



GOODBYO

**MULTI-COMMODITIES MICROBIAL-DRIVEN BIOREFINERY
BASED ON FOOD-PROCESSING INDUSTRY WASTES, BIOGENIC CO₂
AND BIOPROCESS WASTEWATERS**

Deliverable 8.1 – Framing the project LCA study: methodological tailoring and input requirements

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Lead: POLITO

COORDINATOR CONTACTS

Center for Sustainable Future Technologies
CSFT@Polito

Dr. Valeria Agostino
valeria.agostino@iit.it

Prof. Fabrizio Pirri
fabrizio.pirri@iit.it



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REVIEWERS	Sebastian Bernacchi, Arne Seifert (KRJ), Valeria Agostino (IIT), Kasper de Leeuw (CC)

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1 EXECUTIVE SUMMARY

The present document outlines the methodological framework of the Life Cycle Assessment (LCA) study within the GoodByO project Work Package 8 (WP8).

The LCA study purpose was contextualized, and its methodological approach was thoroughly described and motivated.

The present document reports an introduction of the GoodByO project from an LCA standpoint (chapter 4), a generic description of LCA framework core concepts (chapter 5), followed by a discussion on the methodological choices that will be applied to the GoodByO LCA study (chapter 6). Lastly, final remarks on the adopted methodology are reported (chapter 7), alongside references used to realize this document (chapter 8), and an annex for additional information (chapter 9).

Chapter 4 introduces a brief description of the GoodByO process and contextualizes the use of LCA in the project.

Concepts outlined in chapter 5 regard the foundations of LCA, i.e. functional unit, multifunctionality, system boundaries and the four phases of LCAs. Despite having discussed LCA foundations, the present report is not aimed at laymen, but rather to readers with a basic understanding of LCA concepts.

Chapter 6 reports a contextualization of the LCA study, reporting the goal of the study, the analyzed process and its boundaries. Also, the functional unit is discussed and reported; similarly, the multifunctionality (i.e., the production of multiple products) is addressed and discussed, as both functional unit and multifunctionality are not trivial matters, when dealing with biorefineries. Moreover, the impact categories that will be assessed by the study are reported, alongside the database that will be used. The geographical and temporal scope of the study are also reported. The Life Cycle Inventory of the study was also discussed, outlining a procedure to assess the quality of data that will be used for the study, despite the data itself not being available now of writing, due to the early stage of the project.

Chapter 7 reports the final remarks on the described methodology.

Chapter 8 reports this report references.

Chapter 9 reports additional information on the Environmental Footprint method.

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3 LIST OF ABBREVIATIONS

CBE-JU	Circular Bio-Based Joint Undertaking
CA	Consortium Agreement
CC	ChainCraft
EC	European Commission
EF	Environmental Footprint
EoL	End of Life
FU	Functional Unit
IPCC	International Panel on Climate Change
ISO	International Organization for Standardization
LC	Life Cycle
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
MMMCZCS	Mærsk Mc-Kinney Møller Center for Zero Carbon Shipping
PCR	Product Category Rules
PEF	Product Environmental Footprint
WP	Work Package

4 INTRODUCTION TO THE GOODBYO PROJECT

The GoodByO project aims at establishing an innovative biorefinery production path for hexanol and octanoic acid at industrial scales, starting from agrifood waste. The GoodByO biorefinery consists of four different *microbial factories*, from which carotenoids are also produced, alongside the hexanol and octanoic acid (labelled as bio-hexanol and bio-octanoic acid, due to their production from biogenic carbon sources). Furthermore, additional co-products are produced, such as bio-fertilizers or methane-enriched biogas, which will be upgraded to biomethane.

The GoodByO biorefinery starts from biogas production through the ChainCraft (CC) process, followed by a chain elongation of the liquid effluent from CC process to produce the bio-octanoic acid. Currently, two different scenarios for bio-octanoic acid are being evaluated; the first scenario performs an additional chain elongation step, starting from the CC process. The second scenario, on the other hand, consists of a modification of the CC process to produce bio-octanoic acid through a single chain elongation step. In both scenarios, liquid effluents from bio-octanoic acid production are used to produce carotenoids. In addition to the liquid effluent treatment, also the raw biogas from CC process is further treated, producing the bio-hexanol at the end of the biogas treatment section.

The GoodByO bio-hexanol, bio-octanoic acid, and carotenoids thus represent alternatives to fossil-based or other bio-based products, starting from biogenic waste. **To assess the process environmental impacts and benefits, the Life Cycle Assessment methodology will be employed**, to identify environmental hotspots and compare the environmental profile of the GoodByO products with conventional fossil and bio-based products. The following impact categories will be analysed: **global warming, water use, land use, freshwater ecotoxicity, use of mineral and metal resources, use of fossil resources**, using the **Ecoinvent 3.10** database on the **OpenLCA** software.

5 INTRODUCTION TO LIFE CYCLE ASSESSMENT METHODOLOGY

Life cycle assessment is a methodology developed to assess the environmental impacts tied to a specific product, service or process (from now on, these three possible subjects of LCAs will just be indicated as “product”). The methodology allows studies to be extended both to the entire life cycle of the product (i.e., from raw material extraction to the end-of-life (EoL) disposal) or to just some parts of the life cycle.

The life cycle (LC) of a product in general is composed of five major stages, namely: *raw materials extractions/collection*, *processing/transformation*, *transportation to consumer*, *usage/consumption*, and *disposal/recycling*. Each stage refers to a unique part of the LC that clearly identifies several activities or processes that occur during the

product life cycle. Usually, to identify the stages encompassed in LCA studies, specific terms, like cradle-to-gate or cradle-to-grave, are used, the meaning of which was reported later in this report.

5.1 Framework Methodologies

Typically, evaluating a product environmental impact requires several aspects to be considered, as the specific raw materials involved, or the possibility of the life cycle having multiple outputs, other than the product subject of the study. Therefore, several methodological choices must be taken, significantly influencing the final result of the assessment. Consequently, the International Organization for Standardization (ISO) developed a series of guidelines and frameworks, reported in ISO 14040 and 14044 standards, first issued in 1997 and 2006, respectively, with an update to ISO 14040 in 2006. The ISO 14040 standard lays the fundamental principles and guidelines for LCA, listing the core phases of LCA studies, the need for transparency to allow correct interpretation and comparison of different studies, and core methodological aspects [1]. ISO 14044 further expands the methodological framework, detailing aspects and procedures such as guidelines on data quality, approaches for multi-output processes (defined as multifunctionality of the process), and mandatory parts of LCA results reports [2].

Therefore, ISO 14040 and 14044 pose a base for harmonized studies, ensuring a certain level of quality and standardization among completely distinct products and LCs. However, ISO guidelines are often not able to totally encompass the peculiarities of several industrial sectors, or no totally standardized approaches are reached, despite the guidelines. Hence, during the years other methodological frameworks were developed and are still being developed, starting and expanding upon ISO guidelines. In recent years, the European Commission has taken action in establishing a standardized LCA methodology, defined as Product Environmental Footprint (PEF) methodology. The PEF methodology sets a series of rules for conduction of LCA studies, called Product Category Rules (PCR), which are specific for each sector and aim to standardize LCAs in a stricter way than the ISO guidelines. Nonetheless, the PEF was still based upon ISO guidelines, following the ISO-defined four core phases of LCA studies:

- **Definition of goal and scope**, which includes the motivations for carrying out the study, the description and boundaries of the analyzed system, the functional unit and the general assumptions.
- **Life Cycle Inventory (LCI)**, requiring the quantifications of inputs and outputs of each step of the analyzed system. LCI may also report the quality of the used data.
- **Life Cycle Impact Assessment (LCIA)**, consisting of the evaluation of the system environmental impacts (e.g. climate change, water depletion).
- **Interpretation of results**, during which the evaluated impacts are used to identify environmental hotspots, discuss potential improvements of the environmental profile, and provide support in the decision-making process.

A more detailed description of the four phases of an LCA analysis is provided in sections 5.2, 5.3, 5.4, and 5.5.

5.2 Goal and scope definition in LCA methodology

5.2.1 Goal definition

Crucial parts of the goal definition are represented by stating the study motivations and intended application, which inevitably shape the applied methodology, such as the approach to multifunctionality or the choice of data sources. Also, the goal should state the intended audience of the study, an aspect that will define the technical and communicative depth of the study; moreover, audience may also define the contextual information provided in the study report.

5.2.2 Scope definition

While the goal defines the rationale behind the study, the scope definition regards the more in-depth technical aspects of it. The scope encompasses the boundaries of the analysed system, possibly coupled with a description of the system, the functional unit and the reference flow. Lastly, the LCA assumptions are usually reported in this phase.

5.2.2.1 System boundaries, process assumptions and description, and study limitations

The system boundaries represent not only the stage of the product life cycle (e.g., raw material extraction, processing, end-of-life, etc.) considered by the process, but might also the single operative steps, depending on the level of detail of the study. While it is possible to group two or more operative steps together, rather than individually report them, the grouping must be stated and motivated. The process assumptions and description are also strictly related to the limitations of the study. Limitations may be represented by parts of the actual system not included in the analysis, uncertainties regarding collected data, or others.

As stated at the start of chapter 5 different terms can identify LCA studies based on the extension of the system boundaries. Generally, studies encompassing the whole life cycle (end-of-life included) are called *cradle-to-grave* studies. Intermediate life stages (e.g., production, utilization, transport of the product) are generally referred to as “gate” stages. Thereby, a study encompassing only the raw material extraction and the production process, stopping at the out-of-factory product (or another gate step) would be called a *cradle-to-gate* study. Furthermore, a study not including the raw materials extraction nor the end-of-life, thus including only gate steps, would be called a *gate-to-gate* study.

Other than these generically used terms, specific sectors may also use specific variants of this concept, such as *well-to-wake*, used for LCAs investigating fuels full life cycles. However, to the best of the authors' knowledge, no biorefinery-specific definitions exist in that regard. Therefore, the general terminology will be employed, since not all of the GoodByO products are biofuels.

System boundaries assumptions regarding waste inputs

When dealing with inputs deriving from waste materials (in the case of GoodByO, the agrifood waste) different assumptions on the embedded impacts of the waste inputs can be made. A usual assumption is the zero-burden concept, where the embedded impacts of waste materials prior to the waste arrival at the centralized collection point (e.g., collection point at the end of a centralized agrifood waste collection value chain) or to the waste exiting the gate of the plant/farm/operational site (e.g., when agrifood waste is removed from fields and thus serve no more function) are not considered.

Thereby, this assumption states that waste inputs to the investigated system enter virtually impact-free, hence being called **zero-burden inputs**. However, despite embedded prior impacts getting cut off, the transportation from the centralized collection point/gate of operational site to the site of new utilization is accounted for. Therefore, even if zero-burden, using waste inputs that require long transportation distances might represent a significant source of impacts.

5.2.2.2 Functional unit and reference flow

The functional unit serves as a quantitative description of the investigated product function. Functional units can cover a wide range of different quantities, from mass production to energy contents, up to areas, or number of items. Functional units are often paired to reference flows, which are flows representing the functional unit while being coherent with the rest of the system streams. Examples of reference flows might be the mass of a fuel corresponding to a functional unit of 1 MJ, or the mass of a plastic bottle corresponding to a functional unit of 1 L of bottling capacity. In these cases, the reference flow allows the fuel or the bottle to be related to the other mass streams in the system.

5.2.2.3 Impact categories and impact calculation methods

The last part of the scope phase includes the statement of the impact categories investigated in the study, coupled with the calculation method chosen for assessing each investigated impact category. While ISO guidelines do not state a specific impact category to be assessed, other methodologies might specify them.

Some examples might be provided by the Renewable Energy Directive, which explicitly states the GHG emissions impacts [3], [4], or the PEF, which states sixteen impact categories compulsory to discuss in PEF-compliant studies [5], [6].

5.3 Life cycle inventory

LCI usually encompasses a report on data quality, a quantitative inventory of the inputs and outputs of the process, and, according to ISO 14044 [2], the approach to multifunctionality.

5.3.1 Data quality report and data classification

The data quality report requires an evaluation of the origin of used data. ISO guidelines define two essential types of data: *primary* and *secondary*. Primary data refers to data collected at laboratory, pilot or industrial scale purposely for the conducted study, either by the LCA study authors or by other parties. Secondary data is an umbrella term for a wider range of data types, encompassing data obtained from simulations, from calculations, from other works in the literature, or estimates. While primary data is often preferred to secondary data, robust simulations represent the most reliable and preferred source of secondary data, while estimates are at the bottom of the secondary data hierarchy [2]. It is important to consider that modelling of flows included in databases is classified as secondary data.

Furthermore, in LCI the outputs are classified as products, waste or emissions. Correct classification of the outputs is paramount since LCA methodology expects the environmental burdens of the several stages to be placed onto products only. Data quality also regards the match between time and geographical frame of the study and of the data. While the time frame refers to the relevant time horizon for the study, the geographical frame contextualizes eventual region or area-specific emissions, or parameters, considered for the study.

An additional data classification is represented by “foreground” and “background” data. Foreground data basically encompass all data and emissions pertaining to the system investigated by the LCA study. As an example, the quantity of GHG gases generated by a reaction occurring in the system investigated by the LCA study would be classified as foreground data, as it is an emission originated by the investigated system.

On the other hand, background data basically represent all data and related emissions not directly originated in the investigated system, i.e., the upstream emissions of input materials or energy used in the analysed process. As an example, electric energy, when supplied by a third party or by the national grid, often represents a case of background data, as it is not generated by the investigated system.

When dealing with foreground and background data definition, it is paramount to notice that background data processes still pertain to the system boundaries, as processes outside of system boundaries would not be considered by the LCA study.

Noticeably, background data is usually implemented in the LCA through the use of already existing databases. However, in some cases it may be required to model a background process. In such cases, secondary data is usually used for modelling background processes. By contrast, no standard can be defined beforehand for

foreground processes modelling; while primary data would be preferred, also the use of secondary data is acceptable, as long as a relevant discussion on data quality is also reported.

5.3.2 Multifunctionality

Both ISO guidelines and other methodologies report more than one possible approach to multifunctionality. Due to one of the approaches rarely being applicable in complex product systems, it will not be discussed in this work. For more information, the reader is referred to ISO 14040 and ISO 14044 [1], [2].

System expansion and allocation

A possible approach is the system expansion, with substitution, which requires the entirety of the environmental burdens to be placed upon one of the products, identified as the main interest of the study. The rest of the products are instead considered as “avoided burdens”. The concept of avoided burdens consists of the co-products substituting equivalent amounts of conventional products on the market (e.g. biofuels substituting conventional fossil fuels, or microbial proteins substituting feed appliances such as fishmeal [7]). Thus, the impacts tied to the production of the substituted conventional product are avoided. The avoided burdens are generally negative in value, thereby sometimes being referred to also as “savings”. The avoided burdens are therefore applied to the impacts placed upon the main product of the system, reducing its overall environmental impact.

Another approach is called allocation, which consists of partitioning the overall impacts of the system between the multiple products. The allocation can either be done based on physical properties or economic considerations, depending on the context and goal of the study. As already mentioned, LCA methodology states that impacts can be allocated only onto products; therefore, the allocation procedure does not take waste outputs or emissions into consideration for the impacts partitioning.

5.3.2.1 Criterion for multifunctionality methodology choice

Due to the different management of the overall impacts, system expansion and allocation might lead to significantly different results, often resulting in a system treated with allocation not being comparable with the same system treated with system expansion. While ISO guidelines state that, when applicable, system expansion is preferred to allocation [1], [2], the choice between the two approaches is usually left to the study conductors. By contrast, PEF Product Category Rules (PCRs) usually dictate the multifunctionality approach to be adopted for the specific sector. In the context of ISO methodology, a series of criteria can be followed to determine the appropriate multifunctionality approach.

Despite being usually applied to the fuel sector, The Mærsk Mc-Kinney Møller Center for Zero Carbon Shipping (MMMCZCS) methodology can support the decision process,

stating that system expansion should be preferred to allocation only when meeting certain requirements [8]:

- Unambiguous ability of the co-product(s) to substitute the respective conventional product(s) on a real market. The co-product fate has also to be certain, admitting no uncertainty on its effective fate after the production.
- Existence of a clearly identified main product, which is the main goal of the process.
- The production of co-products is relatively small, when compared to the main product.

All the product systems that do not comply with these criteria should therefore be treated with allocation. Moreover, the chosen basis of the allocation should be motivated and pertaining to the study goal and scope.

However, as mentioned, in PEF-compliant studies the multifunctionality approach is dictated by the PCR, removing the burden of choice from the study performers, unless stated otherwise.

5.4 Life Cycle Impact Assessment

The LCIA phase itself can be composed of more than one part. Usually, the assessed value can be reported in more than one way; however, only one of them is mandatory for LCA studies, whereas the others are optional. The mandatory report is the *characterization*, which multiplies the inputs and emissions of the process with characterization factors (usually characterized by a certain measure unit, such as *g CO₂ equivalent/measure unit of stream*), with the values of the latter being determined by the chosen calculation method. Hence, this coupling returns the assessed impacts of the process. The optional assessment reports are *normalization*, *weighting* and *grouping*. However, due to them being outside the scope of this work, no further information will be provided on their regards. For more information, the readers are referred to ISO 14040 and 14044 [1], [2]. Regarding PEF-compliant studies, the calculation method is required to be the EF (Environmental Footprint) method, which assesses sixteen different impact categories (reported in

Table 9-1 in the ANNEX section), all of which are compulsory to be reported in PEF-compliant studies. By contrast, ISO does not state mandatory methods, nor mandatory impact categories to be reported. In particular, studies using the EF method but not fully adhering to PEF methodology are not obliged to report all the sixteen impact categories.

5.5 Results interpretation

The interpretation phase generally encompasses a discussion of the obtained results, coupled with a comparison with other studies (either academical or technical) and the

identification of environmental hotspots. Also, limitations on the study assumptions and data quality must be considered when reporting the interpretation. Regarding comparison with other studies, fair comparisons can only be performed under strict requirements. The utmost requirement consists of the compared systems having the same functional unit, followed by the systems having the same overall boundaries (e.g., both LCAs as cradle-to-gate). Also, the same calculation method and database should be used to ensure a completely fair comparison. Even if the specific operative steps of the system may differ, as long as the overall system boundaries do not the comparison remains fair.

Lastly, additional aspects of the interpretation are tied to the study goal. Studies directed toward the optimization of a process might propose impact mitigation solutions, whereas studies directed to policy makers may rely on the assessed results to propose certain aspects of the policies, or to direct policy makers to a more informed formulation of regulations.

5.6 ISO and PEF methodologies comparison

Despite PEF methodology using ISO methodology as its core, several notable differences can be observed between the two. In particular, PEF methodology aims to standardize LCA studies while also accounting for all the characteristics or practices of specific production sectors. As shown in Table 5-1, ISO methodology lets the LCA practitioner define aspects such as functional unit, or the impact categories analysed in the study. On the other hand, PEF methodology imposes certain aspects such as the functional unit, or the approach to multifunctionality, through the Product Category Rules. Several specific PCRs exist under PEF methodology. However, some common rules can be observed, which need to be applied in PEF-compliant studies.

When performing an ISO-based study, some aspects of PEF methodology can be used to approach some of the decisions faced by the practitioner; however, to identify the study as PEF-compliant, all of the requirements of PEF methodology must be fulfilled.

Table 5-1 Comparison of main characteristics of ISO and PEF methodologies.

	ISO 14040 and 14044	PEF
Targeted products	No specific targeted products	Various possible targets, determined by individual Product Category Rules
Functional Unit	Up to the practitioner	Specified by the individual Product Category Rule; if not specified/PCR not existing, up to the practitioner, based on four criteria
Reference flow	Up to the practitioner	Specified by the individual Product Category Rule; if not specified/PCR not existing, up to the practitioner

System boundary	Cradle-to-grave or reduced scopes	Cradle-to-grave for finished products; Cradle-to-gate for intermediate products. Different boundaries need to be motivated.
Multifunctionality	Up to the practitioner, although a hierarchy of approaches exists	Specified by individual Product Category Rules; if a specific PCR does not exist, up to the practitioner, following the same hierarchy as ISO methodology.
Specific database required?	No	Yes, although some proxy database can be used, as specified by the guidance documentation [6]
Impact categories	Up to the practitioner	16 categories calculated through EF method
Fundamental documents	ISO 14040 and ISO 14044 [1], [2]	Overall PEF guidance documentation [6], specific PCR documentation

While PEF methodology returns a highly standardized study, the request for a specific database could severely hinder its application, at the moment of this document writing. Nonetheless, ISO-complying studies can be further standardized through a literature review of previously performed LCA studies, to identify the most common practices and adhering to them.

6 GOODBYO LCA METHODOLOGY

6.1 LCA in GoodByO project context

In the context of the GoodByO project, LCA will act as a tool for detecting environmental hotspots, which will be addressed during further development of the process, while also allowing a value comparison with impacts of other similar processes or with similar products obtained from fossil sources.

Generally, biorefineries such as the GoodByO plant need robust LCA models, with clearly reported assumptions and methodological choices, to ensure a fair comparison with other similar, fossil-based products and other biorefineries.

Thus, although an entirely PEF-compliant study will not be performed, the PEF methodology will be used to determine certain aspects of the methodology, while also accounting for common practices in literature studies regarding biorefineries, to further standardize the present work. Nonetheless, the study will be mainly ISO-compliant.

6.2 Goal of LCA study and intended audience

The goals of the LCA study are:

- Assessing the environmental impacts tied to the operation of the GoodByO integrated refinery plant, to produce hexanol, carotenoids, octanoic acid and other products.
- Identifying environmental hotspots, to address them during the development of the GoodByO technology.
- Comparing the assessed impacts with other bio-based and fossil-based product benchmarks.

The LCA study will target two groups of recipients, the **GoodByO consortium partners**, for an informed development of the last stages of the project, and **the stakeholders**, aiming at an informed characterization of the environmental profile of the products.

"The goal of this LCA study is to assess the environmental impacts associated with the operation of the GoodByO integrated biorefinery, to identify environmental hotspots and guide the development phase."

6.3 Scope of LCA study

6.3.1 Process description and System boundary

The GoodByO process, represented in Figure 6-1 alongside the LCA system boundary, consists of an integrated biorefinery. It is paramount to specify that, despite a description of the current schemes in Figure 6-1 will follow, the reported schemes are used only with the scope of describing the methodological elements in this deliverable, and not to represent the updated status of the project.

The core objective of the process and system boundary description is to identify the process products, waste, and emissions. The reader is thereby redirected to other documentation (see the Deliverable 6.1 related to the Front Engineering Design of each Microbial Factory) on the GoodByO project for fully updated information on other current elements of the process.

As illustrated in Figure 6-1, the GoodByO process can be divided in three different sections: the first section can be labeled as "ChainCraft section" ("CC section"), which includes the operations of the already existing ChainCraft process from which the GoodByO process is developed. The second section regards the treatment of liquid effluents from the "CC section" to produce bio-octanoic acid and carotenoids and is thus called the "liquid treatment section" in this report. The third section consists of the treatment of the "CC section" raw biogas to produce bio-hexanol and is thus called the "gas treatment section" in this report.

Currently, two different scenarios for the GoodByO process are being evaluated: the “C6” scenario and the “EtOH” scenario. Depending on the scenario, the “CC section” is composed of the ChainCraft process, or by modified version of the CC process.

The “C6” scenario (Figure 6-1.A) includes the already existing CC process in the “CC section”. The hexanoic-acid-rich liquid effluent produced in the CC process is then sent to the MF1 reactor in the “liquid treatment section”. Alongside the CC process liquid effluent, electron donors are also fed to the MF1 reactor, where a further chain elongation reaction produces **bio-octanoic acid**, which is separated from the MF1 liquid effluents downstream of MF1. A CO₂ stream is also produced downstream of MF1, which will be evaluated for feeding to the subsequent MF4 reactor.

In the “EtOH” scenario (Figure 6-1.B), the “CC section” is constituted by a modified version of the CC process, constituted of a fermentation reactor (FR reactor). The MF1 reactor allows the chain elongation to produce **bio-octanoic acid** starting from ethanol and short-chain volatile fatty acids coming from FR reactor. Also, an H₂ stream is produced from the chain elongation reaction. Similar to the “C6” scenario, also in the “EtOH” scenario, a CO₂ stream is produced downstream of MF1, albeit in different amounts (the reader is referred to document D6.1 for further details).

Aside from the differences reported above, the rest of the “liquid treatment section” does not differ between the two scenarios. In both scenarios, after bio-octanoic acid separation, the MF1 liquid effluent stream is filtered through membranes. The permeate is then sent to the MF4 reactor, whereas the retentate is recirculated back to the “CC” section. The permeate sent to MF4 serves as a nutrient substrate for mixotrophic microalgae growth. The microalgae then use CO₂ as a substrate to produce **carotenoids**, which are then extracted and subsequently separated from the **microalgae debris** (treated as co-products due to their protein content), leaving a wastewater flow as a waste stream. The CO₂ used in MF4 will be derived from MF1 reactor downstream processes; in the “EtOH” scenario, however, the CO₂ derived from MF1 downstream may not satisfy the MF4 requirements, and thus external CO₂ inputs might be needed. However, such possibility will be evaluated after one of the two scenarios is established as the definitive one, in later stages of the project. In both scenarios, the CO₂ will be diluted with fresh air prior to entering MF4.

In the “gas treatment section” (Figure 6-1.A and Figure 6-1.B), the raw biogas is sent to an anaerobic biological purification step (MF3) to remove H₂S, purifying the biogas and at the same time producing a sulphur-rich microbial biomass, valorised as **biofertilizer**. The purified biogas is then sent to MF2, where a microbial fermentation process uses biogas and green hydrogen to produce **bio-hexanol**, also obtaining **microbial biomass** as a co-product, and producing a wastewater stream. Off-gas exiting MF2 (a **methane-enriched biogas**, shown in Figure 6-1) is sent to an external site for methanation. However, the methanation reaction will currently be placed outside of the current system boundaries, thus treating the biogas as a co-product, instead of biomethane, as shown in Figure 6-1.

Other than including the operative steps of the GoodByO process, the LCA system boundary will encompass the raw/waste feedstock extraction/production and related transport, shaping the study as a **cradle-to-gate** LCA. On the other hand, transportation of the products was not included, thus stopping the study at the plant gate.

The raw materials and energy extraction/production will be considered as background processes. Additionally, in “C6” path, the ChainCraft process will be treated as a background process. In both scenarios, the rest of the operations in Figure 6-1 (including the FR reactor in “EtOH” path) will be considered as foreground processes.

The possibility of recirculating MF4 wastewaters to MF2 (or recirculating MF2 liquid effluents to MF1) will be further evaluated during future development of the project, due to current mass balances having shown the recirculation to have low influence on MF2 and MF1 feed requirements (for further information, the reader is referred to report D6.1); in case of a positive evaluation, the recirculating streams will be subsequently included in the LCA study. Regardless of the evaluation outcome, the presence or lack of recirculating wastewaters would not affect the methodology presented in this document in any relevant way.

6.3.2 Main assumptions

In the LCA study, the agri-food waste will be assumed as a zero-burden input; however, transportation of agri-food waste to plant will be included in the boundaries of the system, as the transportation occurs downstream of waste exiting their initial production site.

Renewable energy will be representative of the renewable energy source (RES) developed within work package 7 of the project.

The hydrogen produced in “EtOH” scenario, should this scenario be the decisive one chosen in later development of the project, will not be considered as a product, and thus no allocation will be placed onto it. This choice stems from the intended use for the hydrogen as input to the biomethanation process, which is placed outside the system boundaries, rather than a placement on the market.

MF1, MF2, MF3, and MF4 steps (Figure 6-1) will be assumed to work in conditions granting similar rates of micro-organisms growth and death, allowing not to consider the necessity of micro-organisms make-up, unless subsequent experimental data from GoodByO partners suggest such make-up to be significant. However, the initial micro-organisms inoculum input will be considered, after being normalized upon the entire lifespan production of the reference flow, i.e., the initial inoculum input will be divided by the reference flow mass produced during the entire lifespan of the plant (e.g., total production over a 25 year lifespan). The normalization will be discussed with partners of the project, to assess the expected lifespan of the plant and the duration of plant operations before maintenance of the bioreactor is necessary. In the case of the normalized initial inoculum input amounting to relatively low values, the possibility of

setting a cut-off threshold (thus, not including the initial inoculum data in the LCA study) will be considered.

The infrastructure of foreground process steps will not be accounted for, as the study focuses on the process itself, rather than on an existing, high-TRL plant.

6.3.3 Functional Unit

Functional unit choice rationale

The choice of the functional unit (FU) for the study of a biorefinery is not a trivial matter and was also discussed in other studies. Gaffey et al. [9] analysed several LCA studies on biorefineries, reporting that the majority (49%) of the studies FUs were based on one of the biorefineries products. Nonetheless, the same review reported that 27% of the studies based their FU on the treated feedstock. Also Ahlgren et al. [10] discussed the importance of FU definition in biorefinery LCAs. Their main recommendation was to define a FU coherent with the goal of the study, but also easily interpretable and open to comparison with other studies.

Both Ahlgren et al. and Gaffey et al. studies reported multiple options for functional units that could be appropriate for the GoodByO process:

- feedstock-based FU;
- product-based FU;
- basing the FU on the biorefinery purpose, thus encompassing all its operations under one extended FU, e.g. production of “x kg of carotenoids, y kg of bio-hexanol, z kg of bio-octanoic acid”, or “operating 1 biorefinery plant”.

While a product-based FU would comply with the majority of biorefinery LCAs, this would require identifying one of the GoodByO process products as the main product, which could be argued, as the goal of biorefineries is to convert the feedstock into several products, rather than just one main product [9], [11]. However, this would be the most transparent choice for communicating and comparing the impacts of each individual product of the biorefinery. Adding to that, the majority of biorefinery studies used a product-based approach, as already reported, thus increasing the possibilities of fair comparison with other studies.

On the other hand, a feedstock-based FU would clearly identify the agri-food waste as the main feedstock of the plant. However, placing the FU on the feedstock would shift the core concept of the study on a waste-management level, rather than on a production level. Moreover, it may be argued that the comparison with fossil-based processes might not be feasible in a transparent way, with such a FU.

The “extended FU” option would be the most appropriate choice for the sole purpose of assessing the plant impacts, at the expense of a difficult comparison with other

biorefinery LCAs, as there is no guarantee that other biorefineries would produce the same products in similar ratios. Adding to that, an “extended FU” might hinder a transparent communication of the impacts of the single products of the GoodByO process and their comparison with fossil-based alternatives. The comparison of the biorefinery with non-integrated-refinery benchmarks would therefore require an analysis of the separate benchmarks, and then the observed benchmark impacts should be summed to match the extended FU of the GoodByO study.

Therefore, the **FU was chosen according to a product-based perspective**, to pursue all the goals set by the LCA study.

Chosen functional unit

To adopt a **product-based FU**, the main product of the process was identified in **the bio-octanoic acid production**.

The choice of bio-octanoic acid as the functional unit was motivated by the GoodByO biorefinery representing a modification and expansion of the already existing ChainCraft process. While the CC process produces hexanoic acid as main product, the GoodByO process enhances the CC chain elongation step, producing (bio-)octanoic acid instead of hexanoic acid. Despite producing different compounds, both processes have the function of producing carboxylic acids; hence, bio-octanoic acid was chosen as the functional unit over the remaining two main products (i.e., bio-hexanol and carotenoids). Moreover, the choice of bio-octanoic acid as FU will allow a more rigorous comparison of GoodByO biorefinery environmental benefits with the ChainCraft process.

Thereby, the **FU of the study will be defined as the production of 1 t of bio-octanoic acid**. The rest of the products will be treated as co-products and their impacts reported accordingly.

6.3.4 Approach to multi-functionality

Chosen multi-functionality approach

Similar to the functional unit, also the multi-functionality of biorefinery plants was discussed in the literature, as it also represents a non-trivial aspect of biorefineries LCAs. ISO 14040 and 14044 state that system expansion should be preferred over allocation; however, the former approach would hinder the additional information report of each singular product impacts. Therefore, the multi-functionality was approached through allocation, which allows partitioning the overall impacts of the biorefinery on the individual products. Thus, the **bio-octanoic acid will be treated as the main product** (owing to its status as FU), whereas impacts of the remaining products will be reported as impacts of co-products.

Other than determining allocation as the multi-functionality approach, a basis for the allocation needs to be determined.

Multi-functionality approach rationale

The allocation basis is to be pondered upon the process functionality and the relationship between products. In the GoodByO process context, an energy basis allocation would not be applicable, as energy of certain products (e.g., carotenoids) is hardly determinable or of interest.

Among the remaining options (i.e., mass and economic bases), the final mass balance of the GoodByO project will be pivotal in determining the allocation basis. Based purely on the products nature, economic allocation would be preferable, as biogas, usually used for energy production purposes, would not be appropriately represented by a mass based allocation; on the other hand, due to biogas prices being usually determined on the base of its energetic content, an economic-based allocation would be suitable, as it would be suitable for the rest of the products, since their definition as products implies the existence of an economic value on the market.

However, carotenoids prices usually range between 2000-7000 USD/kg [12], which is significantly higher than the prices of other products of the biorefinery, based on initial communications by GoodByO partners [13]. Hence, depending on the carotenoids productivity, an economic-based allocation could place almost the entirety of the overall impacts on the carotenoids, leading to an abysmal share of impacts for the rest of the products.

On the other hand, a mass-based allocation, even if not appropriate for biogas, would still be possible. Nonetheless, due to the usually low yield of carotenoids in industrial-scale productions, a low productivity might lead to an abysmal share of impacts to be placed on carotenoids. Due to the carotenoids being one of the main biorefinery products (albeit not being the FU), such an abysmal share for one of the main products would not be up to good LCA practices.

The current preliminary mass balance (reported in the D6.1 deliverable of the project) shows an economic-based allocation to place almost the entirety of overall impacts on the carotenoids, whereas an initial communication within the GoodByO partners [13] showed the economic-based allocation to be a more balanced approach than the mass-based, demonstrating the strong influence of the mass balances on the allocation suitability.

Hence, despite economic allocation being the most suitable base on a concept level, due to the profound influence of the final process mass balance on the allocation factors (both economic and mass-based), **the most appropriate allocation might change in the time period occurring between the writing of this report and the finalization of the LCA inventory to start the study**, following simulations and refining of the preliminary mass balances in the future development of the project. In case both allocation bases provide a comparable share of impacts among products, economic-based allocation will be preferred over the mass-based one, due to the reasons discussed above.

6.3.5 Database, method and impact categories

The Ecoinvent 3.10 database will be used to include background processes and emissions in the study.

The study will investigate the following impact categories, reported in Table 6-1 alongside the chosen calculation methods [5], [14].

Table 6-1 impact categories and related calculation methods chosen for the GoodByO LCA study.

Impact category	Measure unit	Calculation method
Global warming	kg CO ₂ eq.	EF v3.1/ReCiPe Midpoint 2016 (H)
Water use	m ³	ReCiPe Midpoint 2016 (H)
Land use	m ²	ReCiPe Midpoint 2016 (H)
Ecotoxicity, freshwater	CTUe	EF v3.1
Resource use, minerals and metals	kg Sb-eq	EF v3.1
Resource use, fossil	MJ	EF v3.1

The use of EF v3.1 method would make the study, at least partially, adhere to standards set by the EU Commission through the PEF methodology. However, the use of additional methods such as ReCiPe 2016 Midpoint (H) can benefit the study, whether to assess robustness of assessed impacts or to assess impacts using a calculation better suited to low-TRL technologies. As an example, in the case of water use, the ReCiPe method calculates the total used water in the examined life cycle stages, allowing to evaluate the need for water consumption optimization.

The global warming indicator will assess the emissions of greenhouse gases (GHG), using both EF v3.1 and ReCiPe Midpoint 2016 (H) methods. Assessing the impact with two different methods allows to determine whether the assessed global warming impact value is robust or highly dependent on the chosen method.

The water depletion impact category was selected based on the emphasis of the GoodByO process on green H₂ use. While wastewater recycling might represent a beneficial aspect for the water depletion, the use of green H₂ would represent a potentially significant water consumption step. The ReCiPe method was selected as its water depletion assessment reports the water consumption of the process, thus allowing a direct and clear indication of the process water request, useful for better efficiency upon TRL development.

The land use category was chosen based on the environmental concerns of palm oil-based products, which the GoodByO project aims to replace.

The freshwater ecotoxicity was selected based on the possible reuse of the wastewaters, which could help reduce the impact.

Minerals and metals use, as well as fossil use, was selected based on the comparison with fossil-based products, which tend to have rather high consumption of minerals or fossil

resources, thus acting as benchmark for the GoodByO biorefineries relinquishment of such resources.

6.3.6 Geographical and temporal scope

The temporal scope of the study was set on 2030. The studies geographical scope will be set in multiple locations in Europe.

6.3.7 Scenarios

At the current stage, no relevant scenarios were yet defined, aside from the main system described in section 6.3.1. Additional scenarios will be defined alongside the project development, building upon the future evolution of the process and on the preliminary results obtained by the first LCA analysis. It is paramount to add that the two process scenarios (“C6” and “EtOH”) do not represent different LCA scenarios, as the definitive process scenario will be defined at a later stage of the project, and the other will not be taken into consideration in the final LCA analysis.

6.3.8 Sensitivity analysis

Sensitivity analyses will be defined during the future development, as they are better defined after observing the preliminary results of the LCA study, or development of other activities within the project. The sensitivity analyses will be aimed at investigating potential interesting alternatives in the process (e.g., in the transportation modalities), or at validating the robustness of the analysis.

6.4 Life Cycle Inventory

The LCI of the study will mainly encompass primary data collected during the GoodByO project. Gaps in the data of foreground processes will be filled using secondary data from literature or, when possible, calculations and simulations. On the other hand, all background processes that require modelling will be modelled using secondary data. Other than filling the LCI, the study will also assess the quality of the used data, beyond the more general classifications of “primary” and “secondary”. The data quality will be assessed through a protocol based on the methodology described by Edelen and Ingwersen [15]. A qualitative pedigree matrix will be used to assess the quality of data, based on the criteria listed in Table 6-2, referring to the individual flows entering the foreground processes. Therefore, data pertaining to each flow will be evaluated.

It is important to specify that while these criteria will be applied to all foreground process data, only background processes which will be modeled and not directly taken from the database will be treated similarly. The rest of database flows will not be examined.

Table 6-2 Description of the applied data quality index, adapted from Edelen and Ingwersen study [15]. FG: foreground processes, BG: background processes.. * Only background processes modelled for the purpose of this specific study will be evaluated through the index; background process deriving from daabase will not be analyzed.

Quality index	Description	Applied to
Reliability	Primary or secondary data	FG, BG
Temporal	Difference between year of collection and year of application in the study	FG, BG
Geographical	Relevance of geographical area of data collection	FG, BG
Technological	Relevance of collected data to the analyzed system processes	FG, BG
Representativeness	How well data represents the overall market and/or common industrial practice pertaining to the described technology or operation	FG

For sake of standardization of quality assessment and to ensure an easy comparison between studies, the four maintained quality indexes were kept as stated by Edelen and Ingwersen. The reader is therefore referred to their study for further details [15].

Additionally, an interesting “model/process” level index was reported by Edelen and Ingwersen, but not fully described. In LCA studies, background data is usually chosen from a database. The choice of the exact database flow represents a quality index of the model, since it is not uncommon in LCA studies to rely on proxies, when no model flow in the database fits the analyzed process unit. On the basis of Edelen and Ingwersen study, the following evaluation of the qualitative index will hence be proposed (Table 6-3).

Table 6-3 Description of background flow quality index proposed for this study, on the basis of Edelen and Ingwersen work.

Background flow quality index				
1	2	3	4	5
Same technology and feedstock, same geographical area	Same technology and feedstock, different (related) geographical area	Same technology and feedstock, non-related geographical area	Same technology, proxy feedstock, same geographic al area	Proxy technology and feedstock

The criteria proposed in Table 6-3 indicate how accurately each upstream operation is represented by the background flow chosen from the database.

The highest quality (index 1) pertains to an accurate representation, meaning that the background flow describes the same technology required by the investigated system, using the same feedstock (if any), and operating in the same geographical area as the investigated process upstream. By contrast, the lower qualities (indexes 4 and 5) represent background flows that either use a proxy feedstock (i.e., a different but similar feedstock to that of the investigated system upstream) or both a proxy feedstock and a proxy technology.

An example of this index can be provided by considering renewable electricity in a specific geographical area. If the specified geographical area mainly relies on wind power for renewable electricity production using a certain size of wind turbines, a quality index of 1 would be applied to a background flow describing “electricity from wind power, using the same wind turbine size, in the specified geographical area”. On the other hand, a background flow describing “electricity from photovoltaic, in the specified geographical area” would obtain a quality index of 5, as the technology would be different, even if still producing renewable energy.

6.4.1 Methodology description for each quality index

Reliability

The reliability criterion is based on the origin of the data. Regarding primary data, the data quality assessment will specify the eventual need for verification through cross-check with literature, if not possible by mass/energy balance closure. Simulated data and calculated data will not be differentiated from the point of view of the quality index; however, the report will specify whether simulations or less accurate calculations were performed.

Verification of data will be performed based on the type of data. For primary data, whenever possible, mass/energy balance closure will be verified. Closures equal or higher than 99% will be accepted, whereas closures between 95 and 99% will be evaluated on the basis of uncertainties of measurements or experiments. Closures between 90 and 95% will be evaluated on the specific case basis, to determine whether the uncertainty could be acceptable (even if not desirable) or the data would remain unverified. Closures lower than 90% will be considered unverified in every case, and other means of verification will be adapted (e.g., cross-check with other literature). In case of verification by cross-check, the literature references will be chosen based on the specific data to be verified, as accuracy of certain data might be more time-sensitive than others.

Temporal

The temporal index will mostly regard secondary data, as primary data will be collected by GoodByO partners. In case of averaged literature data, the state of the technology will also be accounted for through verification. For instance, already well-established technologies may be less affected by longer time frames and thus also be verified by older data, as opposed to novelty applications. Thereby, the quality assessment will not

be altered, but the verification will be less restrained for already established technologies.

Geographical

The geographical area of the study will be set in several locations in Europe.

In cases where no background flows should be available in the used database, for the specific European country considered, background flows pertaining to a generalized European area might be used, and seen as a different (but related) area, since there is no guarantee that the “European-level” background flow will be similar to the “country-specific” flow.

On the other hand, non-EU countries will be treated as non-related areas. Lastly, regarding Switzerland, it will still be considered a related area due to its geographical location, even if not an EU Member State.

Technological

One of the parameters considered by the technological index is the process scale. Since one of the objectives of the project is to upgrade the TRL of the process, a scale-up is likely to be expected. Hence, the industrial scale will be considered as the most accurate scale for secondary data.

Representativeness

As the foreground processes will mostly derive from the GoodByO project, there might be a high possibility that these data could be less representative for the overall market and/or industrial practice, thus attaining a low quality index value. In these cases, the quality score will be discussed, contextualizing whether the low index value is tied to poorly collected data, or to the innovations of the GoodByO project. For example, attributing a low quality to data regarding innovative processes (thus not diffused in common industrial practice or overall market) would be penalizing towards the concept of innovation itself.

On the other hand, as modelled background processes will mostly rely on secondary data, the quality index will be applied as intended by its original proposers [15].

Background flow quality

This index, proposed for the GoodByO biorefinery on basis of Edelen and Ingwersen work, will be applied to all background flows, both modelled and already existing in databases. As different operations will present different characteristics, it may not always be possible to apply every criterion listed in Table 6-3.

In cases where the type of feedstock will be irrelevant (e.g., transportation of non-hazardous materials, transportation of solids, etc.), only technology and geographical area will be considered for the index. By contrast, in cases where technology and feedstock are inherently tied (e.g., renewable electricity production, where the feedstock dictates the necessary technology for producing electricity), both, technology and

feedstock will either be the same as the investigated process upstream or be both proxies.

Obviously, operations suited to be evaluated by the listed criteria (e.g., relevance of feedstock for the operation, but feedstock not inherently tied to technology) will be evaluated following criteria listed in Table 6-3.

Lastly, as the name implies, foreground data will not be examined according to this criterion.

7 FINAL REMARKS ON CHOSEN METHODOLOGY

The chosen methodology will cover the main steps of the GoodByO process, adhering to the set goals of the study. In particular, the functional unit and multifunctionality approach will be targeted at allowing the assessment of each products impact and their comparison with fossil and other bio-based products.

Although a definitive basis for the allocation cannot be determined at this stage, due to possible changes in the process mass balance which could significantly affect the allocation factors, preferring an economic-based allocation over a mass-based allocation would allow to avoid issues trying to determine the function of energy carriers (i.e., biogas) based on their mass, rather than on their energy content. Moreover, discarding an energy-based allocation will avoid issues in trying to define an energetic content of carotenoids.

The functional unit being placed on one of the products (i.e., bio-octanoic acid) is also in line with the most common practices in similar LCA studies, further standardizing the study.

The impact categories chosen to be investigated will address the environmental concerns tied to different fossil-based and bio-based materials, from the GHG emissions of fossil-based fuels to the concerns on land use for production of palm oil.

Lastly, the analysis on quality data will create a sounder final assessment, suggesting which data to refine or optimize, in view of the future development of the GoodByO process.

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9 ANNEX

9.1 EF v3.1 impact categories

The EF v3.1 method assesses sixteen impact categories, which are compulsory to report in PEF-compliant study, but are not in any other LCA methodology. The impact categories are reported in

Table 9-1.

Table 9-1 EF v3.1 impact categories and related measure unit [5].

Impact category	Measure unit
Climate change	kg CO ₂ eq
Ozone depletion	kg CFC-11 eq
Human toxicity, cancer effects	CTUh
Human toxicity, non-cancer effects	CTUh
Particulate matter	kg PM _{2.5}
Ionising radiation	kg U235 eq
Photochemical ozone formation	kg NMVOC eq
Acidification	mol H ⁺ eq
Eutrophication, terrestrial	mol N eq
Eutrophication, freshwater	kg P eq
Eutrophication, marine	kg N eq
Ecotoxicity, freshwater	CTUe
Land use	Pts
Water use	m ³
Resource use, fossils	MJ
Resource use, minerals and metals	kg Sb eq