1.00E+01	kg
	Electricity	input	2.52E-01	MJ
	Clean water	output	1.05E+01	kg
	PE	output	6.39E-01	kg
	<i>Al + PET</i>	output	2.61E-01	kg
<b>Recovery of solution 1</b>	Contaminated solution 1	input	3.02E+00	kg
	Dry ice/CO2	input	5.25E-01	kg
	Recovered lauric acid	output	5.20E-04	kg
	<i>HCO3<sup>-</sup>TEA<sup>+</sup></i>	output	3.55E+00	kg
<b>Recovery of solution 2</b>	Contaminated solution 2	input	4.50E+00	kg
	Dry ice/CO2	input	2.11E-01	kg
	Recovered lauric acid	output	1.07E-03	kg
	<i>HCO3<sup>-</sup>NH4OH</i>	output	4.71E+00	kg
<b>Recovery of solution 3</b>	Contaminated solution 3	input	4.00E+00	kg
	Dry ice/CO2	input	1.27E-01	kg
	Recovered lauric acid	output	8.00E-04	kg
	HCO3 <sup>-</sup>	output	4.13E+00	kg
<b>WWTP</b>	<i>HCO3<sup>-</sup>TEA<sup>+</sup></i>	input	3.55E+00	kg
	<i>HCO3<sup>-</sup>NH4OH</i>	input	4.71E+00	kg
	<i>HCO3<sup>-</sup></i>	input	4.13E+00	kg
	Treated water	output	1.24E+01	kg

Table 3 inventory data collected for scenario 3

process	flows	Input / output	amount	measurement
TEA laurate preparation	Lauric acid	input	1.15E-02	kg
	Triethanolamine.	input	1.28E-02	kg
	Thermal energy	input	4.00E+00	kg
	Water	input	6.69E-01	MJ
	<i>Triethanolamine laurate – TEA – laurate</i>	output	4.02E+00	kg
Delamination	Coffee bags	input	9.00E-01	kg
	TEA-laurate	input	4.02E+00	kg
	Electricity	input	7.56E-01	MJ
	Thermal energy	input	1.18E+00	MJ
	<i>Multilayer Al + PET/PE scrap + TEA – laurate % + water%</i>	output	1.90E+00	kg
	<i>TEA – laurate % + water% (contaminated solution 1)</i>	output	3.02E+00	kg
NH4OH preparation	<i>NH3/Ammonia</i>	input	1.51E-03	kg
	Water	input	1.59E-03	kg
	<i>Ammonium hydroxide/NH4OH</i>	output	3.10E-03	kg
washing with basic solution	<i>Al/PET + PE + TEA – laurate % + water%</i>	input	1.90E+00	kg
	NH4OH	input	3.10E-03	kg
	Electricity	input	2.52E-01	MJ
	Water	input	4.00E+00	kg
	<i>TEA – laurate % + water% + NH4OH (contaminated solution 2)</i>	output	4.50E+00	kg
	<i>Multilayer Al + PET/PE scrap + TEA – laurate % + water%</i>	output	1.40E+00	kg
washing with water	<i>Multilayer Al + PET/PE scrap + TEA – laurate % + water%</i>	input	1.40E+00	kg
	Water	input	4.00E+00	kg
	<i>TEA – laurate % + water% (contaminated solution 3)</i>	output	4.00E+00	kg
	<i>PE/AL + PET + water%</i>	output	1.40E+00	kg
separation tank	PE/AL+PET	input	1.40E+00	kg
	Water	input	1.00E+01	kg
	Electricity	input	2.52E-01	MJ
	Clean water	output	1.05E+01	kg
	PE	output	6.39E-01	kg
	<i>Al + PET</i>	output	2.61E-01	kg

<b>Recovery of solution 1</b>	Contaminated solution 1	input	3.02E+00	kg
	Dry ice/CO2	input	5.25E-01	kg
	Recovered lauric acid	output	5.20E-04	kg
	HCO3-TEA+	output	3.55E+00	kg
<b>Recovery of solution 2</b>	Contaminated solution 2	input	4.50E+00	kg
	Dry ice/CO2	input	2.11E-01	kg
	Recovered lauric acid	output	1.07E-03	kg
	HCO3-NH4OH	output	4.71E+00	kg
<b>Recovery of solution 3</b>	Contaminated solution 3	input	4.00E+00	kg
	Dry ice/CO2	input	1.27E-01	kg
	Recovered lauric acid	output	8.00E-04	kg
	HCO3-	output	4.13E+00	kg
<b>CO2 Recovery part 1</b>	HCO3-TEA+	input	3.55E+00	kg
	electricity	input	4.20E-01	MJ
	thermal energy	input	1.04E+00	MJ
	recovered CO2	output	5.25E-01	kg
	TEA water solution/waste	output	3.02E+00	kg
<b>WWTP</b>	TEA water solution/waste	input	3.02E+00	kg
	HCO3-NH4OH	input	4.71E+00	kg
	HCO3-	input	4.13E+00	kg
	treated water	output	1.19E+01	kg

Table 4 inventory data collected for scenario 4

process	flows	Input / output	amount	measurement
<b>TEA laurate preparation</b>	Lauric acid	input	1.15E-02	kg
	Triethanolamine.	input	1.28E-02	kg
	Thermal energy	input	6.69E-01	MJ
	Water	input	4.00E+00	kg
	<i>Triethanolamine laurate – TEA – laurate</i>	output	4.02E+00	kg
<b>Delamination</b>	Coffee bags	input	9.00E-01	kg
	TEA-laurate	input	4.02E+00	kg
	Electricity	input	7.56E-01	MJ
	Thermal energy	input	1.18E+00	MJ

	<i>Multilayer Al + PET/PE scrap + TEA – laurate % + water%</i>	output	1.90E+00	kg
	<i>TEA – laurate % + water% (contaminated solution 1)</i>	output	3.02E+00	kg
<b>NH4OH preparation</b>	NH3/Ammonia	input	1.51E-03	kg
	Water	input	1.59E-03	kg
	<i>Ammonium hydroxide/NH4OH</i>	output	3.10E-03	kg
<b>washing with basic solution</b>	<i>Al/PET + PE + TEA – laurate % + water%</i>	input	1.90E+00	kg
	NH4OH	input	3.10E-03	kg
	Electricity	input	2.52E-01	MJ
	Water	input	4.00E+00	kg
	<i>TEA – laurate % + water% + NH4OH (contaminated solution 2)</i>	output	4.50E+00	kg
	<i>Multilayer Al + PET/PE scrap + TEA – laurate % + water%</i>	output	1.40E+00	kg
<b>washing with water</b>	<i>Multilayer Al + PET/PE scrap + TEA – laurate % + water%</i>	input	1.40E+00	kg
	Water	input	4.00E+00	kg
	<i>TEA – laurate % + water% (contaminated solution 3)</i>	output	4.00E+00	kg
	<i>PE/AL + PET + water%</i>	output	1.40E+00	kg
<b>separation tank</b>	<i>PE/AL + PET</i>	input	1.40E+00	kg
	Water	input	1.00E+01	kg
	Electricity	input	2.52E-01	MJ
	Clean water	output	1.05E+01	kg
	PE	output	6.39E-01	kg
	<i>Al + PET</i>	output	2.61E-01	kg
<b>Recovery of solution 1</b>	Contaminated solution 1	input	3.02E+00	kg
	Dry ice/CO2	input	5.25E-01	kg
	Recovered lauric acid	output	5.20E-04	kg
	HCO3-TEA+	output	3.55E+00	kg
<b>Recovery of solution 2</b>	Contaminated solution 2	input	4.50E+00	kg
	Dry ice/CO2	input	2.11E-01	kg
	Recovered lauric acid	output	1.07E-03	kg
	HCO3-NH4OH	output	4.71E+00	kg
<b>Recovery of solution 3</b>	Contaminated solution 3	input	4.00E+00	kg
	Dry ice/CO2	input	1.27E-01	kg
	Recovered lauric acid	output	8.00E-04	kg

	HCO <sub>3</sub> <sup>-</sup>	output	4.13E+00	kg
<b>CO<sub>2</sub> Recovery part 1</b>	HCO <sub>3</sub> -TEA <sup>+</sup>	input	3.55E+00	kg
	electricity	input	4.20E-01	MJ
	thermal energy	input	1.04E+00	MJ
	recovered CO <sub>2</sub>	output	5.25E-01	kg
	TEA water solution/waste	output	3.02E+00	kg
<b>CO<sub>2</sub> Recovery part 2</b>	HCO <sub>3</sub> -NH <sub>4</sub> OH	input	4.71E+00	kg
	electricity	input	3.28E-01	
	thermal energy	input	1.38E+00	MJ
	recovered CO <sub>2</sub>	output	2.11E-01	kg
	NH <sub>4</sub> OH	output	3.10E-03	
	clean water	output	4.50E+00	kg
<b>CO<sub>2</sub> Recovery part 3</b>	HCO <sub>3</sub> <sup>-</sup>	input	4.13E+00	kg
	electricity	input	2.52E-01	MJ
	thermal energy	input	1.21E+00	MJ
	recovered CO <sub>2</sub>	output	1.27E-01	kg
	clean water	output	4.00E+00	kg
<b>WWTP</b>	TEA water solution/waste	input	3.02E+00	kg
	treated water	output	3.02E+00	kg

## 4.2. Models' implementation using GaBi software

### Clarification and Considerations for Modelling in Gabi Software

In the context of modelling the scenarios for the coffee bag delamination process, some adjustments and considerations had to be made due to the limitations of the available datasets in GaBi software. Specifically, two key areas required additional processes and clarifications:

- **Ammonium Hydroxide Dataset:** The production dataset for ammonium hydroxide (NH<sub>4</sub>OH) was not available in the standard GaBi databases. To accurately model its environmental impacts, a custom process was created. This was achieved by calculating the impacts based on the required amounts of ammonia (NH<sub>3</sub>) and water, as ammonium hydroxide is essentially a 25% aqueous solution of ammonia. The dataset for ammonia production and water were obtained from available sources in the GaBi database, and the combination of these two inputs was used to

model the production of ammonium hydroxide. This ensured that the environmental impact of NH<sub>4</sub>OH was accurately represented across all scenarios.

- **Carbon Dioxide Flow in Precipitation Process:** For the precipitation process where CO<sub>2</sub> is involved in the recovery of Lauric acid, an additional challenge was encountered. GaBi software did not have a direct dataset supporting the waste CO<sub>2</sub> flow needed for the precipitation process. As a solution, a dataset from **Ecoinvent** (carbon dioxide production, liquid ecoinvent 3.9.1) was utilized to model CO<sub>2</sub> input. This assumption was applied consistently across all scenarios to ensure uniformity in the environmental impact evaluation of the CO<sub>2</sub> flow.

I must mention some information about carbon dioxide production, liquid ecoinvent 3.9.1 source to more clarifying:

The functional unit represents 1 kg of liquid carbon dioxide. Data are based on a Swiss study about different cooling mediums.

Extraction of carbon dioxide out of waste gas streams from different production processes with a 15-20% MEA (monoethanolamine) solution, followed by a purification and a liquefaction step, using each electricity as energy source.

This module contains material and energy input and emissions for the production of liquid carbon dioxide out of waste gases from different production processes. Water consumption and infrastructure have been estimated. This dataset has been extrapolated from year 1999 to the year of the calculation (2015). The uncertainty has been adjusted accordingly. (ecoquery.ecoinvent report 2023)

For simplification, we assumed that the entire amount of CO<sub>2</sub> and NH<sub>4</sub>OH after recovery returns to the cycle with no losses. Fortunately, all the scenarios were successfully take place in Laboratory, and the exact quantities of materials used were made available, thanks to the dedicated efforts of the laboratory research group (Prof. Samorì, Project Merlin).

Following models are my case study scenario models that created in Gabi Software:

### 4.2.1. First scenarios modeled:

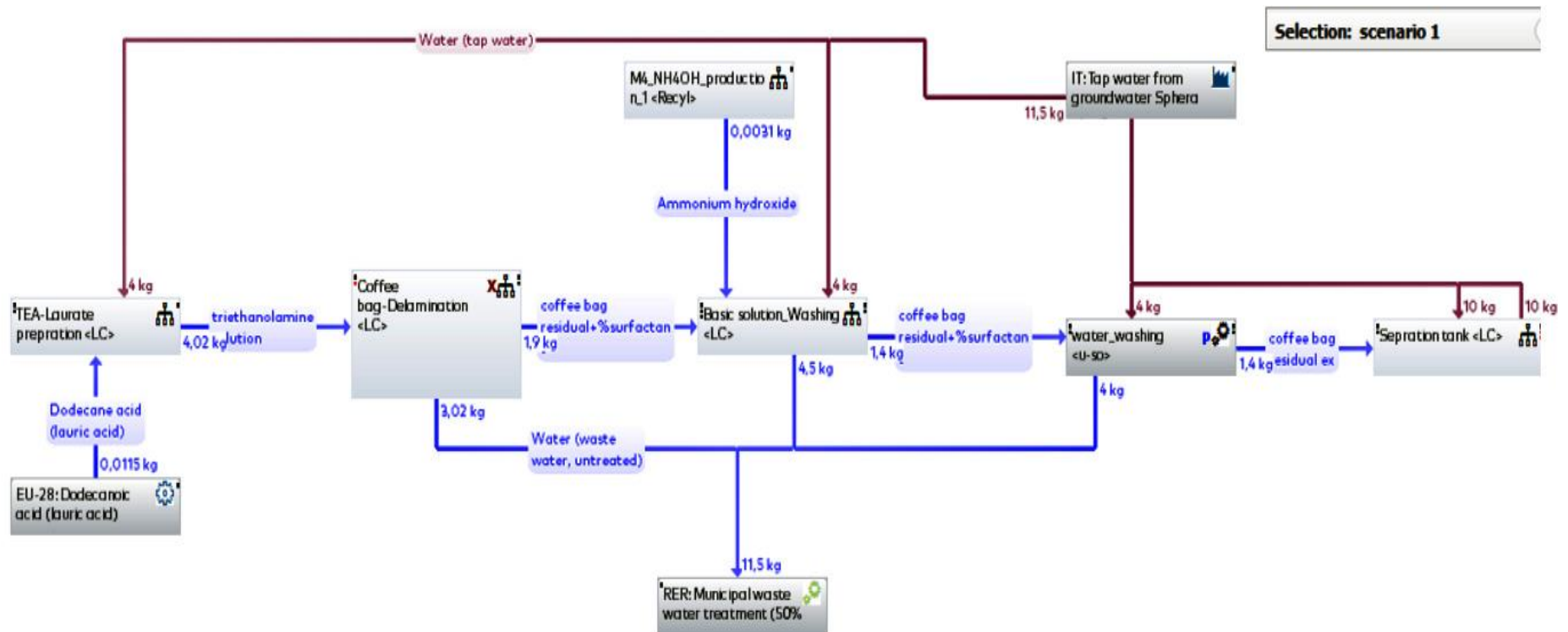


Figure 11 First scenario modeled with Gabi software

## 4.2.2. Second scenarios modeled

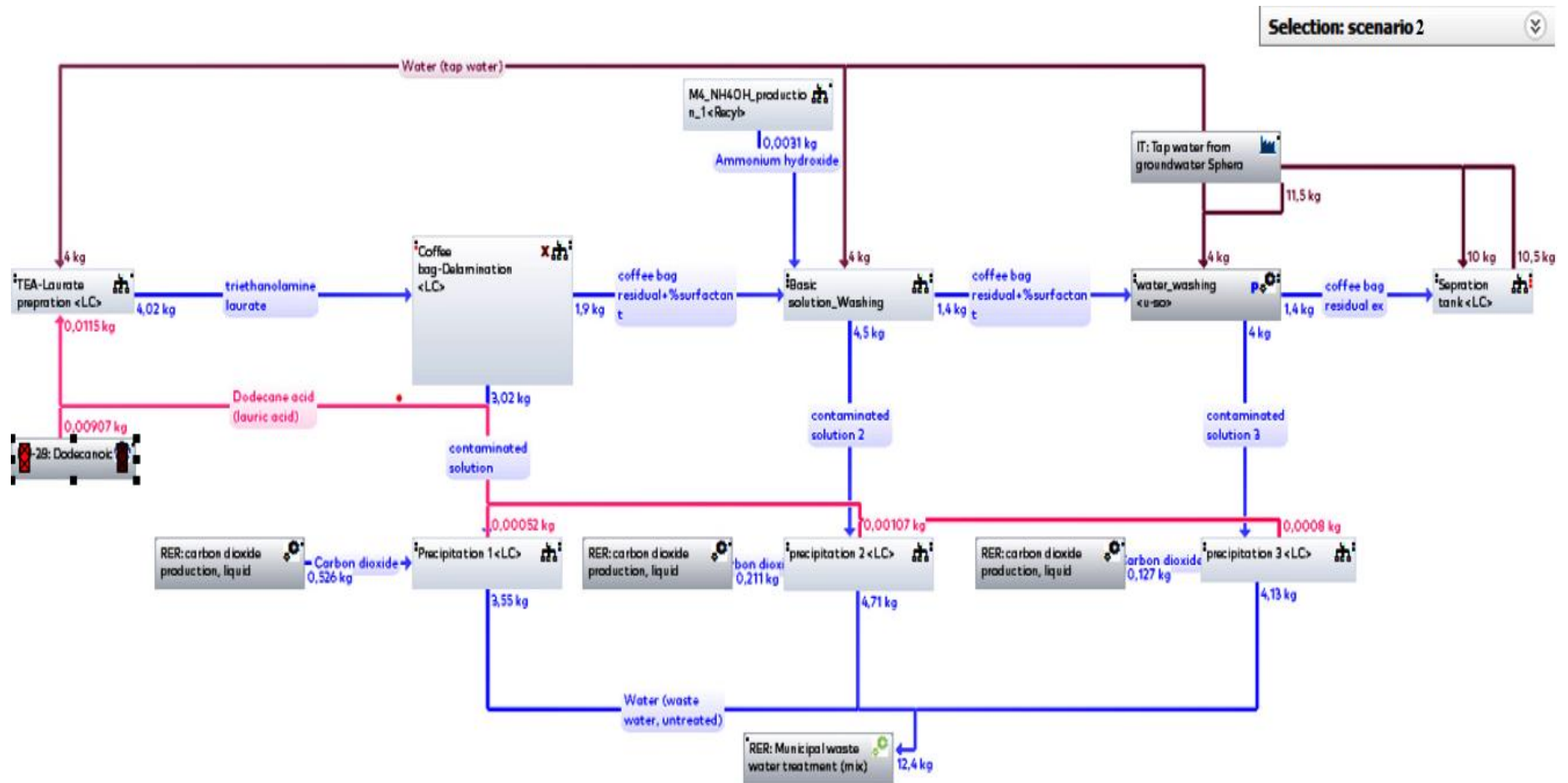


Figure 12 Second scenario modeled with Gabi software

### 4.2.3. Third scenarios modeled:

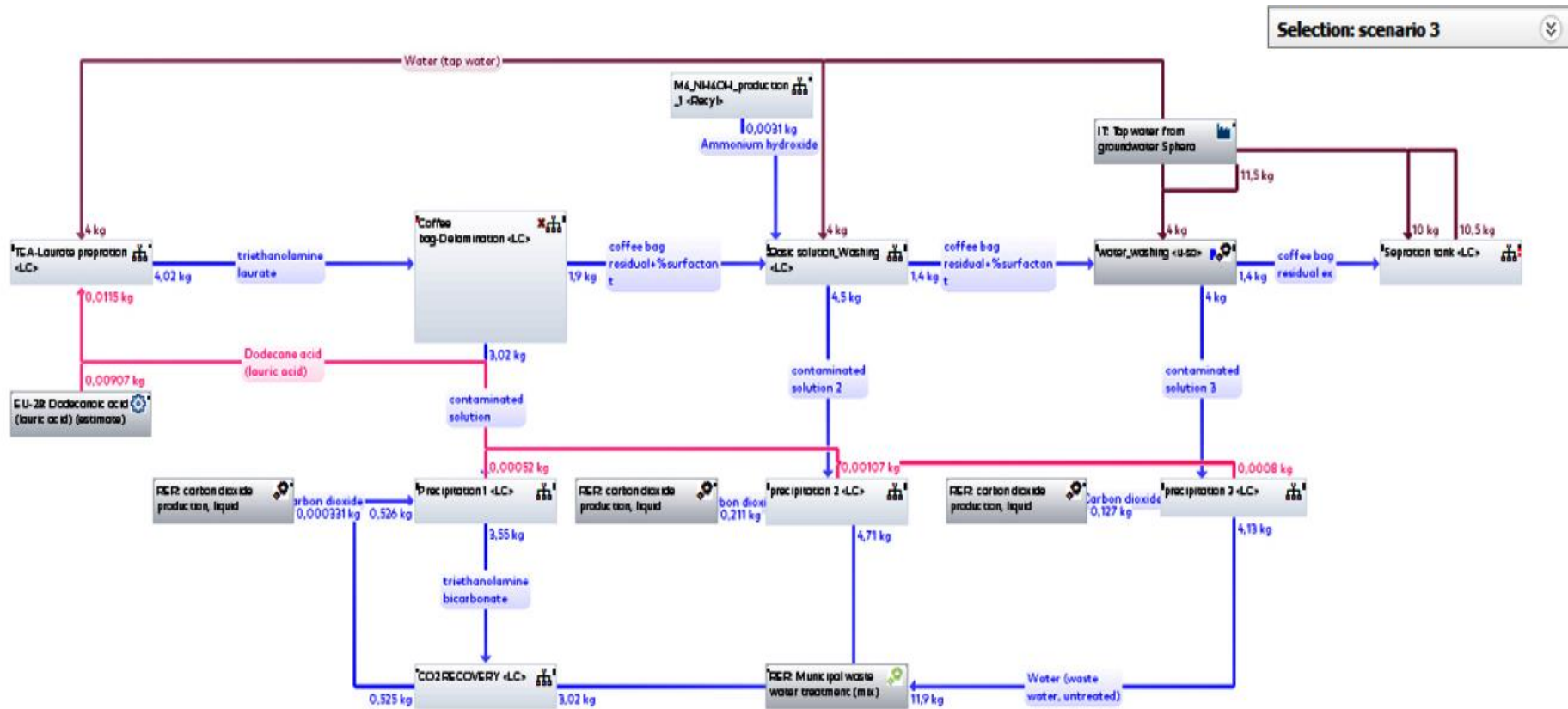


Figure 13 Third scenario modeled with Gabi software

#### 4.2.4. Forth scenarios modeled:

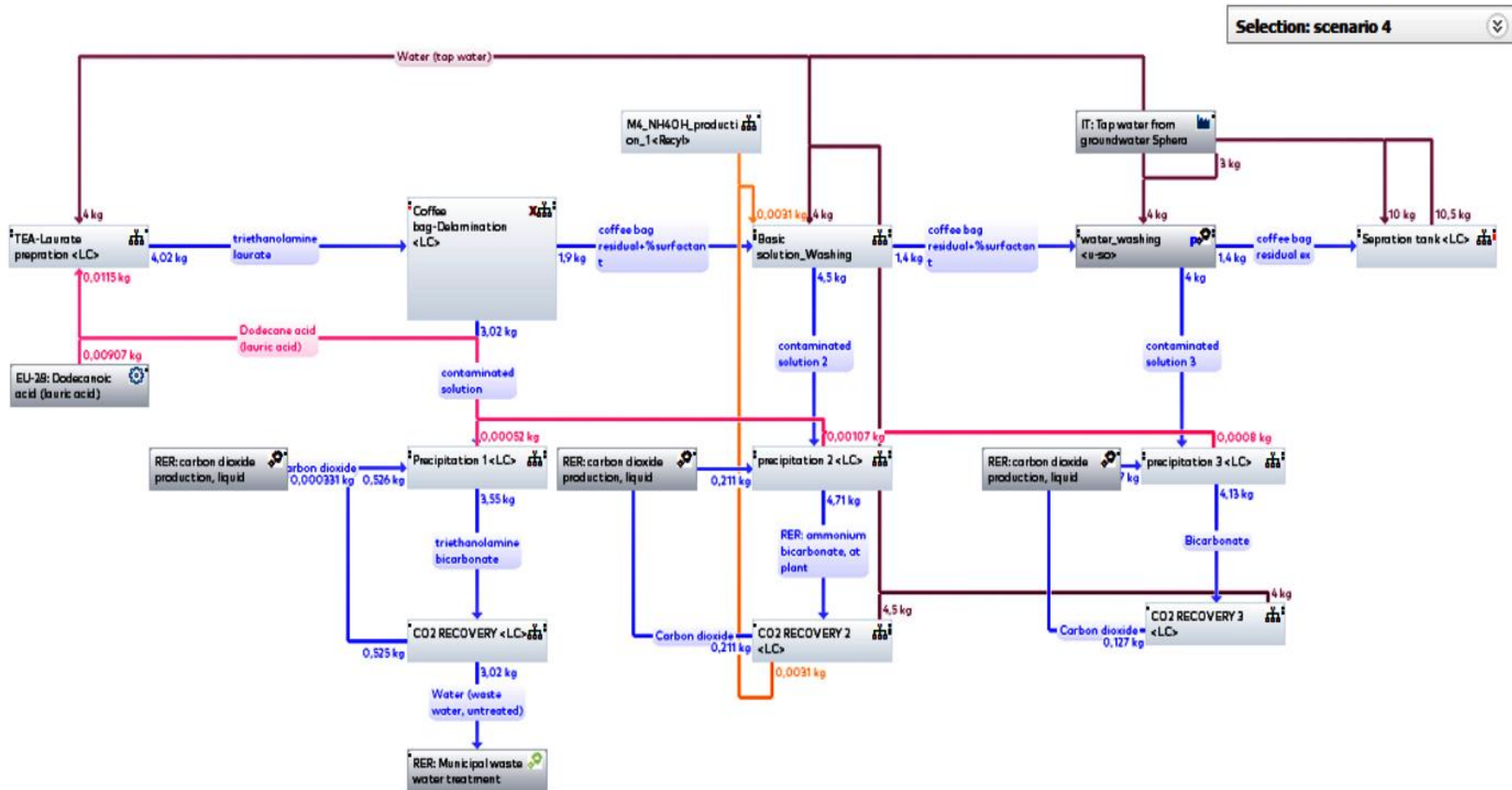


Figure 14 Fourth scenario modeled with Gabi software

These process flow diagrams, modeled using Gabi software, represent the systematic life cycle stages for the delamination process of coffee bags. The functional unit for this analysis is focused specifically on Delamination process.

The progression from Scenario 1 to Scenario 4 illustrates a clear engineering objective: to improve material recovery efficiency and reduce environmental impacts by integrating more complex and closed-loop systems.

Each iteration enhances the reuse of CO<sub>2</sub> and reduces the load on wastewater treatment, resulting in a more sustainable and resource-efficient process. From an engineering standpoint, the models were developed to progressively reduce the consumption of raw materials and minimize waste, following key LCA principles to optimize environmental performance at each stage of the process.

### **4.3. Life Cycle Impact Assessment (LCIA)**

This is a third stage of life cycle assessment methodology which used of PEF.3.1 frameworks.

EF.3.1 framework has 4 main steps to obtain a reliable and comprehensive result due to Identification of hotspots:

- The most-relevant impact categories
- The most-relevant life-cycle stages
- the most-relevant processes
- the most-relevant elementary flows

There is an important operational difference between most-relevant impact categories, and life-cycle stages on one hand and most-relevant processes, and elementary flows on the other. In particular, most-relevant impact categories and life-cycle stages may be mainly relevant in the context of communicating the results of an EF study. They might serve to highlight environmental areas where the organisation should focus their attention.

Identifying the most-relevant processes and elementary flows is more important for the engineers and designers to identify actions for improving the overall footprint e.g. by-passing or changing a process, further optimising a process, or applying anti-pollution technology. This is particularly relevant for internal studies, to look deeper into how to improve the product's environmental performance. (*European Commission, 2021*).

The procedure that shall be followed to identify the most-relevant impact categories, life-cycle stages, processes, and elementary flows is described in the following table:

*Table 5 European Commission, 2021*

<b>item</b>	<b>At what level does relevance need to be identified?</b>	<b>threshold</b>
Most-relevant impact categories	Single overall score	Impact categories that together contribute to at least 80% of the single overall score.
Most-relevant life-cycle stages	For each most-relevant impact category	All life-cycle stages that together contribute more than 80% to that impact category. If the use stage accounts for more than 50% of the total impact of a most-relevant impact category, the procedure shall be re-run, excluding the use stage.
Most-relevant processes	For each most-relevant impact category	All processes that together contribute (along the entire life cycle) more than 80% to that impact category, considering absolute values
Most-relevant elementary flows	For each most-relevant process considering the most-relevant impact categories	All life-cycle stages that together contribute more than 80% to that impact category. If the use stage accounts for more than 50% of the total impact of a most-relevant impact category, the procedure shall be re-run, excluding the use stage.

The 80% rule states that when identifying the most relevant impact categories, life cycle phases, processes, or flows, any category, phase, or process that contributes more than 80% to the total environmental impact in any given category should be considered a hotspot. The aim of this rule is to focus on the most significant contributors to the environmental footprint, making it easier to prioritize areas for improvement and sustainability interventions. (PEFCR\_guidance.2018)

In this study, we focused solely on interpreting the first two steps.

### **4.3.1. Environmental impact results for each scenario**

After extracting the data from each model in GaBi software, the contribution of individual phases to the total impact for each category, as well as the analysis of the relative contribution of individual phases, is presented in the following tables and graphical charts

Table 6 Result of the first scenario.

IMPACT CATEGORY	TEA-Laurate preparation	Coffee bag-Delamination	Basic solution Washing	NH4OH_production	Separation tank	Municipal wastewater treatment	EU-28: Dodecanoic acid (lauric acid) (estimate) ts	IT: Tap water from groundwater Sphera/total
EF 3.1 Acidification [Mole of H+ eq.]	1.00E-04	1.90E-04	4.43E-05	1.60E-06	4.43E-05	1.86E-05	2.30E-04	1.87E-06
EF 3.1 Climate Change - total [kg CO2 eq.]	8.72E-02	1.66E-01	2.68E-02	4.18E-03	2.68E-02	8.06E-03	3.20E-02	9.92E-04
EF 3.1 Ecotoxicity, freshwater - total [CTUe]	1.72E-01	9.18E-01	3.02E-01	8.24E-03	3.02E-01	2.64E-01	4.85E-02	9.78E-03
EF 3.1 Eutrophication, freshwater [kg P eq.]	9.55E-06	4.48E-07	1.48E-07	2.57E-09	1.48E-07	7.13E-06	3.86E-07	1.35E-07
EF 3.1 Eutrophication, marine [kg N eq.]	8.81E-05	5.27E-05	1.12E-05	2.55E-06	1.12E-05	3.09E-05	4.34E-05	9.55E-07
EF 3.1 Eutrophication, terrestrial [Mole of N eq.]	4.56E-04	5.82E-04	1.23E-04	5.77E-06	1.23E-04	4.52E-05	6.74E-04	4.66E-06
EF 3.1 Human toxicity, cancer - total [CTUh]	1.39E-10	3.24E-11	7.41E-12	2.63E-13	7.41E-12	3.31E-11	7.59E-12	6.49E-13
EF 3.1 Human toxicity, non-cancer - total [CTUh]	6.31E-10	7.90E-10	1.12E-10	1.21E-11	1.12E-10	3.28E-09	2.06E-10	4.54E-11
EF 3.1 Ionising radiation, human health [kBq U235 eq.]	2.62E-03	9.76E-03	3.24E-03	1.01E-04	3.24E-03	1.09E-03	7.41E-05	3.89E-05
EF 3.1 Land Use [Pt]	6.92E-02	7.09E-01	2.36E-01	1.81E-03	2.36E-01	2.02E-02	5.48E+00	1.89E-03
EF 3.1 Ozone depletion [kg CFC-11 eq.]	1.11E-09	1.81E-12	6.04E-13	5.06E-15	6.04E-13	4.26E-14	5.23E-16	5.26E-15
EF 3.1 Particulate matter [Disease incidences]	1.48E-09	1.33E-09	3.08E-10	1.29E-11	3.08E-10	1.41E-10	1.68E-09	3.17E-11
EF 3.1 Photochemical ozone formation, human health [kg NMVOC eq.]	1.46E-04	1.49E-04	2.93E-05	1.60E-06	2.93E-05	1.13E-05	1.33E-04	1.31E-06
EF 3.1 Resource use, fossils [MJ]	1.67E+00	2.42E+00	3.56E-01	5.67E-02	3.56E-01	5.72E-02	1.69E-01	1.31E-02
EF 3.1 Resource use, mineral and metals [kg Sb eq.]	3.55E-07	1.59E-08	5.00E-09	6.12E-11	5.00E-09	3.91E-10	1.16E-07	4.65E-11
EF 3.1 Water use [m³ world equiv.]	2.41E-02	3.41E-02	1.13E-02	1.07E-04	1.13E-02	-4.93E-01	4.40E-03	5.17E-01

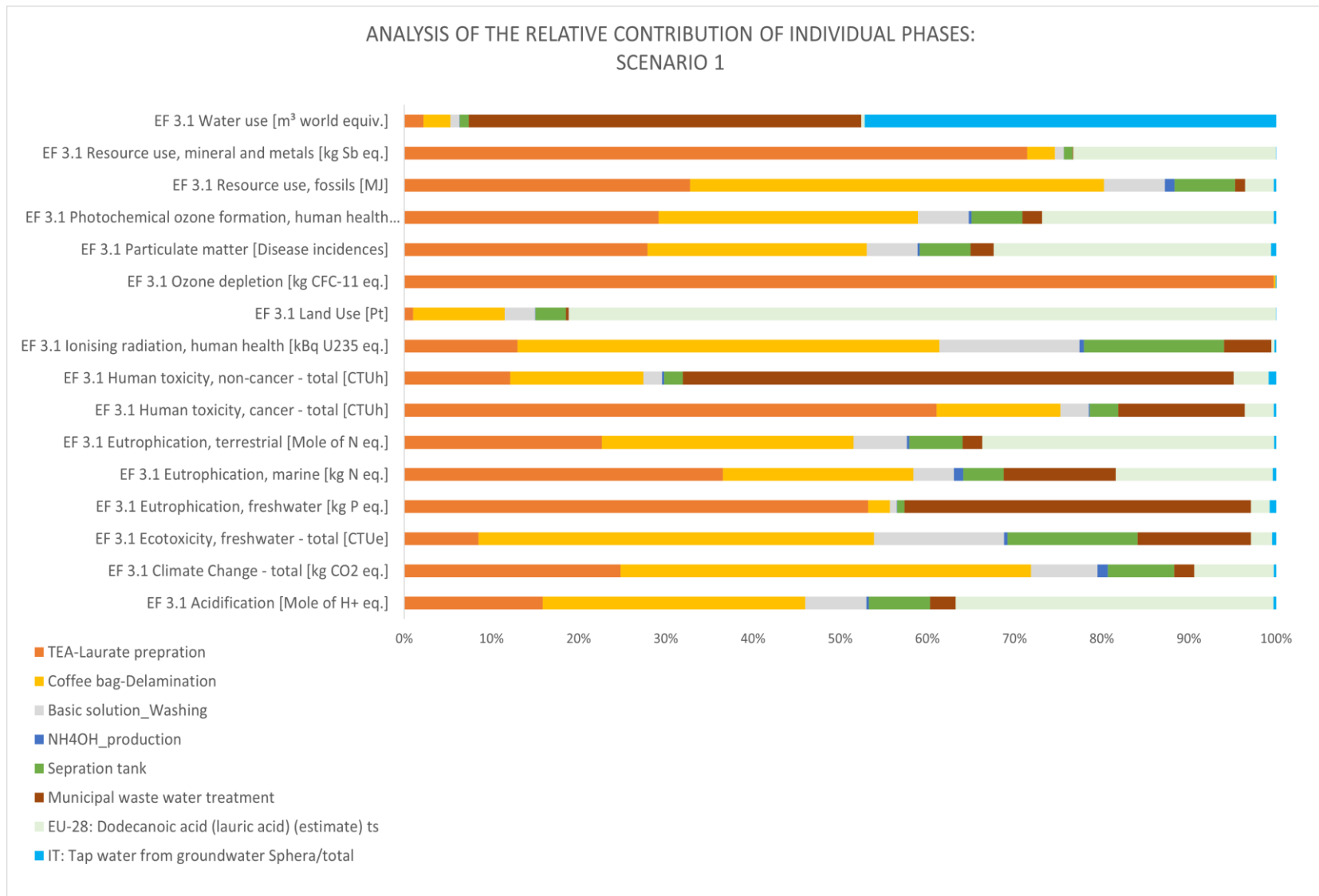


Figure 15 Analysis of the relative contribution of individual phases-scenario one.

Table 7 Results of scenario two

IMPACT CATEGORY	TEA-Laurate preparation	Coffee bag-Delamination	Basic solution_Washing	NH4OH_production	Separation tank	lauric acid recovering / precipitation	RER: carbon dioxide production, liquid ecoinvent 3.9.1/CO2 -1	RER: carbon dioxide production, liquid ecoinvent 3.9.1/CO2 -2	RER: carbon dioxide production, liquid ecoinvent 3.9.1/CO2 -3	Municipal wastewater treatment	EU-28: Dodecanoic acid (lauric acid) (estimate)ts	IT: Tap water from groundwater Sphera/total
EF 3.1 Acidification [Mole of H+ eq.]	1.00E-04	1.90E-04	4.43E-05	1.60E-06	4.43E-05	0.00E+00	3.50E-04	1.41E-04	8.49E-05	1.77E-05	1.82E-04	1.87E-06
EF 3.1 Climate Change - total [kg CO2 eq.]	8.72E-02	1.66E-01	2.68E-02	4.18E-03	2.68E-02	0.00E+00	3.85E-01	1.55E-01	9.33E-02	7.02E-03	2.53E-02	9.92E-04
EF 3.1 Ecotoxicity, freshwater - total [CTUe]	1.72E-01	9.18E-01	3.02E-01	8.24E-03	3.02E-01	0.00E+00	1.05E+00	4.20E-01	2.53E-01	2.80E-01	3.84E-02	9.78E-03
EF 3.1 Eutrophication, freshwater [kg P eq.]	9.55E-06	4.48E-07	1.48E-07	2.57E-09	1.48E-07	0.00E+00	1.12E-04	4.48E-05	2.71E-05	7.67E-06	3.06E-07	1.35E-07
EF 3.1 Eutrophication, marine [kg N eq.]	8.81E-05	5.27E-05	1.12E-05	2.55E-06	1.12E-05	0.00E+00	2.26E-04	9.07E-05	5.47E-05	3.26E-05	3.44E-05	9.55E-07
EF 3.1 Eutrophication, terrestrial [Mole of N eq.]	4.56E-04	5.82E-04	1.23E-04	5.77E-06	1.23E-04	0.00E+00	1.69E-03	6.78E-04	4.09E-04	4.20E-05	5.34E-04	4.66E-06
EF 3.1 Human toxicity, cancer - total [CTUh]	1.39E-10	3.24E-11	7.41E-12	2.63E-13	7.41E-12	0.00E+00	2.62E-10	1.05E-10	6.36E-11	3.53E-11	6.01E-12	6.49E-13
EF 3.1 Human toxicity, non-cancer - total [CTUh]	6.31E-10	7.90E-10	1.12E-10	1.21E-11	1.12E-10	0.00E+00	1.08E-08	4.35E-09	2.62E-09	3.51E-09	1.63E-10	4.54E-11
EF 3.1 Ionising radiation, human health [kBq U235 eq.]	2.62E-03	9.76E-03	3.24E-03	1.01E-04	3.24E-03	0.00E+00	5.46E-02	2.19E-02	1.32E-02	9.09E-04	5.86E-05	3.89E-05
EF 3.1 Land Use [Pt]	6.92E-02	7.09E-01	2.36E-01	1.81E-03	2.36E-01	0.00E+00	9.24E-01	3.71E-01	2.24E-01	1.77E-02	4.33E+00	1.89E-03
EF 3.1 Ozone depletion [kg CFC-11 eq.]	1.11E-09	1.81E-12	6.04E-13	5.06E-15	6.04E-13	0.00E+00	6.01E-09	2.41E-09	1.46E-09	3.69E-14	4.14E-16	5.26E-15
EF 3.1 Particulate matter [Disease incidences]	1.48E-09	1.33E-09	3.08E-10	1.29E-11	3.08E-10	0.00E+00	5.73E-09	2.30E-09	1.39E-09	1.37E-10	1.33E-09	3.17E-11
EF 3.1 Photochemical ozone formation, human health [kg NMVOC eq.]	1.46E-04	1.49E-04	2.93E-05	1.60E-06	2.93E-05	0.00E+00	6.58E-04	2.64E-04	1.59E-04	1.05E-05	1.05E-04	1.31E-06
EF 3.1 Resource use, fossils [MJ]	1.67E+00	2.42E+00	3.56E-01	5.67E-02	3.56E-01	0.00E+00	3.31E+00	1.33E+00	8.01E-01	3.75E-02	1.34E-01	1.31E-02
EF 3.1 Resource use, mineral and metals [kg Sb eq.]	3.55E-07	1.59E-08	5.00E-09	6.12E-11	5.00E-09	0.00E+00	4.39E-06	1.76E-06	1.06E-06	2.48E-10	9.15E-08	4.65E-11
EF 3.1 Water use [m³ world equiv.]	2.41E-02	3.41E-02	1.13E-02	1.07E-04	1.13E-02	0.00E+00	1.25E-01	5.03E-02	3.04E-02	-5.30E-01	3.48E-03	5.17E-01

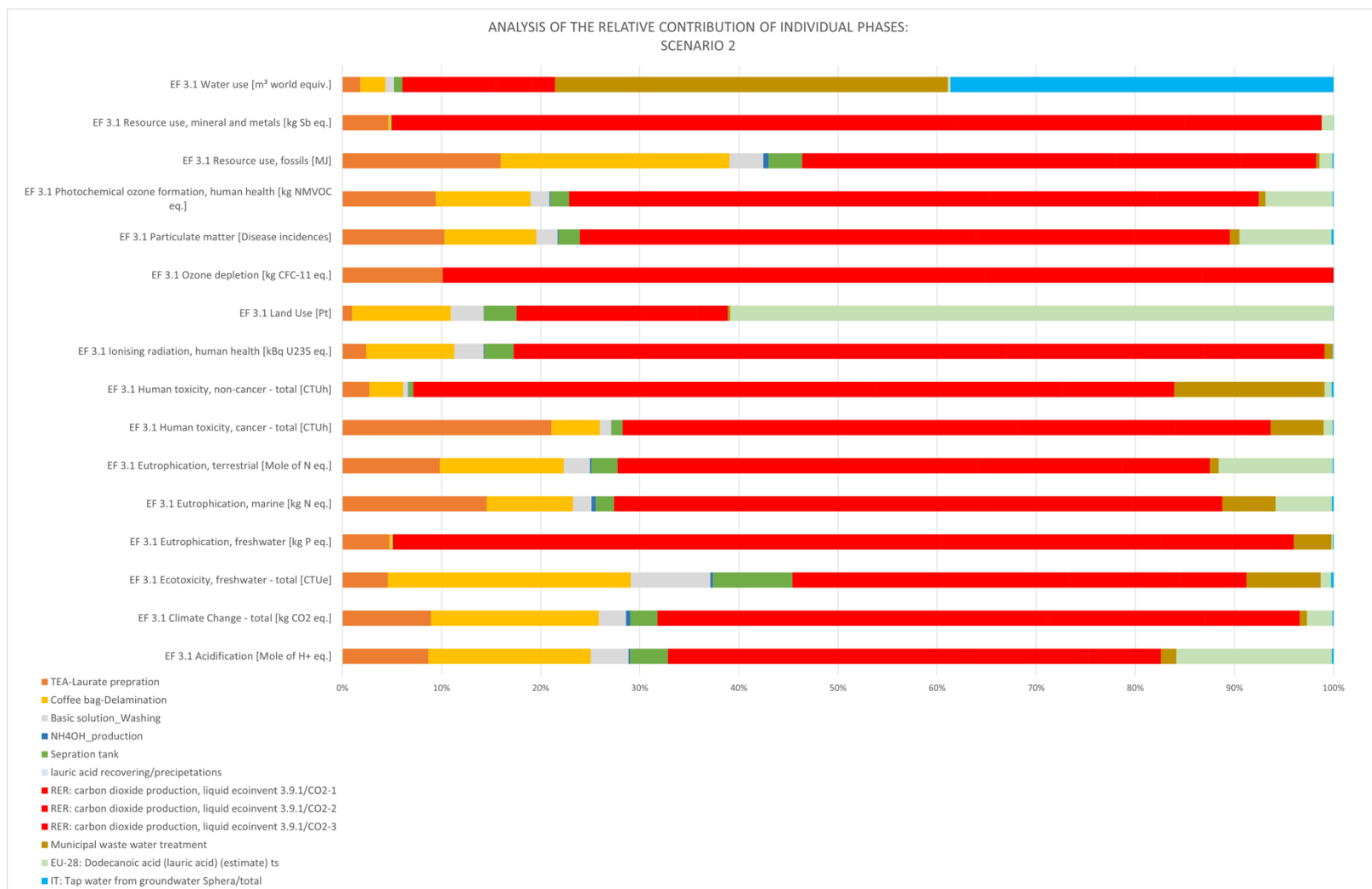


Figure 16 Analysis of the relative contribution of individual phases-scenario two.

Table 8 Results of scenario three

IMPACT CATEGORY	TEA-Laurate preparation	Coffee bag - Delamination	Basic solution Washing	NH4OH production_1	Separation tank	lauric acid recovering / precipitation	CO2 partial recovering	RER: carbon dioxide production, liquid ecoinvent 3.9.1/CO2-1	RER: carbon dioxide production, liquid ecoinvent 3.9.1/CO2-2	RER: carbon dioxide production, liquid ecoinvent 3.9.1/CO2-3	Municipal wastewater treatment	EU-28: Dodecanoic acid (lauric acid) (estimate) ts	IT: Tap water from groundwater Sphera/total
EF 3.1 Acidification [Mole of H+ eq.]	1.00E-04	1.90E-04	4.43E-05	1.60E-06	4.43E-05	0.00E+00	1.24E-04	2.21E-07	1.41E-04	8.49E-05	1.69E-05	1.82E-04	1.87E-06
EF 3.1 Climate Change - total [kg CO2 eq.]	8.72E-02	1.66E-01	2.68E-02	4.18E-03	2.68E-02	0.00E+00	1.20E-01	2.43E-04	1.55E-01	9.33E-02	6.72E-03	2.53E-02	9.92E-04
EF 3.1 Ecotoxicity, freshwater - total [CTUe]	1.72E-01	9.18E-01	3.02E-01	8.24E-03	3.02E-01	0.00E+00	5.15E-01	6.59E-04	4.20E-01	2.53E-01	2.68E-01	3.84E-02	9.78E-03
EF 3.1 Eutrophication, freshwater [kg P eq.]	9.55E-06	4.48E-07	1.48E-07	2.57E-09	1.48E-07	0.00E+00	2.51E-07	7.04E-08	4.48E-05	2.71E-05	7.34E-06	3.06E-07	1.35E-07
EF 3.1 Eutrophication, marine [kg N eq.]	8.81E-05	5.27E-05	1.12E-05	2.55E-06	1.12E-05	0.00E+00	3.55E-05	1.42E-07	9.07E-05	5.47E-05	3.12E-05	3.44E-05	9.55E-07
EF 3.1 Eutrophication, terrestrial [Mole of N eq.]	4.56E-04	5.82E-04	1.23E-04	5.77E-06	1.23E-04	0.00E+00	3.92E-04	1.06E-06	6.78E-04	4.09E-04	4.02E-05	5.34E-04	4.66E-06
EF 3.1 Human toxicity, cancer - total [CTUh]	1.39E-10	3.24E-11	7.41E-12	2.63E-13	7.41E-12	0.00E+00	2.13E-11	1.65E-13	1.05E-10	6.36E-11	3.38E-11	6.01E-12	6.49E-13
EF 3.1 Human toxicity, non-cancer - total [CTUh]	6.31E-10	7.90E-10	1.12E-10	1.21E-11	1.12E-10	0.00E+00	5.87E-10	6.82E-12	4.35E-09	2.62E-09	3.36E-09	1.63E-10	4.54E-11
EF 3.1 Ionising radiation, human health [kBq U235 eq.]	2.62E-03	9.76E-03	3.24E-03	1.01E-04	3.24E-03	0.00E+00	5.43E-03	3.44E-05	2.19E-02	1.32E-02	8.70E-04	5.86E-05	3.89E-05
EF 3.1 Land Use [Pt]	6.92E-02	7.09E-01	2.36E-01	1.81E-03	2.36E-01	0.00E+00	3.95E-01	5.82E-04	3.71E-01	2.24E-01	1.70E-02	4.33E+00	1.89E-03
EF 3.1 Ozone depletion [kg CFC-11 eq.]	1.11E-09	1.81E-12	6.04E-13	5.06E-15	6.04E-13	0.00E+00	1.01E-12	3.79E-12	2.41E-09	1.46E-09	3.53E-14	4.14E-16	5.26E-15
EF 3.1 Particulate matter [Disease incidences]	1.48E-09	1.33E-09	3.08E-10	1.29E-11	3.08E-10	0.00E+00	8.74E-10	3.61E-12	2.30E-09	1.39E-09	1.31E-10	1.33E-09	3.17E-11
EF 3.1 Photochemical ozone formation, human health [kg NMVOC eq.]	1.46E-04	1.49E-04	2.93E-05	1.60E-06	2.93E-05	0.00E+00	1.03E-04	4.15E-07	2.64E-04	1.59E-04	1.01E-05	1.05E-04	1.31E-06
EF 3.1 Resource use, fossils [MJ]	1.67E+00	2.42E+00	3.56E-01	5.67E-02	3.56E-01	0.00E+00	1.79E+00	2.08E-03	1.33E+00	8.01E-01	3.59E-02	1.34E-01	1.31E-02
EF 3.1 Resource use, mineral and metals [kg Sb eq.]	3.55E-07	1.59E-08	5.00E-09	6.12E-11	5.00E-09	0.00E+00	9.10E-09	2.77E-09	1.76E-06	1.06E-06	2.37E-10	9.15E-08	4.65E-11
EF 3.1 Water use [m³ world equiv.]	2.41E-02	3.41E-02	1.13E-02	1.07E-04	1.13E-02	0.00E+00	1.90E-02	7.89E-05	5.03E-02	3.04E-02	-5.08E-01	3.48E-03	5.17E-01

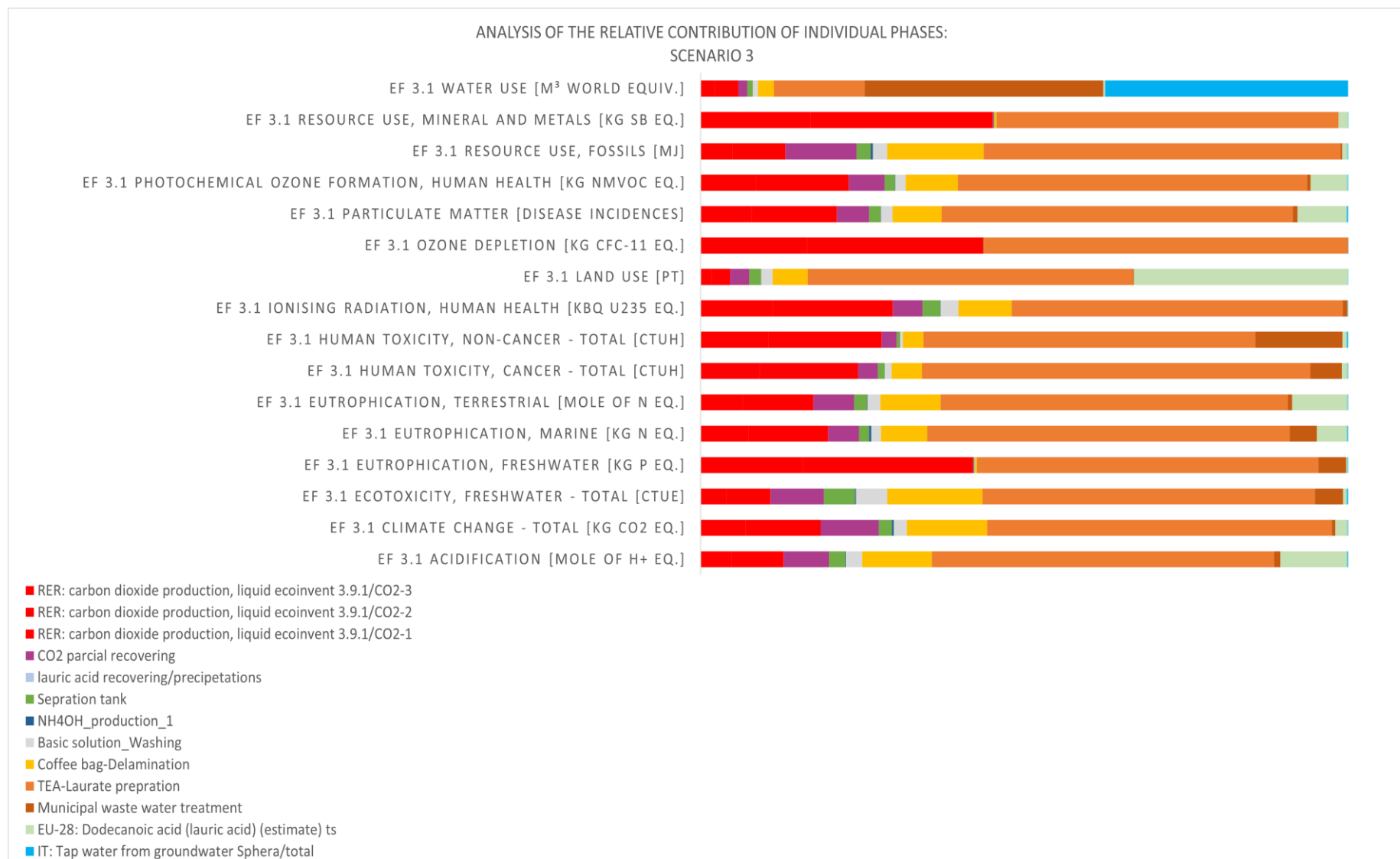


Figure 17 Analysis of the relative contribution of individual phases-scenario three.

Table 9 Result of the scenario four

IMPACT CATEGORY	TEA-Laurate preparation	Coffee bag-Delamination	Basic solution Washing	NH4OH_production_1	Separation tank	lauric acid recovering/precipitation	CO2 recovery 1	CO2 recovery 2	CO2 recovery 3	RER: carbon dioxide production, liquid ecoinvent 3.9.1/CO2-1	RER: carbon dioxide production, liquid ecoinvent 3.9.1/CO2-2	RER: carbon dioxide production, liquid ecoinvent 3.9.1/CO2-3	Municipal waste treatment	EU-28: Dodecanoic acid (lauric acid) (estimates)	IT: Tap water from groundwater Sphera/total
EF 3.1 Acidification [Mole of H+ eq.]	1,00E-04	1,90E-04	4,43E-05	1,55E-06	4,43E-05	0,00E+00	1,24E-04	1,24E-04	1,03E-04	2,21E-07	6,66E-08	1,85E-08	4,31E-06	1,82E-04	4,88E-07
EF 3.1 Climate Change - total [kg CO2 eq.]	8,72E-02	1,66E-01	2,68E-02	4,06E-03	2,68E-02	0,00E+00	1,20E-01	1,35E-01	1,14E-01	2,43E-04	7,33E-05	2,04E-05	1,71E-03	2,53E-02	2,59E-04
EF 3.1 Ecotoxicity, freshwater - total [CTUe]	1,72E-01	9,18E-01	3,02E-01	8,01E-03	3,02E-01	0,00E+00	5,15E-01	4,08E-01	3,15E-01	6,59E-04	1,99E-04	5,53E-05	6,84E-02	3,84E-02	2,55E-03
EF 3.1 Eutrophication, freshwater [kg P eq.]	9,55E-06	4,48E-07	1,48E-07	2,49E-09	1,48E-07	0,00E+00	2,51E-07	1,98E-07	1,53E-07	7,04E-08	2,13E-08	5,90E-09	1,87E-06	3,06E-07	3,52E-08
EF 3.1 Eutrophication, marine [kg N eq.]	8,81E-05	5,27E-05	1,12E-05	2,48E-06	1,12E-05	0,00E+00	3,55E-05	3,70E-05	3,08E-05	1,42E-07	4,30E-08	1,19E-08	7,95E-06	3,44E-05	2,49E-07
EF 3.1 Eutrophication, terrestrial [Mole of N eq.]	4,56E-04	5,82E-04	1,23E-04	5,61E-06	1,23E-04	0,00E+00	3,92E-04	4,09E-04	3,40E-04	1,06E-06	3,21E-07	8,93E-08	1,02E-05	5,34E-04	1,22E-06
EF 3.1 Human toxicity, cancer - total [CTUh]	1,39E-10	3,24E-11	7,41E-12	2,56E-13	7,41E-12	0,00E+00	2,13E-11	2,15E-11	1,78E-11	1,65E-13	4,99E-14	1,39E-14	8,61E-12	6,01E-12	1,69E-13
EF 3.1 Human toxicity, non-cancer - total [CTUh]	6,31E-10	7,90E-10	1,12E-10	1,17E-11	1,12E-10	0,00E+00	5,87E-10	6,78E-10	5,78E-10	6,82E-12	2,06E-12	5,73E-13	8,58E-10	1,63E-10	1,19E-11
EF 3.1 Ionising radiation, human health [kBq U235 eq.]	2,62E-03	9,76E-03	3,24E-03	9,79E-05	3,24E-03	0,00E+00	5,43E-03	4,26E-03	3,27E-03	3,44E-05	1,04E-05	2,89E-06	2,22E-04	5,86E-05	1,01E-05
EF 3.1 Land Use [Pt]	6,92E-02	7,09E-01	2,36E-01	1,76E-03	2,36E-01	0,00E+00	3,95E-01	3,10E-01	2,38E-01	5,82E-04	1,76E-04	4,88E-05	4,33E-03	4,33E+00	4,94E-04
EF 3.1 Ozone depletion [kg CFC-11 eq.]	1,11E-09	1,81E-12	6,04E-13	4,92E-15	6,04E-13	0,00E+00	1,01E-12	7,88E-13	6,06E-13	3,79E-12	1,14E-12	3,18E-13	9,00E-15	4,14E-16	1,37E-15
EF 3.1 Particulate matter [Disease incidences]	1,48E-09	1,33E-09	3,08E-10	1,25E-11	3,08E-10	0,00E+00	8,74E-10	8,80E-10	7,27E-10	3,61E-12	1,09E-12	3,03E-13	3,34E-11	1,33E-09	8,27E-12
EF 3.1 Photochemical ozone formation, human health [kg NMVOC eq.]	1,46E-04	1,49E-04	2,93E-05	1,55E-06	2,93E-05	0,00E+00	1,03E-04	1,10E-04	9,20E-05	4,15E-07	1,25E-07	3,48E-08	2,57E-06	1,05E-04	3,42E-07
EF 3.1 Resource use, fossils [MJ]	1,67E+00	2,42E+00	3,56E-01	5,51E-02	3,56E-01	0,00E+00	1,79E+00	2,05E+00	1,74E+00	2,08E-03	6,29E-04	1,75E-04	9,16E-03	1,34E-01	3,43E-03
EF 3.1 Resource use, mineral and metals [kg Sb eq.]	3,55E-07	1,59E-08	5,00E-09	5,95E-11	5,00E-09	0,00E+00	9,10E-09	7,53E-09	5,89E-09	2,77E-09	8,36E-10	2,32E-10	6,05E-11	9,15E-08	1,22E-11
EF 3.1 Water use [m³ world equiv.]	2,41E-02	3,41E-02	1,13E-02	1,04E-04	1,13E-02	0,00E+00	1,90E-02	1,48E-02	1,14E-02	7,89E-05	2,38E-05	6,62E-06	-1,29E-01	3,48E-03	1,35E-01

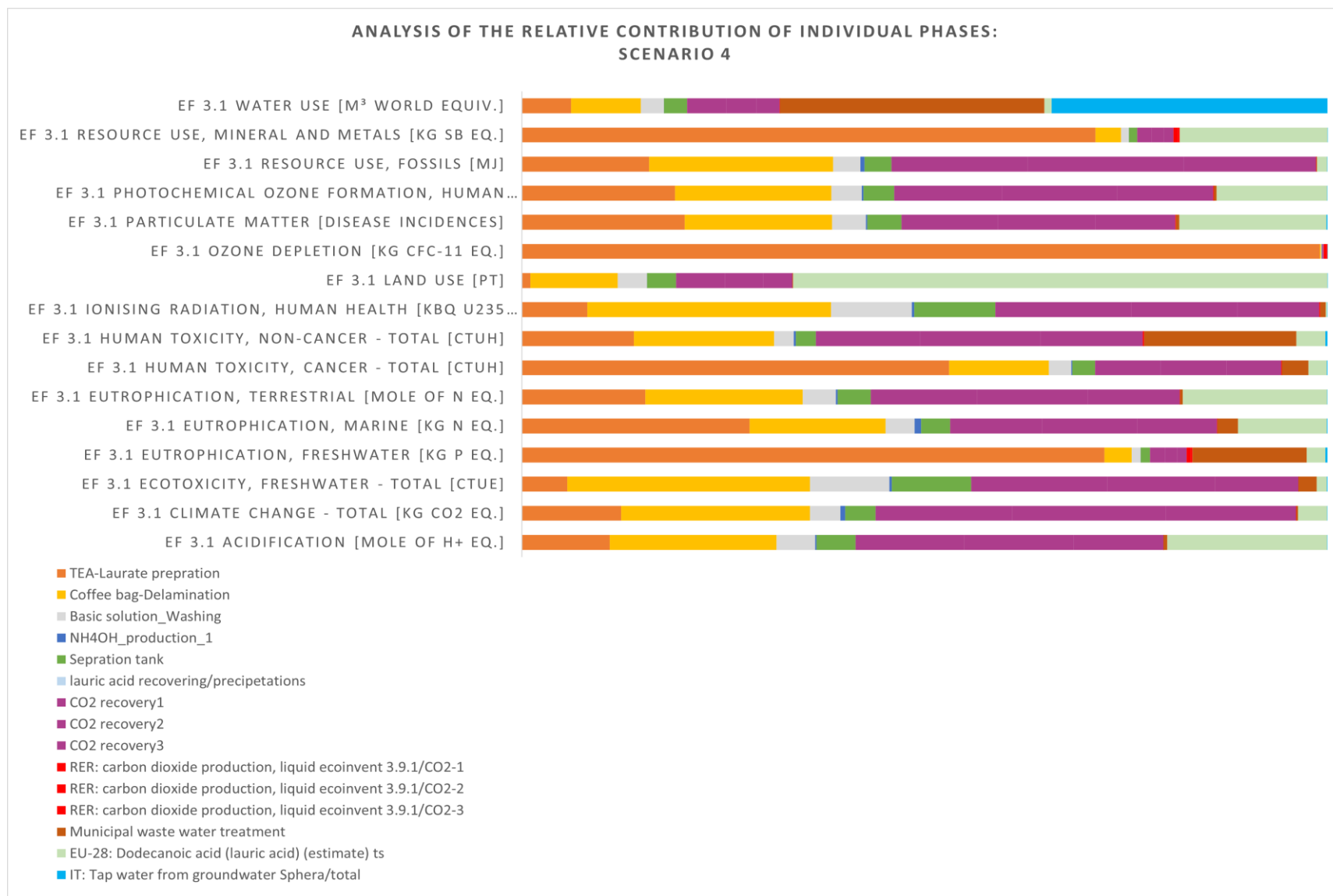


Figure 18 Analysis of the relative contribution of individual phases-scenario four.

### 4.3.2. Graph's Explanation

In Scenario One (Figure 15), the most significant environmental impacts come from the TEA-Laurate preparation phase, which contributes heavily to categories such as ozone depletion (around 98%), as well as mineral and metal resource use, human toxicity (cancer), and eutrophication (freshwater). A large part of this impact is due to the use of lauric acid in this process, which also affects acidification and land use, contributing approximately 40% and 80%, respectively.

The coffee bag delamination phase also plays a major role, particularly impacting fossil resource use, freshwater ecotoxicity, ionizing radiation (human health), and climate change. This is largely due to the consumption of electricity, thermal energy, and water, which are likely major contributors to these impacts. Additionally, municipal wastewater treatment contributes to the environmental impacts, but to a lesser extent. In contrast, phases like  $\text{NH}_4\text{OH}$  production and water-based washing show minimal contributions across all categories.

In the second scenario (Figure 16), the inclusion of the recovery phase plays a prominent role, as previously mentioned. The scenarios become progressively more comprehensive with the addition of this phase, which aims to recover surfactant through the  $\text{CO}_2$  precipitation process, impacting all environmental categories.

The majority of the contributions in this phase are attributed to the three  $\text{CO}_2$  flows, which significantly affect climate change, resource use (mineral and metal), human toxicity, and freshwater eutrophication. This sharp change is due to the upscale in the  $\text{CO}_2$  production process used in the dataset.

Following this, TEA-Laurate preparation and Delamination become the next largest contributors across most impact categories, particularly in resource use (fossil fuels) and human toxicity (cancer).

As the scenarios progress into Scenario Three (Figure 17), additional phases such as  $\text{CO}_2$  recovery are introduced for extracting  $\text{CO}_2$ , which is used to recover lauric acid. This process consumes electricity and thermal energy, impacting resource use (fossil fuels) and climate change. However, the majority of the environmental impact still comes from the carbon dioxide production flows, significantly affecting categories such as resource use (mineral and metal), ozone depletion, and freshwater eutrophication.

As seen in the graph, while CO<sub>2</sub> production remains the dominant contributor, TEA-Laurate preparation is the second largest contributor and has nearly equal impacts across multiple categories. At this stage, the LCA reflects a broader life cycle, with environmental impacts more evenly distributed across various phases. It is important to note that in this scenario, partial CO<sub>2</sub> recovery is implemented, allowing some CO<sub>2</sub> to re-enter the cycle. This results in a more balanced distribution of environmental impacts compared to the previous scenario.

By the time we reach Scenario Four (Figure 18), the life cycle is fully aligned with the inclusion of all relevant phases, making this the most comprehensive representation. In this scenario, the impact categories show a more balanced distribution of contributions across the various phases compared to the previous scenario, reflecting the true complexity of the product's life cycle.

While TEA-Laurate preparation still plays a significant role in some categories like resource use mineral and metal, ozone depletion, and eutrophication freshwater, its dominance is reduced by the growing contributions from phases like CO<sub>2</sub> recovery mostly in resource use fossil and climate change.

The delamination process, alongside TEA-Laurate preparation, also re-emerges and impacts categories such as resource use (fossil fuels), ionizing radiation (human health), eutrophication freshwater, and climate change.

The graph shows that climate change and eutrophication impacts are now more evenly distributed, with each phase contributing a more proportionate share to the overall environmental burden.

This point should be mentioned that in all four scenarios, the consumption of lauric acid impacts the land use category. Additionally, tap water and municipal wastewater treatment play significant roles in the water use impact category. Their effects remain consistent and are equal across all scenarios.

#### **Trends Observed in Environmental Categories:**

- **Resource Use (Minerals and Fossils):**

In the early scenarios, TEA-Laurate preparation overwhelmingly dominates this category, indicating that this phase consumes the most raw materials.

As more phases are added in Scenarios 3 and 4, resource use is better distributed, reflecting the input from other processes like lauric acid recovery and CO<sub>2</sub> production.

- **Climate Change (kg CO<sub>2</sub> eq.):**

Initially, TEA-Laurate preparation and Coffee bag delamination are responsible for a large portion of CO<sub>2</sub> emissions and as a result a large part of climate change. With the inclusion of CO<sub>2</sub> recovery phases in the later scenarios, the total CO<sub>2</sub> impact is shared more evenly, giving a more accurate picture of where emissions are coming from throughout the life cycle.

- **Human Toxicity and Ionizing Radiation:**

These categories show a steady shift in burden as the phases expand. While municipal waste water treatment and TEA-Laurate process contribute notably in Scenario 1 for Human toxicity, the introduction of phases like CO<sub>2</sub> recovery spreads the impact in later scenarios. This suggests that toxic emissions and radiation impacts are more intricately linked to a combination of phases rather than a single dominant phase, as initially implied.

- **Eutrophication (Freshwater, Marine, Terrestrial):**

As the scenarios progress, TEA-Laurate preparation is the dominant contributor to eutrophication in Scenario 1. However, with the introduction of CO<sub>2</sub> recovery in Scenario 2, it quickly overtakes TEA-Laurate, becoming the largest contributor to terrestrial, marine, and freshwater eutrophication. By Scenario 4, CO<sub>2</sub> recovery remains the primary driver of eutrophication impacts.

#### **Final Alignment in Scenario 4**

By Scenario 4, the life cycle is complete, with all relevant phases contributing to the impact categories. This scenario provides the most accurate and comprehensive understanding of the environmental burden, as it includes the full set of processes from resource extraction to end-of-life treatment. The comparison across scenarios shows that Scenario 4, by incorporating CO<sub>2</sub> recovery phases, tap water consumption, and wastewater treatment phases and surfactant preparation, ensures that no single phase disproportionately dominates the environmental profile, reflecting the complex interconnections between phases in the full life cycle.

#### **4.3.3. Applied Normalization in case study**

Different impact categories (e.g., climate change, acidification, eutrophication) have different measurement units and scales. Normalization allows for comparison across these categories by expressing the results relative to a common reference point, such as the global or regional environmental impact per capita. This makes it easier to

understand which impact categories are more or less significant in relation to others. Normalization in LCIA helps translate the raw impact assessment data into meaningful information by providing context and enabling comparisons across different impact categories.

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The following charts are based on normalization factors (EF 2021 Annex 1 - List of EF normalization factors and weighting factors) and show which categories have a higher impact compared to others in each scenario. We should divide the total amount of each impact category by its corresponding normalization factor.

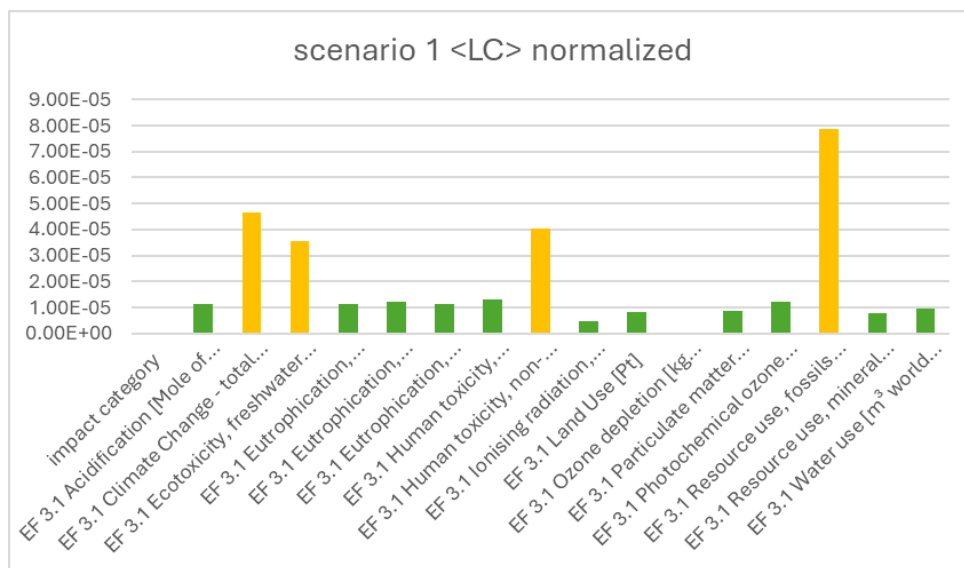


Figure 19 Normalized numbers in impact category-scenario One.

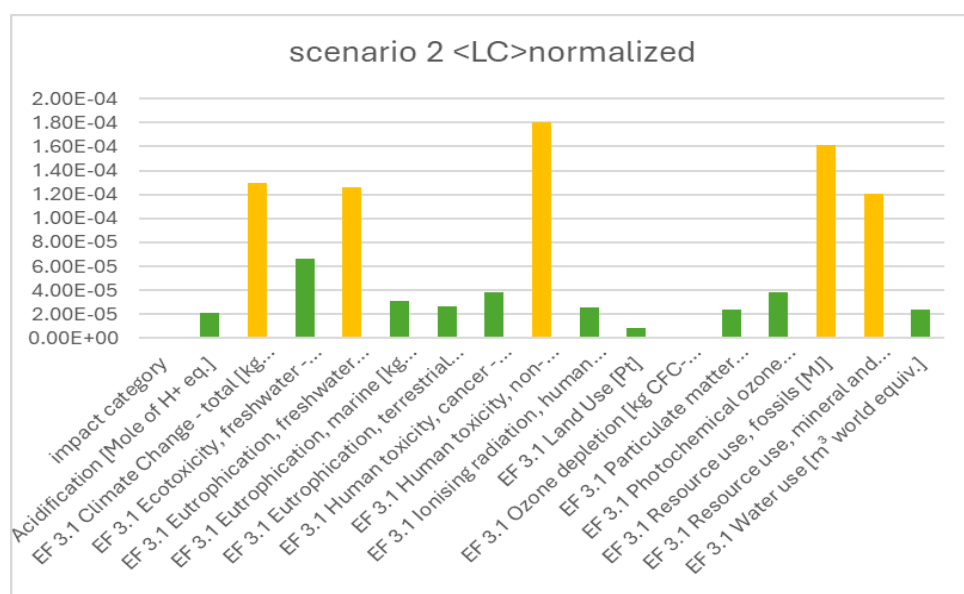


Figure 20 Normalized numbers in impact category-scenario Two.

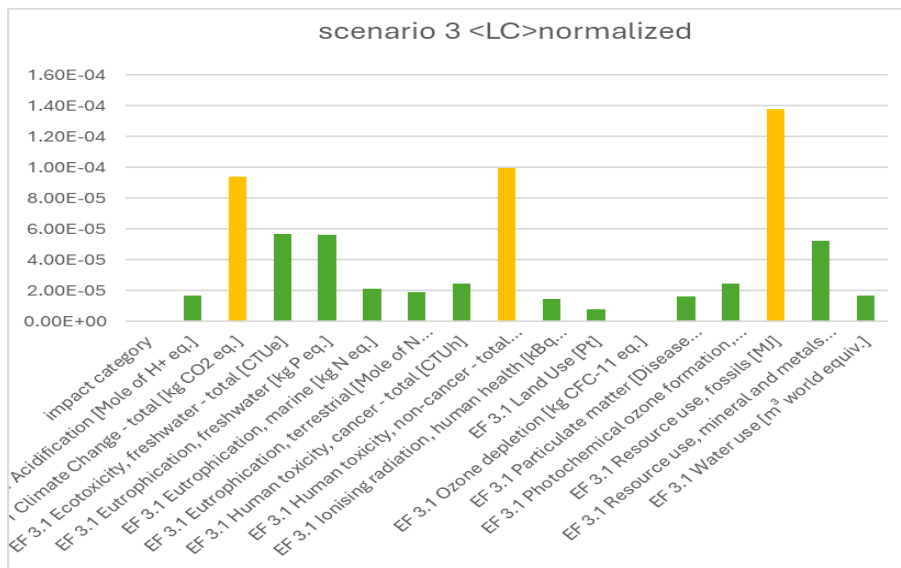


Figure 21 Normalized numbers in impact category-scenario Three.

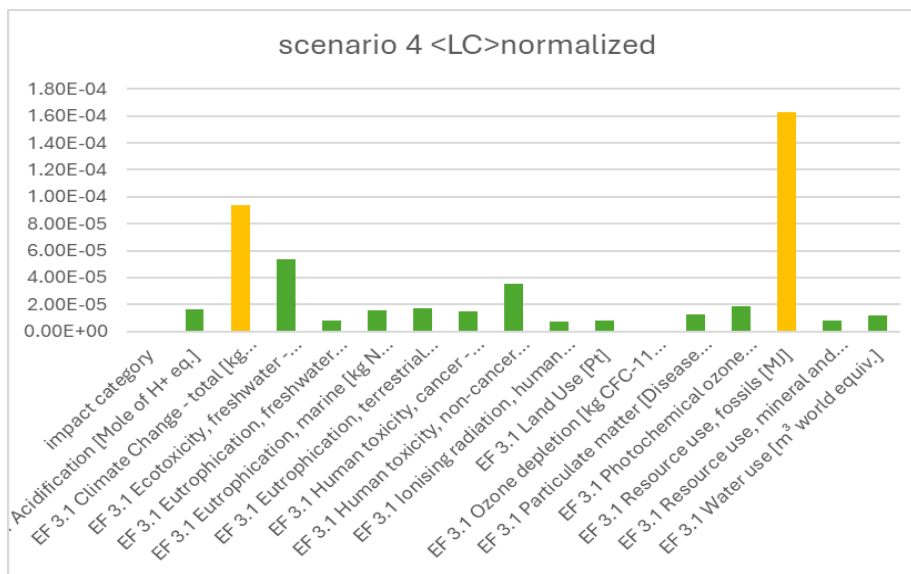


Figure 22 Normalized numbers in impact category-scenario Four.

The normalized bar charts for the four scenarios offer valuable insights into the relative importance of different environmental impact categories by expressing them on a common reference scale. This approach allows us to understand which categories have a greater overall impact on the environment. The environmental impacts of four scenarios are evaluated based on categories such as Resource Use (fossil), Climate Change, Human Toxicity (non-cancer), and Ecotoxicity (freshwater). In figure 19, Scenario 1, the highest impact is seen in Resource Use (fossil) (~8.00E-05), followed by Climate Change (~4.50E-05), Human Toxicity (non-cancer)

(~4.00E-05) and Ecotoxicity freshwater (~3.50E-05). Categories like Ionizing Radiation and Ozone Depletion show minimal impacts. Moving to Scenario 2, figure 20, the largest contributor is Human Toxicity (non-cancer) (1.85E-04), significantly higher than in Scenario 1, indicating greater health risks.

Resource Use (fossil) (1.60E-04) and Climate Change (1.30E-04) also present high values, and Eutrophication, freshwater emerges as a concern.

In Scenario 3, figure 21, the major impact is again Resource Use (fossil) (1.40E-04), with Climate Change (1.00E-04) and Human Toxicity (non-cancer) (~4.00E-05) following.

Finally, Scenario 4, figure 22, exhibits the highest Resource Use (fossil) (1.70E-04), with substantial Climate Change effects (8.00E-05), although impacts on Human Toxicity and Eutrophication are lower compared to other scenarios.

Comparing the four, Scenario 1 shows the lowest overall impacts, particularly in fossil fuel consumption and human toxicity, making it the most environmentally sustainable. In contrast, Scenario 2 has the highest impact across several categories, indicating greater environmental and health risks, especially from toxic substances and climate change. Following in scenario 3 and 4 we can observe obviously this trend related to the former highest impact categories.

In all scenarios, resource use (fossils) emerges as the most significant category, with the highest normalized values, signaling its critical role in the environmental burden. Climate change also shows considerable impacts, though its influence slightly fluctuates across the scenarios. In overall categories such as eutrophication (freshwater), human toxicity (non-cancer), and photochemical ozone formation maintain lower normalized values, indicating they are less pressing environmental concerns in comparison. This normalization process is essential for translating raw impact data into actionable insights, showing which environmental issues should be prioritized. As the scenarios evolve, the charts make it clear that tackling resource use (fossils) and climate change would yield the most substantial environmental benefits, guiding decision-makers on where to focus sustainability efforts.

#### 4.3.4. Applied weighting in the case study

In this part, by multiplying the weighting factor with the normalized value, the weighted result is obtained, indicating which impact category has the greatest significance or effectiveness.

It is important to mention for using these optional steps (normalization and weighting) must be use of the total amount of each impact category for each scenario.

Table 10 weighed data for all scenarios

impact category	Normalized factor	Weighting factor	scenario 1	scenario 2	scenario 3	scenario 4
EF 3.1 Acidification [Mole of H+ eq.]	5,56E+01	0,06200	7,03E-07	1,29E-06	1,04E-06	1,02E-06
EF 3.1 Climate Change - total [kg CO2 eq.]	7,55E+03	0,21060	9,80E-06	2,72E-05	1,98E-05	1,97E-05
EF 3.1 Ecotoxicity, freshwater - total [CTUe]	5,67E+04	0,01920	6,85E-07	1,27E-06	1,09E-06	1,03E-06
EF 3.1 Eutrophication, freshwater [kg P eq.]	1,61E+00	0,02800	3,13E-07	3,52E-06	1,57E-06	2,29E-07
EF 3.1 Eutrophication, marine [kg N eq.]	1,95E+01	0,02960	3,65E-07	9,16E-07	6,26E-07	4,72E-07
EF 3.1 Eutrophication, terrestrial [Mole of N eq.]	1,77E+02	0,03710	4,23E-07	9,75E-07	7,03E-07	6,25E-07
EF 3.1 Human toxicity, cancer - total [CTUh]	1,73E-05	0,02130	2,81E-07	8,15E-07	5,15E-07	3,24E-07
EF 3.1 Human toxicity, non-cancer - total [CTUh]	1,29E-04	0,01840	7,41E-07	3,31E-06	1,83E-06	6,49E-07
EF 3.1 Ionising radiation, human health [kBq U235 eq.]	4,22E+03	0,05010	2,39E-07	1,30E-06	7,19E-07	3,83E-07
EF 3.1 Land Use [Pt]	8,19E+05	0,07940	6,54E-07	6,90E-07	6,39E-07	6,33E-07
EF 3.1 Ozone depletion [kg CFC-11 eq.]	5,23E-02	0,06310	1,34E-09	1,32E-08	6,01E-09	1,34E-09
EF 3.1 Particulate matter [Disease incidences]	5,95E-04	0,08960	7,96E-07	2,16E-06	1,43E-06	1,10E-06
EF 3.1 Photochemical ozone formation, human health [kg NMVOC eq.]	4,09E+01	0,04780	5,86E-07	1,82E-06	1,17E-06	8,99E-07
EF 3.1 Resource use, fossils [MJ]	6,50E+04	0,08320	6,53E-06	1,34E-05	1,15E-05	1,36E-05
EF 3.1 Resource use, mineral and metals [kg Sb eq.]	6,36E-02	0,07550	5,90E-07	9,13E-06	3,93E-06	5,90E-07
EF 3.1 Water use [m <sup>3</sup> world equiv.]	1,15E+04	0,08510	8,09E-07	2,06E-06	1,43E-06	1,00E-06

Based on the numbers in Table 10, we can create graphical charts to compare the four scenarios, highlighting the contribution of different impact categories to the total impact in each scenario:

Contribution of the different impact categories to the total impact for each scenario

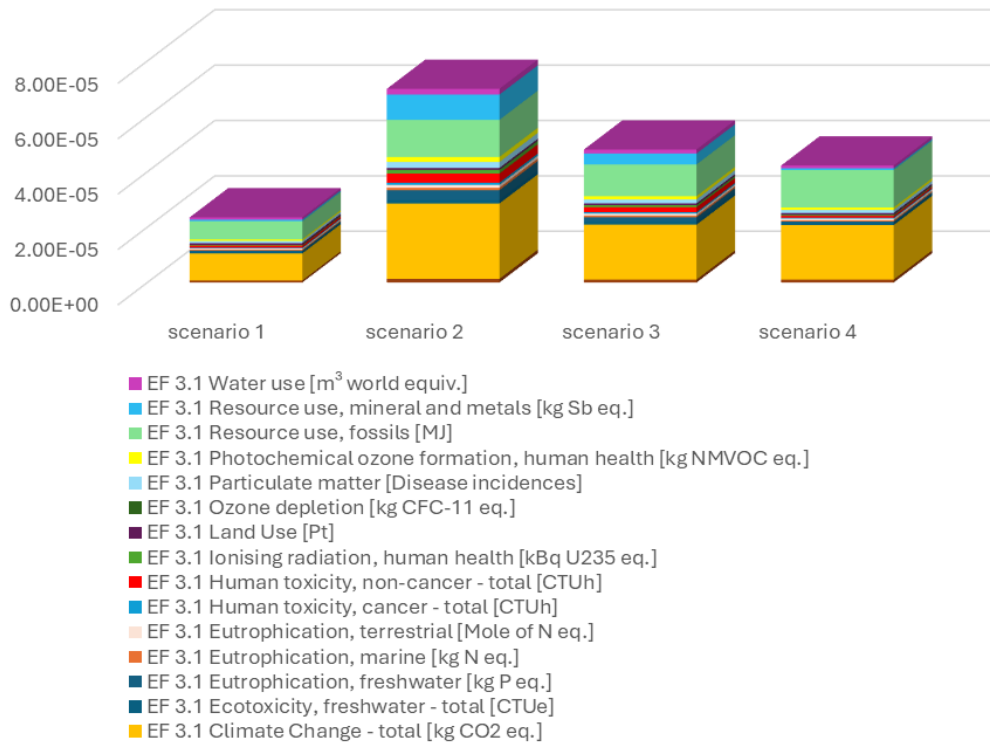


Figure 23 Contribution of the different impact categories to the total impact for each scenario.

The bar chart (figure 23) presents the weighted environmental impacts across four scenarios after applying weighting factors to normalized impact categories, providing a clearer understanding of which environmental aspects are most significant.

Each bar represents the total environmental burden of a scenario, broken down into individual categories such as climate change, resource use (fossils), water use, and eutrophication and etc.

In Scenario 1, the overall environmental impact is the lowest, with relatively balanced contributions across categories with playing the main role of climate change and resource use (fossils), However the total impact increases significantly in Scenario 2, which shows the highest overall burden. This is primarily due to larger contributions from climate change and resource use (fossils), indicating that these categories are driving the environmental footprint in this scenario. What has changed

is the surfactant recovery part that has been added to the scenario 2 which make it very impactful.

Scenario 3 demonstrates a reduction in total impact compared to Scenario 2, although the key contributors—such as climate change and resource use (fossils)—remain significant. This suggests that some improvements or optimizations have been implemented. That would be partial CO<sub>2</sub> recovery has been introduced for one of the precipitation processes after obtaining recovered lauric acid, thereby reducing the overall environmental burden.

Finally, Scenario 4 presents a further reduction in impact, with a total value similar to Scenario 1. The environmental impacts in this scenario are more evenly distributed except 2 main indicators that mentioned before.

In an overall view, the chart highlights the progression of environmental impacts across the scenarios. Scenario 2 represents the highest burden, while Scenario 4 showcases a more sustainable and optimized life cycle compared to Scenarios 2 and 3. However, despite being a more complete cycle, Scenario 4 still has a greater environmental impact than Scenario 1. This outcome is not what we expected, indicating the importance of how we design the recovery processes, the choice of energy sources, and the source of carbon dioxide involved. These factors play a crucial role in minimizing environmental impacts

#### **4.3.5. Hotspot analysis: most-relevant impact categories**

Due to apply the main steps of Analyzing in our applied methods we should go for first obtaining the most-relevant impact categories. The most relevant impact category method is based on weighted results. It involves considering only those categories that when added together, starting with the one with the largest contribution at least 80 percent to the overall impact of the method (EC, 2021).

This table shows Percentage contributions of the different impact categories to the different scenarios:

Table 11 the most relevant impact categories percentages.

Impact Category	Scenario 1	Scenario 2	Scenario 3	Scenario 4
EF 3.1 Acidification [Mole of H+ eq]	3.0%	1.8%	2.2%	2.4%
EF 3.1 Climate Change - total [kg CO2 eq.]	41.7%	39.0%	41.3%	46.7%
EF 3.1 Ecotoxicity, freshwater - total [CTUe]	2.9%	1.8%	2.3%	2.4%
EF 3.1 Eutrophication, freshwater [kg P eq.]	1.3%	5.0%	3.3%	0.5%
EF 3.1 Eutrophication, marine [kg N eq.]	1.6%	1.3%	1.3%	1.4%
EF 3.1 Eutrophication, terrestrial [Mole of N eq.]	1.8%	1.4%	1.5%	1.5%
EF 3.1 Human toxicity, cancer - total [CTUh]	1.2%	1.2%	1.1%	0.8%
EF 3.1 Human toxicity, non-cancer - total [CTUh]	3.2%	4.7%	3.8%	1.5%
EF 3.1 Ionising radiation, human health [kBq U235 eq.]	1.0%	1.9%	1.5%	0.9%
EF 3.1 Land Use [Pt]	2.8%	1.0%	1.3%	1.5%
EF 3.1 Ozone depletion [kg CFC-11 eq.]	0.0%	0.0%	0.0%	0.1%
EF 3.1 Particulate matter [Disease incidences]	3.4%	3.1%	3.0%	2.6%
EF 3.1 Photochemical ozone formation, human health [kg NMVOC eq.]	2.5%	2.6%	2.4%	2.1%
EF 3.1 Resource use, fossils [MJ]	27.8%	19.2%	23.9%	32.1%
EF 3.1 Resource use, mineral and metals [kg Sb eq.]	2.5%	13.1%	13.2%	1.4%
EF 3.1 Water use [m <sup>3</sup> world equiv.]	3.4%	2.9%	3.0%	2.4%
Sum of the most relevant impact	82.4%	81.0%	80.5%	81.4%

As illustrated, applying the 80% rule allows us to sum the percentages of the most relevant impact categories, which together account for the majority of the environmental burden. A graphical representation has been provided in the following figure to facilitate easier comparison between the scenarios, highlighting how the most impactful categories contribute across different phases of the life cycle.

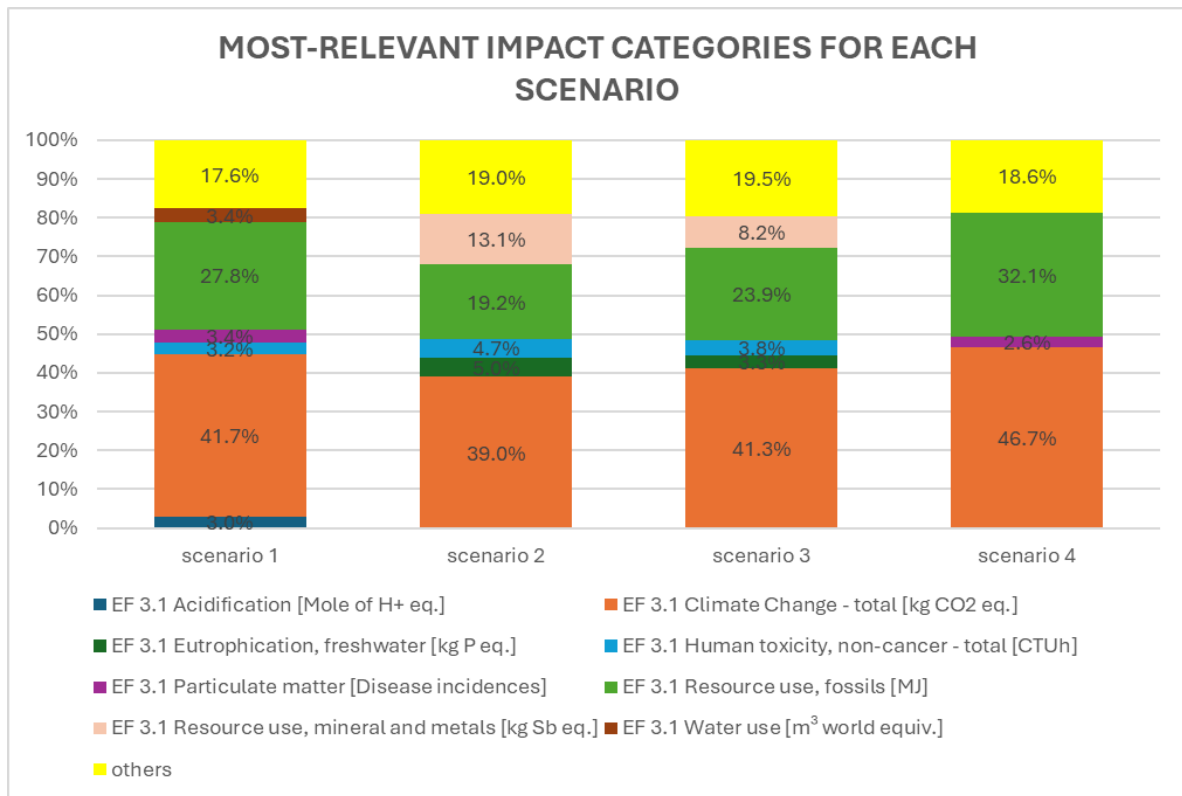


Figure 24 the most relevant impact categories contribution.

Table 12 the most relevant impact categories for each scenario.

Scenario One	Scenario Two
EF 3.1 Acidification (Mole of H+ eq.)	EF 3.1 Climate Change - total [kg CO2 eq.]
EF 3.1 Climate Change - total [kg CO2 eq.]	EF 3.1 Eutrophication, freshwater [kg P eq.] (5%)
EF 3.1 Human toxicity, non-cancer - total [CTUh]	EF 3.1 Human toxicity, non-cancer - total [CTUh]
EF 3.1 Particulate matter [Disease incidences]	EF 3.1 Resource use, fossils [MJ]
EF 3.1 Resource use, fossils [MJ]	EF 3.1 Resource use, mineral and metals [kg Sb eq.]
EF 3.1 Water use [m³ world equiv.]	
Scenario Three	Scenario Four
EF 3.1 Climate Change - total [kg CO2 eq.]	EF 3.1 Climate Change - total [kg CO2 eq.]
EF 3.1 Eutrophication, freshwater [kg P eq.] (5%)	EF 3.1 Particulate matter [Disease incidences]
EF 3.1 Human toxicity, non-cancer - total [CTUh]	EF 3.1 Resource use, fossils [MJ]
EF 3.1 Resource use, fossils [MJ]	EF 3.1 Resource use, mineral and metals

According to the PEF method, the most-relevant life cycle stages are those that together contribute more than 80% to any of the most relevant impact categories identified (EC, 2021). This approach helps prioritize the categories with the greatest significance, ensuring that efforts are focused on the most impactful areas.

As illustrated in the table and bar chart (table12) and (figure 24), climate change emerges as the dominant impact category across all four scenarios.

In Scenario 1, climate change accounts for 41.7% of the total environmental impact, followed by resource use (fossils) at 27.8%, with other categories like eutrophication, acidification, human toxicity (non-cancer), water use, and particulate matter contributing smaller, evenly distributed percentages.

In Scenario 2, climate change (39%) and resource use (fossils) (19.2%) still have the highest contributions, followed by resource use (mineral and metals), which increases to about 13%. Eutrophication and human toxicity remain smaller contributors. It's worth noting that the percentages for climate change and resource use (fossils) decrease slightly, while the sharp rise in resource use (mineral and metals) is likely due to the impact of CO<sub>2</sub> usage in this stage.

In Scenario 3, climate change and resource use continue to play the most impactful roles, with a slight increase in their contributions. The other impact categories show no notable changes compared to Scenario 2. This indicates that, from the perspective of the most relevant impact categories, Scenarios 2 and 3 are in a similar situation.

In Scenario 4, the results largely mirror those of the previous scenarios, but with notable differences in the distribution of environmental impacts. The contribution of climate change reaches 46.7%, and resource use (fossils) rises to 32.1%, marking the highest values across all scenarios. Additionally, particulate matter contributes 2.6%, which is the only other category with a noticeable impact in this scenario.

These results indicate that as the scenarios progress, the environmental impacts become increasingly concentrated in two key categories: climate change and resource use (fossils). The dominance of these two categories suggests that the life cycle is heavily influenced by processes that emit significant levels of CO<sub>2</sub> and rely on fossil resources.

This concentration also highlights a potential oversight in the system design, as other impact categories such as eutrophication, acidification, and human toxicity have gradually diminished in significance, despite being critical for a more comprehensive assessment of environmental sustainability. The increasing focus on climate change and fossil resource use underscores the importance of addressing energy sources and carbon management to minimize the overall environmental burden, while ensuring that impacts in other categories are not neglected.

### **4.3.6. Hotspot analysis: most-relevant stages**

First, we need to define the stages from the phases involved in each scenario. For this purpose, I have identified 5 main stages, which include:

- Surfactant preparation
- Delamination stage
- Washing stage
- Recovery stage
- Wastewater treatment stage

It is important to note that each scenario will gradually become more complex, and as a result, the number of stages will increase with each subsequent scenario. To avoid repetition, I will only describe the most complex scenario which is number four.

The surfactant stage involves only one process, which is the preparation of TEA-Laurate. The next stage is the Delamination stage, which includes the processes for EU-28: Dodecanoic acid (lauric acid) (estimate) and the delamination of coffee bags. Additionally, there is a washing stage, which consists of all processes involving the washing of coffee bag residues with water or a basic solution, such as NH<sub>4</sub>OH production, IT: Tap Water from Groundwater Sphera/total, and the Separation Tank. The recovery stage includes all processes related to the recovery of lauric acid and CO<sub>2</sub>. Finally, the wastewater treatment stage involves only municipal wastewater treatment.

The following bar charts were generated by focusing on the most relevant impact categories in each scenario, assessing the contribution of the most relevant stages in them. These charts provide a clear visual comparison, helping to identify which stages are the most significant contributors to environmental impacts across the different scenarios:

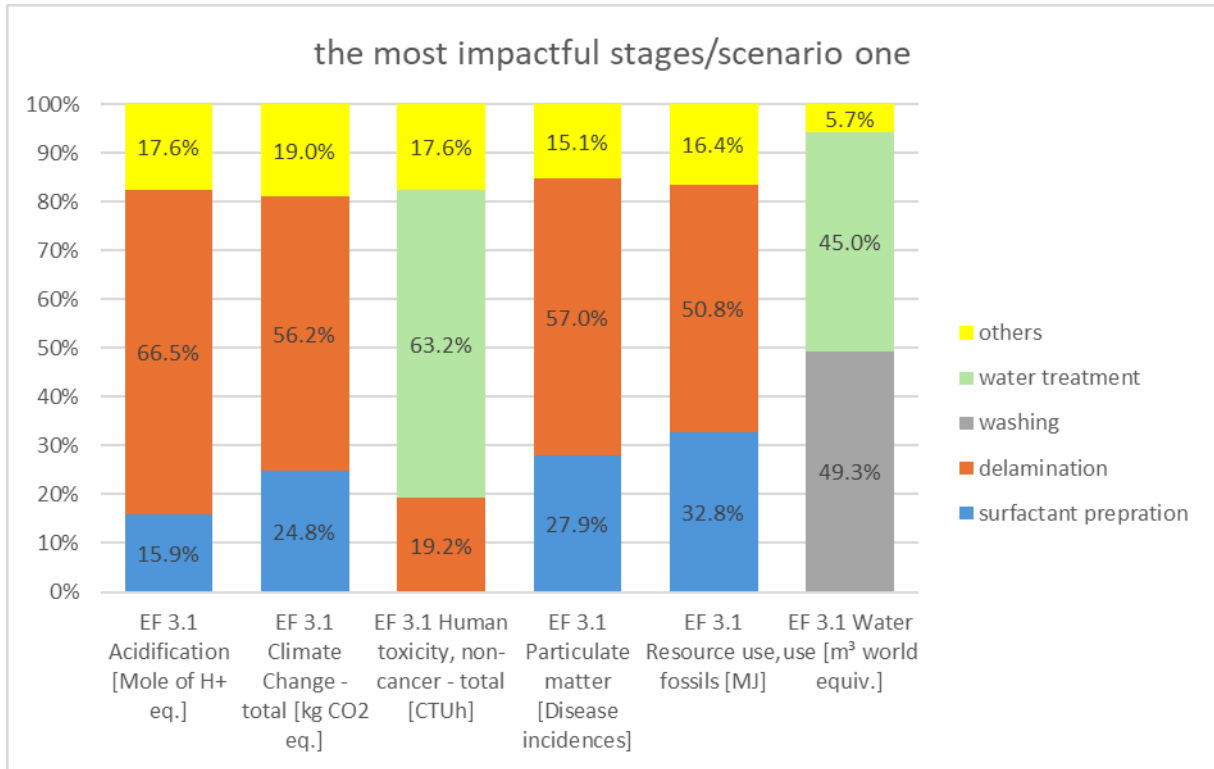


Figure 25 the most impactful stages-scenario One.

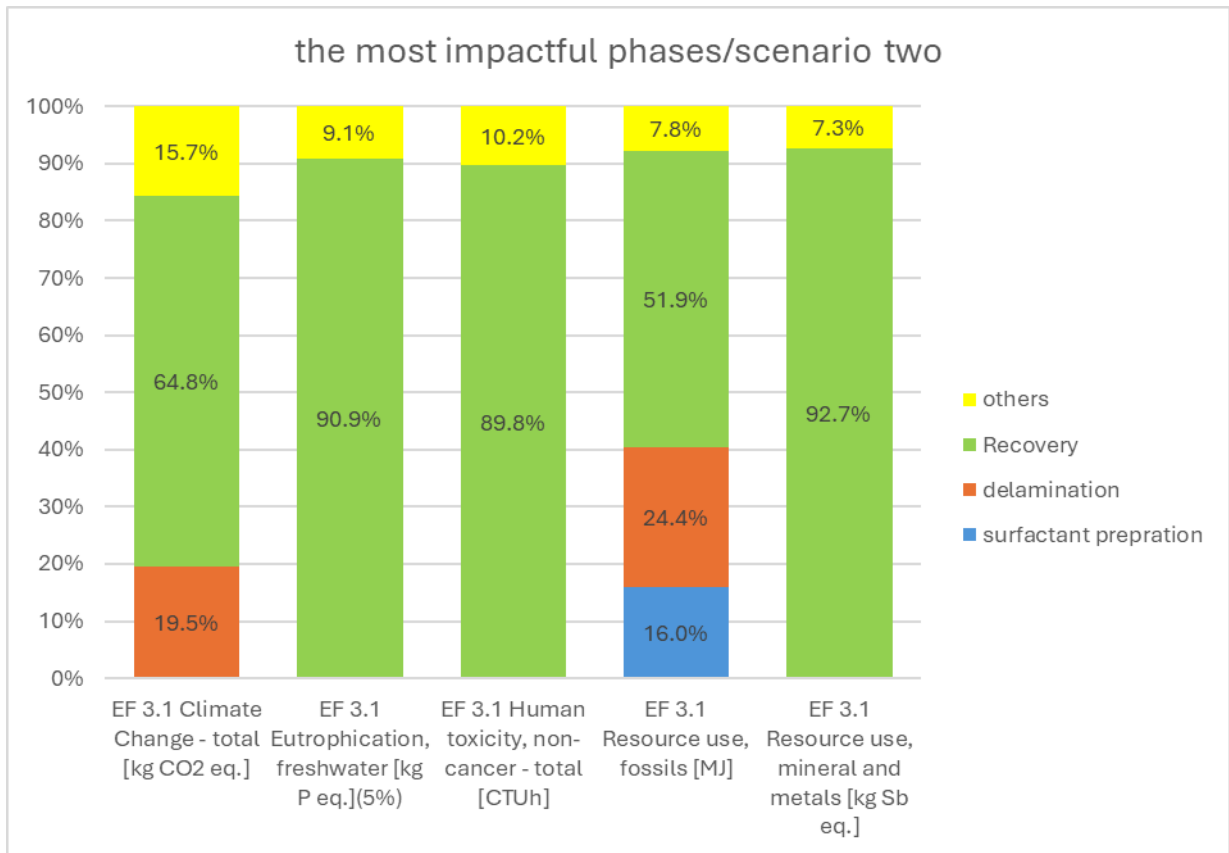


Figure 26 the most impactful stages-scenario Two.

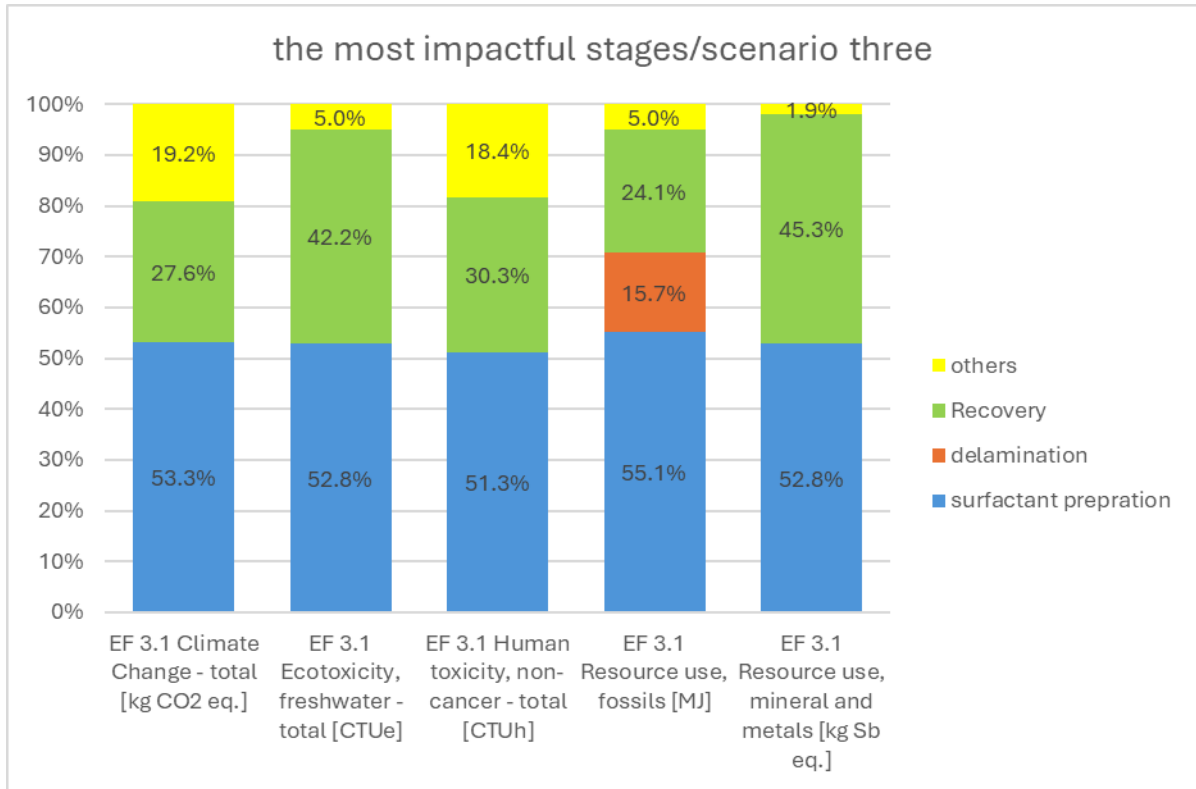


Figure 27 the most impactful stages-scenario Three.

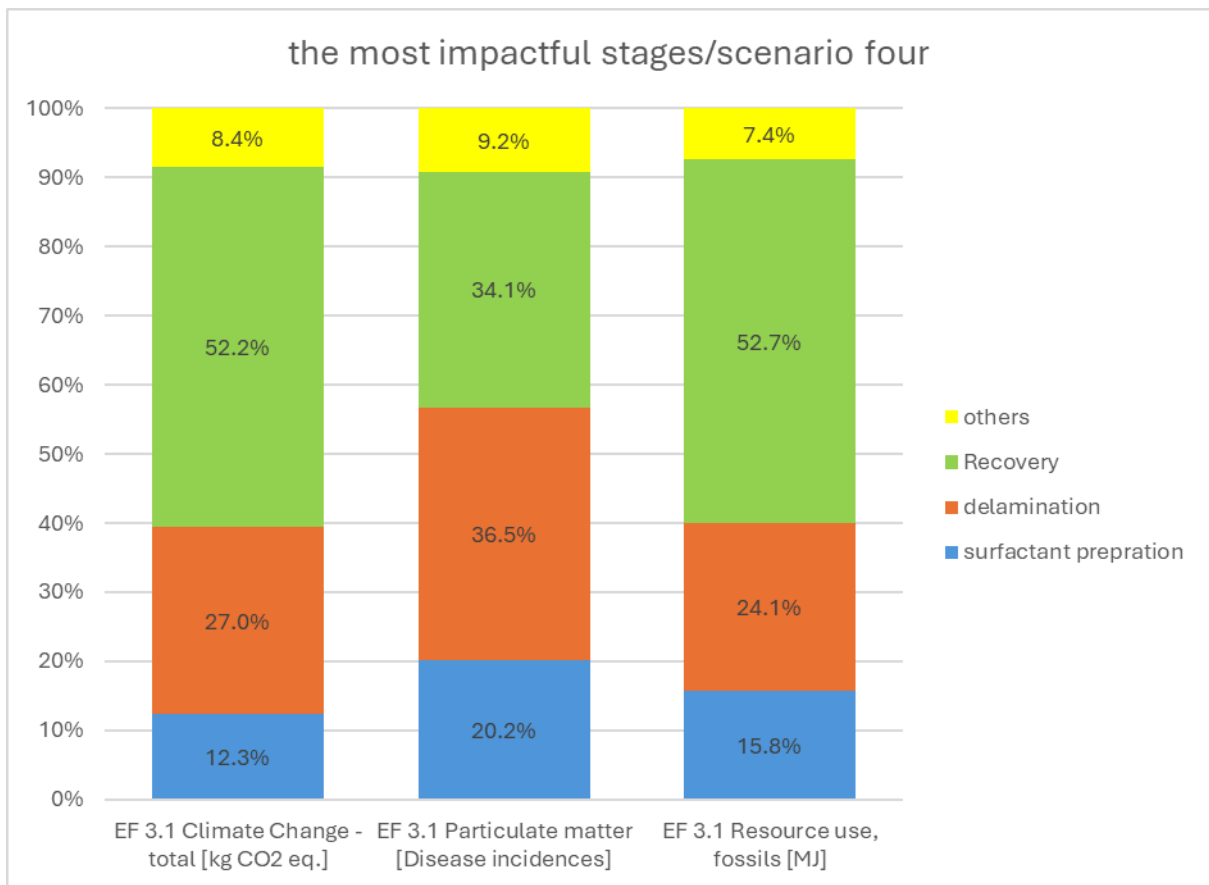


Figure 28 the most impactful stages-scenario Four.

The hotspot analysis for the four scenarios (figures 25-28) focuses on identifying the most-relevant life cycle stages that contribute significantly to the environmental impact categories established in the earlier phases of the study.

These stages—surfactant preparation, delamination, washing, recovery, and wastewater treatment—are analyzed to determine their respective contributions to key environmental categories such as climate change, resource use (fossils), human toxicity, and eutrophication.

As the scenarios become progressively more complex, with additional stages and processes being introduced, the relative contribution of each stage shifts, revealing important insights into the areas that most affect the overall environmental footprint.

The graph shows that delamination is the most impactful stage in Scenario 1, contributing significantly to acidification (66.5%), climate change (56.2%), and particulate matter formation (57%), primarily due to its high energy use.

Surfactant preparation also has notable impacts, especially on climate change (24.8%) and resource use (32.8%), driven by the production of chemicals like TEA-laurate.

Water treatment dominates human toxicity (63.2%) and water use (45%), highlighting the resource-intensive nature of cleaning processes. And Washing plays a major role in water use (49.3%). Overall, the major environmental hotspots are delamination and surfactant preparation while water management is critical for reducing impacts on toxicity and water use.

As the system expands in Scenario 2, its graph shows that Recovery is the most significant contributor across all categories, particularly for eutrophication (90.9%) and human toxicity (89.8%), indicating high environmental burdens from this phase.

Climate change impacts are primarily driven by recovery (64.8%) but also see notable contributions from delamination (19.5%).

Resource use (fossils) shows that percentages of recovery (51.9%), delamination (24.4%), and surfactant preparation (16%), suggesting that these phases especially Recovery stage heavily rely on fossil fuels.

For resource use (minerals and metals), recovery dominates (92.7%), implying the extensive use of materials in recovery processes, additionally the graph highlights recovery as the critical phase needing improvement to reduce environmental impacts, especially in toxicity, resource consumption, and climate change.

As well as there are some evidences pointing out that while there is no direct energy consumption for CO<sub>2</sub> precipitation in Scenario 2, the environmental impact seen in the graph is largely due to the source of the CO<sub>2</sub> used. The liquid CO<sub>2</sub> comes from waste gas streams, which, as indicated by the Ecoinvent dataset, involves significant upstream processes such as CO<sub>2</sub> extraction using Monoethanolamine (MEA) solutions to capture CO<sub>2</sub> from industrial waste gases and Purification and liquefaction of CO<sub>2</sub>, both of which require electricity as the energy source.

Material and energy inputs, water consumption, and infrastructure associated with these processes contribute to the overall environmental burden.

Thus, while the precipitation process itself doesn't consume energy, the production of liquid CO<sub>2</sub> used in the process contributes to environmental impacts in categories like climate change and resource use. The electricity needed for CO<sub>2</sub> extraction, purification, and liquefaction explains the relatively higher impacts seen for recovery in Scenario 2. These upstream processes are responsible for the increase in climate change (CO<sub>2</sub> emissions), resource depletion, and eutrophication, as reflected in the graph. Therefore, the percentages related to recovery are linked to the indirect impacts of sourcing and processing the liquid CO<sub>2</sub>, not just the precipitation stage.

The graph for Scenario 3 illustrates Surfactant preparation is consistently the largest contributor across all categories, accounting for over half of the impacts in climate change (53.3%), resource use fossil (55.1%), and resource use in mineral metal (52.8%). This indicates that the production of chemicals like TEA-laurate remains highly energy- and resource-intensive.

Recovery has a significant impact, particularly in categories like human toxicity (non-cancer) (30.3%) and freshwater ecotoxicity (42.2%), as we mentioned in scenario 2 showing that chemical recovery processes introduce substantial environmental burdens. The delamination phase while less impactful overall, contributes 15.7% to fossil resource use, reflecting the energy demand during material separation.

In this scenario the introduction of partial CO<sub>2</sub> recovery marks a significant development compared to Scenario 2. This new process allows some of the CO<sub>2</sub> used to be recovered and cycled back, reducing the need for fresh CO<sub>2</sub> inputs. As seen in the graph, surfactant preparation remains the dominant environmental hotspot across, but the inclusion of CO<sub>2</sub> recovery in Scenario 3 helps shift some impacts to the recovery phase which are mentioned already.

When comparing to Scenario 2, where CO<sub>2</sub> recovery was not present, Scenario 3 achieves better material efficiency by recycling CO<sub>2</sub>, thereby lowering the demand for fresh resources

Other impacts remain minor but still contribute noticeably to climate change (19.2%). Scenario 3 shows that surfactant preparation and recovery are key environmental hotspots, requiring attention to reduce the system's overall footprint.

By the time we reach Scenario 4, the recovery stage becomes the most dominant contributor across multiple environmental categories, marking a shift from earlier scenarios. For instance, recovery accounts for 52.2% of the impact in climate change, 52.7% in resource use (fossils), and 34.1% in particulate matter, reflecting the heavy reliance on the recovery of Lauric Acid and CO<sub>2</sub>. This shows how resource recovery, as the system becomes more optimized, plays a central role in reducing the overall environmental footprint.

In Scenario 4, while recovery emerges as key, delamination still makes substantial contributions, particularly in particulate matter formation (36.5%) and fossil resource use (24.1%). This indicates that material separation processes remain energy-intensive and environmentally significant even in this more complex and circular setup. Interestingly, surfactant preparation plays a reduced role compared to earlier scenarios, which suggests that its environmental impacts have been somewhat mitigated, likely due to improvements in resource efficiency and recovery processes. Finally, wastewater treatment continues to have the smallest impact across all categories, reinforcing that it does not significantly drive the overall environmental burden.

Scenario four highlights the importance of **recovery optimization** but also underscores that challenges remain in delamination and resource use, despite the improvements achieved.

And also, I create a comparing table and chart regarding the most relevant stages due to better understanding their differences together:

Table 13 comparing the most relevant stages for all scenarios.

	stages					sum of 80%
	surfactant prepration	delamination	washing	recovery	water treatment	
<b>scenario one</b>						
EF 3.1 Acidification [Mole of H+ eq.]	15,9%	66,5%	14,6%	-	2,9%	82,4%
EF 3.1 Climate Change - total [kg CO2 eq.]	24,8%	56,2%	16,7%	-	2,3%	81,0%
EF 3.1 Human toxicity, non-cancer - total [CTUh]	12,2%	19,2%	5,4%	-	63,2%	82,4%
EF 3.1 Particulate matter [Disease incidences]	27,9%	57,0%	12,5%	-	2,7%	84,9%
EF 3.1 Resource use, fossils [MJ]	32,8%	50,8%	15,3%	-	1,1%	83,6%
EF 3.1 Water use [m³ world equiv.]	2,2%	3,5%	49,3%	-	45,0%	94,3%
<b>scenario two</b>						
EF 3.1 Climate Change - total [kg CO2 eq.]	8,9%	19,5%	6,0%	64,8%	0,7%	84,3%
EF 3.1 Eutrophication, freshwater [kg P eq.](5%)	0,0%	0,0%	13,8%	74,1%	12,1%	87,9%
EF 3.1 Human toxicity, non-cancer - total [CTUh]	0,0%	0,0%	0,1%	95,8%	4,0%	95,9%
EF 3.1 Resource use, fossils [MJ]	16,0%	24,4%	7,5%	51,9%	0,4%	92,2%
EF 3.1 Resource use, mineral and metals [kg Sb eq.]	4,6%	1,4%	0,1%	93,8%	0,0%	93,8%
<b>scenario three</b>						
EF 3.1 Climate Change - total [kg CO2 eq.]	53,3%	14,3%	4,4%	27,6%	0,5%	80,8%
EF 3.1 Eutrophication, freshwater [kg P eq.](5%)	52,8%	0,4%	0,3%	42,2%	4,3%	95,0%
EF 3.1 Human toxicity, non-cancer - total [CTUh]	51,3%	3,8%	1,1%	30,3%	13,5%	81,6%
EF 3.1 Resource use, fossils [MJ]	55,1%	15,7%	4,8%	24,1%	0,2%	95,0%
EF 3.1 Resource use, mineral and metals [kg Sb eq.]	52,8%	1,7%	0,2%	45,3%	0,0%	98,1%
<b>scenario four</b>						
EF 3.1 Climate Change - total [kg CO2 eq.]	12,3%	27,0%	8,2%	52,2%	0,2%	91,6%
EF 3.1 Particulate matter [Disease incidences]	20,2%	36,5%	8,7%	34,1%	0,5%	90,8%
EF 3.1 Resource use, fossils [MJ]	15,8%	24,1%	7,3%	52,7%	0,1%	92,6%

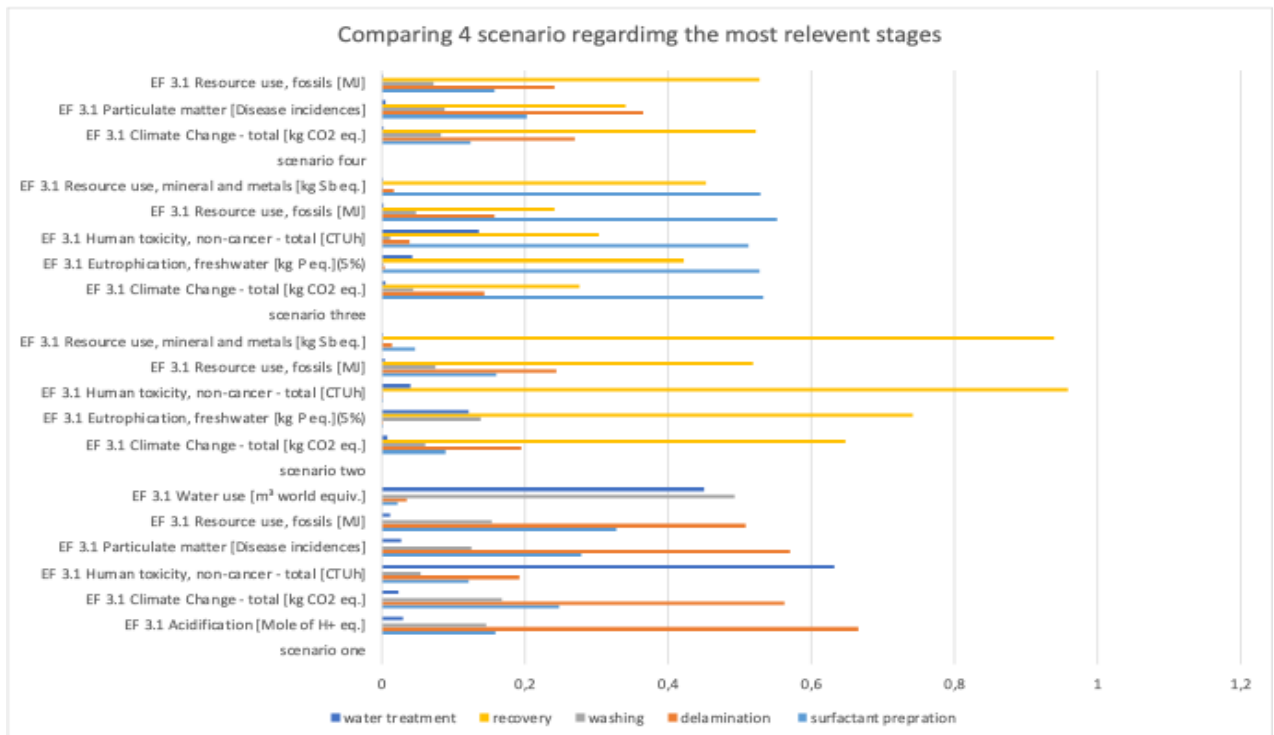


Figure 29 comparing integrated most impactful stages.

Figure 29 emphasizes the shifting importance of various life cycle stages as more processes are incorporated and optimized throughout the scenarios. Recovery processes emerge as the most impactful in later scenarios, particularly in Scenario 4, indicating their increasing environmental significance. Meanwhile, the delamination stages, which include coffee bag delamination and lauric acid production, along with the surfactant preparation stages, remain consistent key contributors across all scenarios.

These findings suggest that further optimization of both recovery, delamination processes and surfactant preparation could significantly reduce the overall environmental impact of the system. Targeting these phases for improvement, particularly in terms of resource efficiency and energy consumption, could lead to more sustainable outcomes in the life cycle.

### **Interpretation and Implications for Sustainability:**

The results of this hotspot analysis illustrate a clear evolution in the significance of various life cycle stages as the system becomes more complex across the scenarios. In the initial scenarios, surfactant preparation and delamination emerge as the most impactful stages, particularly in critical categories such as climate change and resource use.

As the system expands with the integration of additional processes, the recovery stage—fully implemented in Scenario 4—assumes a central role, especially in mitigating impacts related to fossil fuel use and greenhouse gas emissions. This shift emphasizes the critical role of material and energy recovery in minimizing the overall environmental footprint of the product system.

Despite the growing importance of recovery, the delamination stage remains a significant contributor in all scenarios, particularly in categories such as human toxicity and resource use (minerals and metals). This suggests that while recovery processes can alleviate some environmental burdens, the delamination processes, especially those involving lauric acid extraction, still warrant attention to further reduce their environmental impact.

The washing stage, though consistently contributing to resource use and water use, shows a declining relative significance in the later scenarios as other stages, such as recovery, become more dominant. This indicates that some efficiency

improvements may have been achieved in washing, but further optimizations—particularly in water use—are still necessary.

Overall, the hotspot analysis offers a strategic pathway for targeting environmental mitigation efforts. The findings demonstrate that recovery processes, particularly those involving the recapture of lauric acid and CO<sub>2</sub>, are crucial for reducing impacts in key categories like climate change and resource use. However, delamination remains a priority for further improvement, particularly in reducing toxic emissions and resource consumption. This analysis underscores the importance of adopting a life cycle perspective, enabling targeted environmental interventions at specific stages to achieve the greatest reductions in overall environmental impact. and move towards a more sustainable product system.

## 5. Discussion

The recycling of multilayer coffee bags using Switchable Anionic Surfactants (SAS) marks a notable advancement in addressing the environmental challenges associated with complex packaging waste.

This Life Cycle Assessment (LCA) study explored the potential of SAS for enabling the separation and recycling of multilayer materials, specifically coffee bags waste in my case study composed of polyethylene (PE), aluminum (AL), and polyethylene terephthalate (PET). While SAS technology offers clear benefits in delaminating complex structures, the study also highlighted critical environmental trade-offs, which must be addressed to maximize sustainability.

This method, developed by the Chemistry Research Laboratory at the University of Bologna, was used as a case study for the application of the Life Cycle Assessment (LCA) methodology. Although there are existing studies and methods similar to those developed by researchers at the University of Bologna—such as other delamination techniques (Niaounakis, 2019; Zawadiak et al., 2017), thermo-delamination (Yin et al., 2019), and dissolution methods (Cervantes-Reyes et al., 2015)—some of the tested approaches use innovative solvents like 2-methyltetrahydrofuran (2-MeTHF) and cyclopentyl methyl ether (CPME). The latter, a hydrophobic ether solvent, offers a promising alternative to other ether solvents like tetrahydrofuran (THF), dioxane, and 1,2-dimethoxyethane (DME) (Watanabe et al., 2007). Additionally, a recent study by the same chemistry research group, focusing on evaluating the appropriate SAS material for delaminating multilayer packaging, served as a key foundation for initiating this experimental work on coffee bag multilayer delamination in my thesis study (Samorì, Vagnoni, 2023).

The advantage of using Switchable Anionic Surfactants (SAS) compared to other methods lies in their ability to switch between active and inactive forms, making them more efficient for processes like delamination and recycling. Specifically in reversibility, SAS materials can be switched on and off (by adjusting pH or using CO<sub>2</sub>), allowing easy recovery and reuse of materials like plastics and aluminum, which reduces the need for harsh chemicals or additional processing steps. The other one is selective delamination, SAS materials are particularly effective at targeting and separating layers in multilayer packaging, making them more efficient than traditional methods like thermo-delamination or solvent-based dissolution.

Additionally their Environmental Benefits are so notable, they often use milder conditions (e.g., water-based solutions or low-toxicity solvents), minimizing environmental impact compared to more aggressive solvents like 2-MeTHF or THF.

The LCA was structured around four distinct scenarios, each progressively introducing more advanced recovery and recycling processes. The study utilized GaBi software and the EF 3.1 method, enabling detailed comparisons of the environmental impacts across scenarios. The impact categories assessed included climate change, resource depletion, water use, and human toxicity and ect.

Scenario one served as the baseline, focusing on the application of SAS to delaminate the multilayer structure. The delamination process utilized Triethanolamine (TEA) and Lauric Acid to separate the layers.

Scenario two introduced precipitation-based recovery of Lauric Acid using CO<sub>2</sub>, but without any significant energy inputs. CO<sub>2</sub> was added to the system to induce precipitation of Lauric Acid, switching it to its hydrophobic state for reuse. This process reduced the need for fresh surfactant inputs and improved material recovery rates. Importantly, the precipitation process did not involve substantial energy consumption, unlike later scenarios.

Scenario three introduced a more energy-intensive process, CO<sub>2</sub> recovery parts. In this scenario, just one the flows of CO<sub>2</sub> was captured and reused to regenerate the surfactant after delamination, further improving the circularity of the system by reducing waste.

Scenario four represented the most advanced system, incorporating a closed-loop process with full recovery of Lauric Acid, NH<sub>4</sub>OH, and CO<sub>2</sub>, along with the reuse of water. This scenario demonstrated the potential for substantial environmental gains by minimizing the need for fresh raw materials and reducing waste generation.

Comparing the scenarios based on the original results shows In the early scenarios TEA-Laurate preparation and delamination dominate environmental impacts, particularly in resource use, climate change, and eutrophication. As additional phases like CO<sub>2</sub> recovery are introduced in later scenarios, the burden becomes more evenly distributed across categories. By Scenario 4, the inclusion of CO<sub>2</sub> recovery and other processes results in a more balanced environmental impact, highlighting the importance of recovery and resource optimization throughout the life cycle.

when we weight the results, it shows Scenario 1 has the lowest overall impact, with climate change and resource use (fossils) that playing the largest roles. Scenario 2 shows the highest burden due to the introduction of surfactant recovery, which increases impacts in key

categories. Scenario 3 demonstrates a reduction in total impact, primarily due to partial CO<sub>2</sub> recovery, while Scenario 4 shows a further reduction, though still higher than Scenario 1.

The results emphasize the importance of optimizing recovery processes, energy sources, and the CO<sub>2</sub> supply to minimize environmental impacts.

As regards the hotspot analysis, it appears that, overall, the categories with the greatest impact are "Climate change", and "Resource use fossils". highlighting the need for renewable energy adoption and improved CO<sub>2</sub> recovery processes.

Additionally, from other point of view in hotspot analyzing in stages we observed in Scenario 1, delamination is the main contributor to environmental impacts, particularly in climate change and acidification. in Scenario 2, recovery processes dominate, driving impacts in eutrophication and human toxicity. By Scenario 3, surfactant preparation leads most categories, while CO<sub>2</sub> recovery helps reduce resource use. And finally in Scenario 4, recovery remains the largest contributor, but delamination still plays a significant role in certain areas like fossil resource use.

Although the primary goal of adding the recovery stage to reuse input materials such as surfactants, CO<sub>2</sub>, and water in the final scenario (Scenario 4) was to reduce environmental impact, we observed that the initial scenario (Scenario 1), which involves only the basic delamination process, resulted in the lowest environmental impacts across most categories. Conversely, in Scenario 4, the impacts became concentrated in just two key indicators, suggesting that the use of recovery processes and the recycling structure reduced the contributions of other impact categories, but did not minimize the overall environmental burden as effectively as expected.

## 6. Conclusion

As global concerns over food and beverage storage continue to grow, the demand for multilayer packaging has surged. This increase in production has brought attention to the end-of-life management of these materials, raising questions about their disposal and recycling. Multilayer materials, while beneficial for product preservation, pose significant environmental challenges due to their complex composition, making their separation and recycling difficult.

This study has contributed to a deeper understanding of the environmental impacts associated with coffee bag recycling using Switchable Anionic Surfactants (SAS). Through the application of Life Cycle Assessment (LCA) across multiple scenarios, we have gained insights into the different phases of the recycling process, from surfactant preparation to recovery, and the associated environmental trade-offs.

The study demonstrates that while recycling technologies like SAS offer potential solutions for delaminating multilayer materials, they also introduce complexities that need to be addressed, particularly in terms of energy consumption, resource use, and toxicity.

In the early scenarios, surfactant preparation and delamination were the most impactful stages, particularly in categories like climate change and resource depletion. The energy demands for producing chemicals such as TEA-laurate and separating the multilayer structure of coffee bags were major contributors to these impacts.

However, as additional recovery processes were introduced—especially in Scenario 4, where CO<sub>2</sub> and Lauric Acid recovery were fully integrated, the increasing impact category has been observed related in Climate changes and Greenhouse gas emission as well as in Fossil fuels resources. This shift highlights the importance of the design the recovery process, the source of energy required in reducing the environmental impacts of multilayer packaging.

the delamination stage remained a significant environmental contributor across all scenarios, especially in categories like human toxicity and resource use (minerals and metals). This indicates that while recovery can mitigate some impacts, the delamination process, particularly involving Lauric Acid extraction, requires further optimization to reduce its environmental burden. Additionally, although the washing stage showed decreasing importance in later scenarios, water management remains an area of concern, particularly in regions where water scarcity is a pressing issue.

The hotspot analysis provided in this study offers valuable guidance for targeting environmental mitigation efforts. By focusing on improving recovery processes, particularly the recapture of Lauric Acid and CO<sub>2</sub>, significant reductions can be achieved in key environmental categories like climate change and resource use. At the same time, ongoing efforts to improve the delamination process and reduce toxic emissions will be critical to minimizing the overall environmental impacts of the recycling system.

This research also emphasizes the importance of a life cycle perspective in addressing environmental sustainability. The use of LCA methodology has proven effective in identifying the most impactful stages and providing a clear path forward for improving the recycling of multilayer materials. By focusing on specific areas for improvement—such as optimizing energy efficiency, enhancing water recycling systems, and integrating renewable energy sources—the coffee bag recycling process can become more aligned with the principles of a circular economy.

While this study has provided valuable insights into the environmental performance of coffee bag recycling, further research and technological advancements are needed. Future work should explore additional optimization of recovery technologies and delamination methods, as well as the broader application of renewable energy in the recycling process. Moreover, scaling these solutions to an industrial level will require continued collaboration between researchers, industry professionals, and policymakers to ensure that the benefits of these technologies can be fully realized while minimizing their environmental impacts.

In conclusion, although the scenarios progressively improved by incorporating positive processes such as recycling and reusing raw materials, water, and the CO<sub>2</sub> used in the recovery stage, the source of carbon dioxide in this case study—captured from waste gas using carbon capture technology—plays a crucial role. As previously mentioned, the energy consumption required for capturing, filtration, and liquefaction of CO<sub>2</sub> significantly impacted the environmental outcomes of the recovery process. Additionally, the production of lauric acid as a surfactant contributed substantially to the overall environmental impact. To develop a more environmentally friendly process for recycling multilayer packaging, it is recommended to adopt renewable energy sources instead of fossil fuels, reducing CO<sub>2</sub> coming from more sustainable methods, and optimizing the delamination process in terms of raw material, water, and energy consumption.

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