Sustainable and cost-effective production process for the upcycling of olive, grape and nut by-products into 4 natural and healthy ingredients for nutraceutical and cosmetic applications

Project number: 888003

D3.1 Life Cycle Methodology definition and template

Version 2

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HISTORY OF CHANGES		
Version	Date	Changes
Version 2	05/07/2021	The scope of the deliverable was change due to the required modifications in the methodology of the S-LCA.

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PROJECT INFORMATION

Project full title: Sustainable and cost-effective production process for the upcycling of olive, grape and nut by-products into 4 natural and healthy ingredients for nutraceutical and cosmetic application

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Abstract:	A Life Cycle Sustainability Assessment (LCSA) will be performed within the project UP4HEALTH. It includes Life Cycle Assessment (LCA) to assess the environmental impacts, Life Cycle Costing (LCC) analysis to assess the economic feasibility and Social Life Cycle Assessment (S-LCA) to evaluate the social impacts of the products developed. Furthermore, the processes will be modelled for simulation and multi-objective optimization by using the own-developed tool by CTA, eco2des. The LCSA should allow further comparisons with products developed after the optimization and for products from other processes or feedstocks. With that aim, the methodology is defined in this deliverable for LCA, LCC and S-LCA, including standards and guidelines to use in the development of the LCSA, functional unit, system boundaries, data needs, data sources and impact assessment methods. Templates for collecting data from partners are included as annex.

1 LCSA METHODOLOGY UP4HEALTH

The Life Cycle Sustainability Assessment (LCSA) methodology will be based on the general recommendations from UNEP (United Nations Environmental Program (UNEP), 2011) and Walter Kloepffer (Kloepffer, 2008). It will consist of three interconnected assessments: Life Cycle Assessment (LCA), Life Cycle Costing (LCC) and Social Life Cycle Assessment (S-LCA). In consequence, the three pillars of sustainability (environmental, economic and social) will be included. As they all have a holistic and life cycle perspective, and they are based on the same normative (ISO 14040), it is possible to interconnect them keeping some common aspects of the goal and scope, having independent life cycle inventories and impact assessment methods and providing an interpretation that will gather the results of the 3 studies. The interconnection among LCA, LCC and S-LCA during the development of S-LCA can be represented as shown in Figure 1.

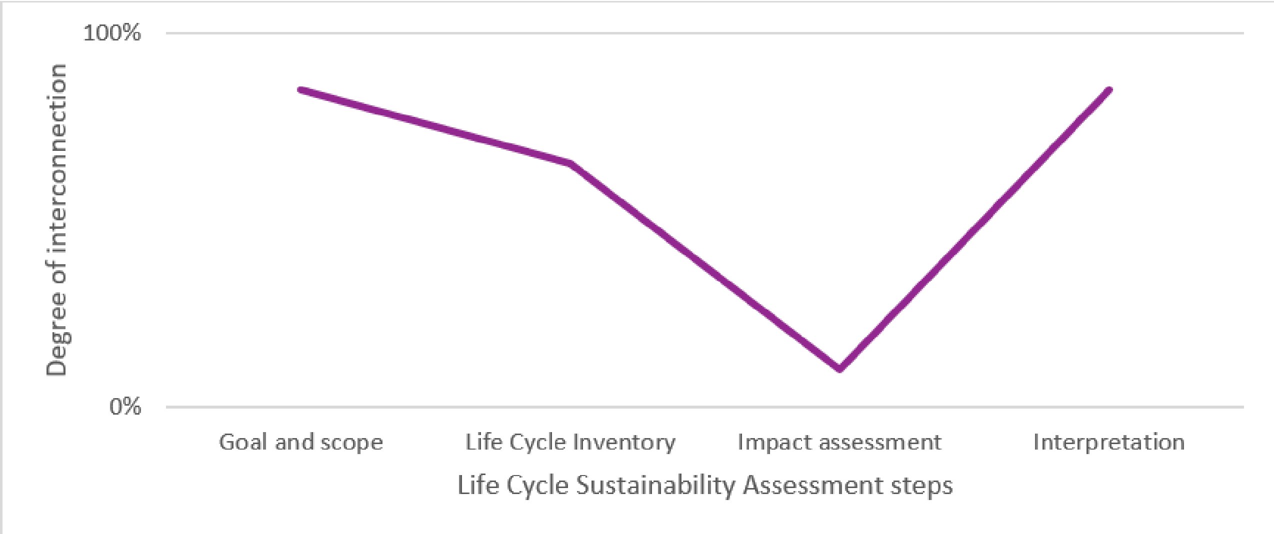

Figure 1. Level of interconnection of LCA, LCC and S-LCA during the LCSA development.

The structure in ISO 14040, main standard for LCA, will be followed for all the three assessments. In the following sections, the approach to develop the goal and scope, the life cycle inventory (LCI), the life cycle impact assessment (LCIA) and the interpretation will be explained. The explanation will include the overall perspective, from the point of view of the sustainable development and the specifications of each assessment will be detailed for each section.

The LCA is the most developed methodology of the three included in LCSA. There are schemes to declare the environmental impacts of products voluntary (type III eco-labels) based on LCAs verified by a third party. These documents are called Environmental Product Declarations (EPDs) and they must be developed under product LCA specific rules: Product Category Rules (PCRs). PCRs can be found for different products under the general rules of several program operators.

In the framework of UP4HEALTH, a research of PCRs will be carried out and draft PCRs will be developed for products. This task feeds from the LCSA methodology definition, particularly from the definition of the LCA.

2 GOAL AND SCOPE

The goal and scope of the LCSA will be the section with more similarities among the three assessments.

The products to be assessed in the UP4HEALTH projects are functional ingredients extracted from biomass. The process will be developed at pilot scale, and an energy production feasibility study will be performed . The biomass is obtained from the agriculture sector and the functional ingredients will be used in food products. The process and value chain will be tested within the UP4HEALTH project and the results obtained will be used for further upscaling of the production processes and improvement of the value chain to ensure product quality.

2.1 Goals of the LCSA

The objectives of the three sustainability assessments are listed below:

- The first goal of the LCSA will be to evaluate and comprehend the environmental, economic and societal impacts of the functional ingredients developed in the UP4HEALTH project.
- Then, the up-scaled process will be modelled and eco-designed in order to optimize the overall sustainability of the functional ingredients production processes and avoid burden shifting among impact categories and among pillars (environment, economic and society).
- At the same time, the feasibility of the energy production in the UP4HEALTH biorefinery will be assessed at different scales.
- The assessment will aim to find the optimal operational parameters to optimize the overall sustainability of the processes at larger scales.
- One specific goal for the LCA will be to evaluate current methodologies and Product Category Rules (PCRs) and, if there are no existing PCRs for UP4HEALTH products, develop draft PCRs.

2.2 Target audience

The LCSA will be addressed for the developers of functional ingredients extraction process to inform them about the most relevant hotspot in their processes in order to improve the sustainability associated in further upscaling plans. In addition, the LCSA will also be addressed to important stakeholders such as the food products producers, who will use the functional ingredients in the future. In addition, further reporting could be made to inform the public about the environmental impacts of the products developed.

2.3 Geographical scope

The LCSA will be located in Spain, where the main production plant is located. This influences directly the LCA results given that the energy used in the project will include the impacts related to the energy production mix of Spain. The economic impacts will also be influenced by the use of Spanish taxes and salaries. The social impacts results will also be determined by this geographical scope by defining the reference scale in relation to Spanish socio-political situation and statistics.

2.4 Main references

The definition of the methodology has been based on specific standards and guidelines in order to allow comparability and provide results with scientific robustness. Many references have been consulted but the following list collects main documents regarding methodological issues of LCA, LCC and S-LCA used for the methodology definition.

- LCSA:
  - Towards a Life Cycle Sustainability Assessment: Making informed choices on products, 2011, UNEP ((United Nations Environmental Program (UNEP), 2011))
- LCA:

    - ISO 14040, ISO 14044 (ISO, 2006a) (ISO, 2006b)
    - Product Environmental Footprint (PEF) guide, 2019, European Commission (Zampori et al., 2019)
- LCC
    - Environmental life-cycle costing: a code of practice (Swarr et al., 2011)

Common and normalized methodologies for products is missing. Only Standards regarding the LCC of buildings is currently released. The mentioned reference has been consulted to link the results of LCC with LCA and S-LCA results.

- S-LCA
    - Guidelines for Social Life Cycle Assessment of Products and Organizations, UNEP 2020. (Benoît Norris et al., 2020)
    - Product Social Impact Assessment Handbook, by the Roundtable for Social Product Metrics - (Goedkoop, M.J.; de Beer, I.M; Harmens, 2020)
    - A Product Social Impact Life Cycle Assessment Database version 3 Documentation, KirillMaister, Claudia Di Noi, Andreas Ciroth, Michael Srocka (all GreenDelta) 2020 (Maister et al., 2020)
    - Social Hotspot Database[1] (NewEarth B, 2015)

The document provided by UNEP has been used as main reference to develop the S-LCA methodology to be followed. The other guidelines consulted were used given that they are compliant with the document from UNEP and they provide useful information about the impact assessment, data needs, reference scale method, data sources, the interpretation of results and communication of results.

2.5 Functional unit

The functional unit for LCA and LCC will be based on physical properties and quality specifications: 1 kg of functional ingredient including packaging and fulfilling the requirements of the final food product producer. In consequence, all the environmental and economic impacts will be expressed in function of 1 kg of functional ingredient. For the S-LCA, the FU will be further discussed after verifying the data availability.

2.6 System boundaries

The system boundaries of the assessment will be adapted for each assessment. social, economic and environmental, which will include all those stages with high relevancy. Some of the life cycle stages will be shared among the three or two assessments and other stages will be independent. The common stages will be the raw material production and the industrial processing. The scheme presented in Figure 2, extracted from United Nations Environmental Program (UNEP), 2011 gives an example of the LCSA system boundaries establishment.

[1] http://www.socialhotspot.org/

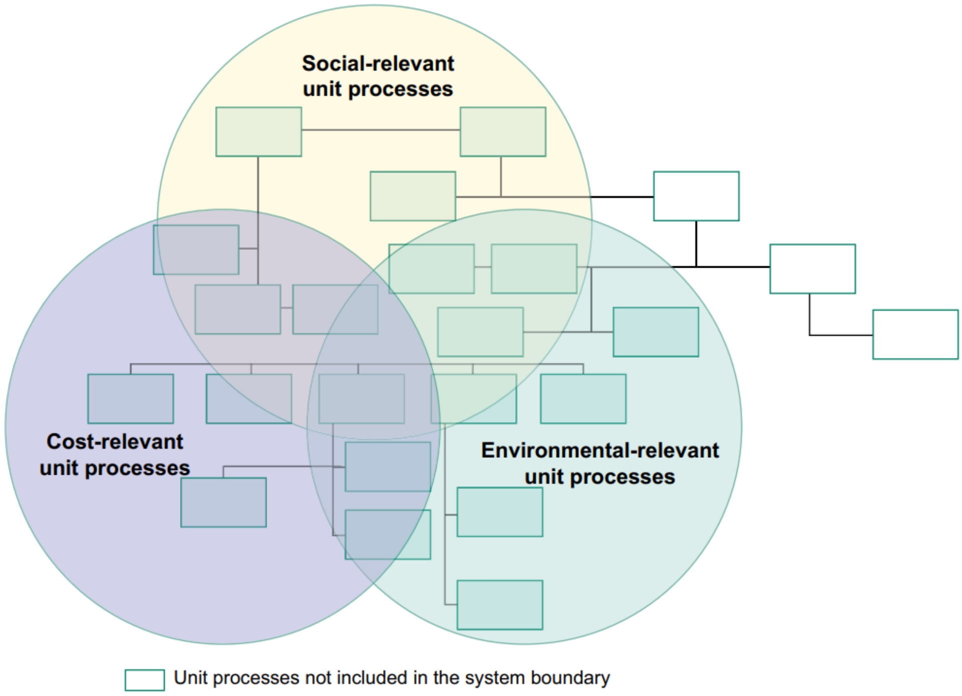

Figure 2. System boundaries for LCSA (United Nations Environmental Program (UNEP), 2011).

In Figure 3, the life cycle stages assessed in LCSA are presented. The impacts related to sustainability will be assessed in a holistic view but the LCA, LCC and S-LCA will consider different stages or aspects of the functional ingredients' life cycle.

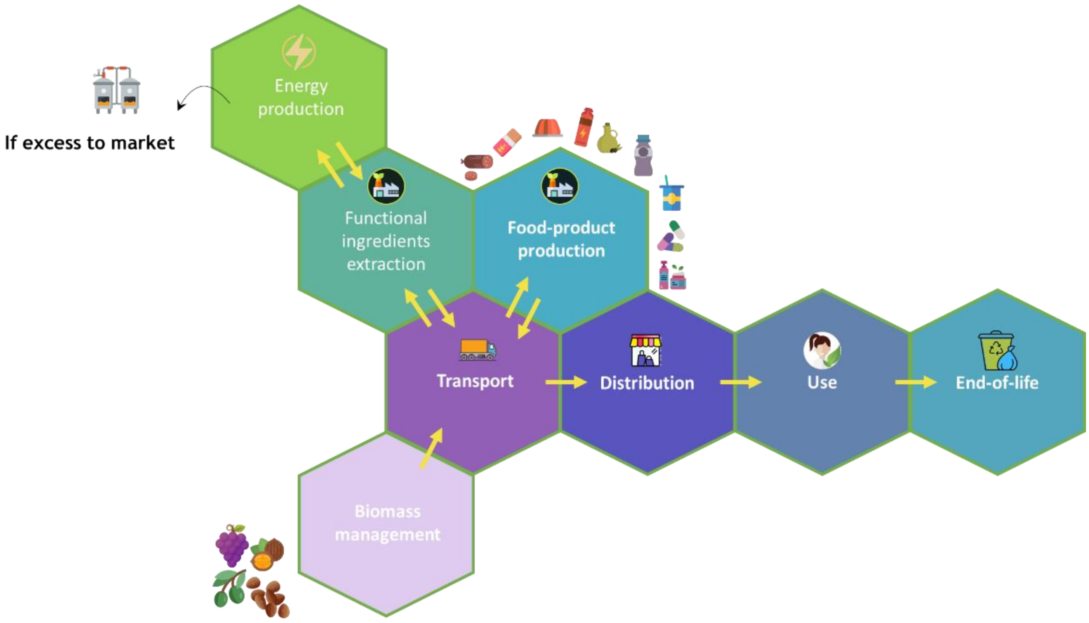

Figure 3. Life cycle of UP4HEALTH products

The final food products production stage is included in the UP4HEALTH project to validate the functional ingredients extracted in different matrixes. Given that final food products are not yet fully developed, and they will not be fully developed within UP4HEALTh, this stage will not be included in the LCSA, due to the low representability for future scenarios.

2.6.1 LCA

Biomass management, transport, functional ingredients extraction, energy production, distribution, use and end-of-life will be incorporated. Given that the validity of the ingredients in final products needs to be tested, the product production will be probably neglected from the study.

2.6.2 LCC

It will address the biomass management, transport, functional ingredients extraction and energy production to assess the viability of the functional ingredient production process and the energy production in the biorefinery.

2.6.3 S-LCA

It will consider the same life cycle stages as the LCA except the transport, distribution and end-of-life, due to the low relevance these stages might present in this assessment. The expected impacts on society of these products are mainly presented in the upstream stages, such as biomass management and functional ingredients extraction, given they are innovative products which boost local community societal aspects (job creation and retention and the impacts on health of final customers). Given the indicators on final customers are not yet fully developed, it is likely the impacts on this stage might not be quantified.

2.7 Selected impact categories

The categories selection is based on relevancy and data availability criteria.

2.7.1 LCA

Impact categories included in the EF method v3 (or most updated version at the moment) will be used. Each impact category will be quantified under a specific method selected by a panel of experts at European level during the Single Market for Green Products (still in course).

Table 1. Environmental impact categories from EF method v3.0.

Impact category	Indicator	Unit	Method and description
Climate change	Radiative forcing as Global Warming Potential (GWP100)	kg CO2 eq	Baseline model of 100 years of the IPCC 2013
Ozone depletion	Ozone Depletion Potential (ODP)	kg CFC11 eq	Steady-state ODPs (WMO 2014)
Ionising radiation, human health	Human exposure efficiency relative to U235	kBq U-235 eq	Human health effect model based on Dreicer et al. 1995 (Frischknecht et al, 2000)
Photochemical ozone formation, human health	Tropospheric ozone concentration increase	kg NMVOC eq	LOTOS-EUROS model (Van Zelm et al, 2008) - ReCiPe 2008
Particulate matter	Impact on human health	disease inc.	PM method recommended by UNEP (UNEP 2016)
Human toxicity, cancer	Comparative Toxic Unit for humans (CTUh)	CTUh	USEtox model 2.1 (Fankte et al, 2017)
Human toxicity, non-cancer	Comparative Toxic Unit for humans (CTUh)	CTUh	USEtox model 2.1 (Fankte et al, 2017)

Impact category	Indicator	Unit	Method and description
Acidification	Accumulated Exceedance (AE)	mol H+ eq	Accumulated Exceedance (Seppälä et al. 2006, Posch et al, 2008)
Eutrophication, freshwater	Fraction of nutrients reaching freshwater end compartment (P)	kg P eq	EUTREND model (Struijs et al, 2009) - ReCiPe
Eutrophication, marine	Fraction of nutrients reaching marine end compartment (P)	kg N eq	EUTREND model (Struijs et al, 2009) - ReCiPe
Eutrophication, terrestrial	Accumulated Exceedance (AE)	mol N eq	Accumulated Exceedance (Seppälä et al. 2006, Posch et al, 2008)
Ecotoxicity, freshwater	Comparative Toxic Unit for ecosystems (CTUe)	CTUe	USEtox model 2.1 (Fankte et al, 2017)
Land use	Soil Quality Index Biotic production erosion resistance Mechanical filtration	Pt	Soil quality index (LANCA v2.2 by JRC)
Water use	User deprivation potential (deprivation-weighted water consumption)	m3 depriv.	Available WAter REmaining (AWARE). Recommended by UNEP, 2016
Resource use, fossils	Abiotic resource depletion – fossil fuels (ADP-fossil)	MJ	CML 2002 (Guinée et al., 2002) and van Oers et al. 2002
Resource use, minerals and metals	Abiotic resource depletion (ADP ultimate reserves)	kg Sb eq	CML 2002 (Guinée et al., 2002) and van Oers et al. 2002.

Deeper analysis will be done on climate change, water use, use of fossil and minerals and metals resources, ozone depletion, terrestrial acidification and photochemical ozone formation, particulate matter, given these categories were identified as most relevant in previous assessments in this plant (NUTRIBIOTA[2] and LIGNOXOS[3] projects). In any case, a new hotspot analysis with updated data will be performed using and the most relevant impact categories will be identified and assessed with more focus.

2.7.2 LCC

The costs will be classified in type of costs categories. Each category will include:

- CAPEX: equipment used in the production of the functional ingredients
- Depreciation: reduction of the value of equipment
- OPEX: products, raw materials, energy, water, salaries, renting, logistics and maintenance
- Taxes: taxes that the company will pay in function of their incomes related to the products assessed

Then, the Net Present Value (NPV) will be calculated, considering all the costs along the lifetime, to estimate the final LCOP. The LCOP will be the main indicator to evaluate the economic feasibility.

[2]Nutribiota: Modulación personalizada de la microbiota mediante el diseño inteligente de alimentos e ingredientes a partir del diagnóstico basado en enterotipos (NUTRIBIOTA), Gobierno de Navarra (https://isanatur.com/the-rd-project-nutribiota-funded-by-the-government-of-navarra/)
[3]Lignoxos: valorización de residuos agroalimentarios lignocelulósicos en ingredientes funcional XOS (https://lignoxos.eu/)

2.7.3 S-LCA

First, a hotspot analysis using SHDB will be performed to evaluate the main hotspots. A literature review will be performed to identify most relevant indicators assessed in similar value chains. Ultimately, the impact categories will be extracted from Guidelines for Social Life Cycle Assessment of Products and Organizations by UNEP, 2020. The job creation/retention indicators have been included following the recommendations of the European Commission for BBI projects, which demands these indicators as a diagnosis to measure the impact of the project. The methodology selected to evaluate it is the one developed by Pillain et al., 2019, which uses Input-Output (IO) tables and process specific data to assess the influence of one activity along the value chain:

- Hotspot analysis: all the impact categories and indicators used in SHDB will be considered, although only those accounting with more than 80% of the weighed impacts will be analysed with special focus. The damage and impact categories in the SHD are presented in Table 2. The social issues included in SHDB have different influence in different impact categories.

Table 2. Damage category and impact categories included in SHDB.

Damage Category	Impact category
Labour Rights & Decent Work	Wage
	Poverty
	Child labour
	Forced labor
	Excessive WkTime
	Freedom of assoc
	Migrant labour
	Social benefits
	Labour Laws/Convs
	Discrimination
	Unemployment
Health & Safety	Occ Tox & Haz
	Injuries & Fatalities
Human Rights	Indigenous Rights
	Gender Equity
	High Conflict Zones
	Non-Communicable Diseases
	Communicable Diseases
Governance	Legal System
	Corruption
Community	Access to drinking water
	Access to Sanitation
	Children out of School
	Access to Hospital Beds
	Smallholder v Commercial Farms

- Job creation potential: the job creation potential will be divided in upstream jobs (direct and indirect) and jobs created within the production life cycle stage.

➢ Additional social information: the UNEP guidelines and current S-LCA methodologies are designed for products on the market and not products in the research and development phase. In consequence, in R&D projects, only few indicators and categories are suitable. A variety of factors determine the selection of categories and indicators for the social assessment: the location of economic activity, the system boundaries, the scope of the study and the availability of high-quality data. The selection also depends on the type of product and value chain to assess. In UP4HEALTH, the selected indicator is the health and safety of users following the criteria set by RPSM, given the availability of documents and studies addressed to evaluate the benefits or harms to human health of proteins.

The categories and indicators selected shall be representative and valid to assess R&D projects. This consideration is important when selecting categories and indicators from recognised international methodologies, such as the ones developed by UNEP or by RSMP. . Firstly, some concepts need to be defined:

- **Stakeholder category: "**cluster of stakeholders that are expected to have shared interests due to their similar relationship to the investigated product systems. Stakeholder categories provide a comprehensive basis for the articulation of the subcategories. The proposed stakeholder categories are deemed to be the main group categories potentially impacted by the life cycle of the product" (Benoît et al., 2013).
- **Social topic:** social areas related to stakeholder groups that should be measured and assessed such as working hours, community engagement, child labour, etc. (Goedkoop, M.J.; de Beer, I.M; Harmens, 2020).
- **Performance indicator:** performance markers for each of the social topics, for example, number of working hours per week, minimum wage paid, etc. (Goedkoop, M.J.; de Beer, I.M; Harmens, 2020)

Table 3.Selected stakeholders, social topics and performance indicators (based on Goedkoop, M.J.; de Beer, I.M; Harmens, 2020).

STAKEHOLDER	SOCIAL TOPIC	DEFINITION	PERFORMANCE INDICATOR	DEFINITION
Consumers	Health and safety	Products are expected to perform their intended functions satisfactorily and not pose a risk to consumers' health and safety. This social topic addresses both risks and the positive impacts that products may have on the health and safety of the end-users of products	Presence of certifications or labels for the product/sites sector	

In addition, some positive impacts could be addressed. Positive social impacts can be addressed in different ways, depending on the scenario that fits the better the types of positive impact according to UNEP, 2020.

In this methodology, type B positive social impacts will be considered. Product life cycles also create positive social impacts through their presence. Products generate impacts on employment, capacity building or infrastructure improvement. These impacts are positive if the company is present in a location and may disappear if there are modifications in the product life cycle, aimed at reducing other negative impacts.

2.8 Treatment of multi-functionality

Functionality will be dealt following the hierarchy described in the PEF guide. First, system expansion or sub-division will be used if possible. If this first approach is not feasible, physical allocation will be used unless economic allocation is preferred. In some cases, the products and co-products sharing some units of the production process have very different functions and mass allocation is not relevant anymore. For example, most food products from agriculture normally use economic allocation due to different function of waste streams, energy produced or final food product.

3 Life Cycle Inventory (LCI)

Three different LCIs will be developed, one for each assessment: LCA, LCC and S-LCA.

The data will be collected from partners through physical interviews and/or online meetings and by using the LCI templates in excel format. The templates have been prepared by CONTACTICA and they are presented in annexes. Note that templates could be modified during the project.

The data needs and sources are described in the following section for each assessment. There will always be two type of data: primary data and secondary data. Primary data are provided by the stakeholders involved in the life cycle stage. Materials, energy, output streams (waste, emissions, products and co-products), operational data (materials, quantities, duration, people involved, etc.) or data to describe the value chain are considered as primary data. Secondary data are obtained from generic databases and includes information that project partners are not able to provide accurately, like the emissions embodied in the materials used or inputs and outputs of downstream and upstream processes.

3.2 Source of data

3.1.1 LCA

The data required for the LCA will be obtained from the following sources:

- Primary data: description of extraction process and value chain, including materials and energy used, amounts, input and output streams, waste streams management scenarios, delivery distance of products used, etc will be provided by partners involved. Data will be asked using the LCI templates found in Annex 1: LCI templates.
- Secondary data: LCA databases will be used to include the emissions associated to the use of materials, energy, industrial processes and transport. Ecoinvent, ELCD, Agribalyse, World Food Database and Industry data (World steel, Plastics Europe, etc) will be used as sources. Default scenarios for end of life or transport will be extracted from PEF guide when no data is available. Additional data can be sought in scientific literature if needed.

Data needed from partners for the LCA will be asked through the template found in Table A 1.

3.1.2 LCC

Costs will be obtained from partners, who must fill the template from Table A 1. with actual cost data. When data is not available, market price will be used. Data concerning taxes or interest rates will be consulted with partners and compared to official indicators for the specific country in which the process takes place.

3.1.3 S-LCA

Data concerning quantities of materials, by-products, waste streams and emissions from industrial processes will be provided. Then this data will be related to process from databases to build the model and calculate the potential environmental impacts. Partners will also provide the cost of their materials, utilities and services.

Data gaps will be filled with data from literature and secondary databases. All the sources previously identified are collected in Table 4.

During the hotspot analysis, the data obtained in the LCI regarding the costs of the inputs and services for the protein extraction will be used together with the SHDB.

Data used to evaluate job creation and job retention potential will be collected from partners (same data used in LCA and LCC) and from specific country data (IO tables).

Data needed for the assessment of the impact categories extracted from S-LCA methodologies and standards will be directly asked to partners. Data gaps will be filled with data from literature and secondary databases. All the sources previously identified are collected in Table 4.

Table 4. Data sources for S-LCA.

STAKEHOLDER	SOCIAL TOPIC	PERFORMANCE INDICATOR	TYPE OF DATA FOR ALEHOOP	SOURCE OF DATA
Consumers	Health and safety/Transparency	Presence of certifications or labels for the product/sites sector	Primary	Partner

The data that need to be collected from partner, will be asked by sending the template found in Table A 1.

4 LIFE CYCLE IMPACT ASSESSMENT (LCIA)

In this third step of the LCSA, the results will be extracted. The impacts will be classified into environmental impact categories (LCA), types of costs (LCC) and social indicators (S-LCA). The methods to calculate the impacts for different categories are presented below for each type of assessment.

4.1.1 LCA

The LCIA method for the LCA will be EF method 3.0 for current scenarios analysis given that it uses the most updated LCIA methods for each category, selected by a panel of European experts. The emissions will be classified and characterized by the use of Characterization Factors (CFs) provided by the method. Normalization and weighting factors included in EF method will also be used to calculate single score results. The SimaPro software which includes the EF method 3.0 will be used. The categories and impact methods are gathered in Table 1.

4.1.2 LCC

The LCC will be based on the calculation of the Net Present Value (NPV) or present Value (PV) and the Levelized Cost of Production (LCOP). This cost represents the value of the final product to equalize costs and sales in a pre-defined time framework. Only exceeding the LCOP, benefits can be obtained. It is a reference value to compare with market price of competence products.

The costs of all categories or type of costs (see section 2.7.2) will be used to calculate the Present Value (PV):

$$PV = \sum_{i=1}^{20} \frac{Costs}{(1+i)^t}$$

Costs: annual operational costs and capital costs performed in year *t*.

$$Costs = EBITDA + taxes$$

$$EBITDA = CAPEX + OPEX + Maintenance + Sales$$

i: nominal discount rate. It is assumed to be 5%, equal to the real discount rate. In consequence, the inflation is not considered.

4.1.3 S-LCA

The S-LCA impacts will be different for job creation and job retention potential and for the other impact categories selected (section 2.7). Job creation potential will be evaluated using following formulas:

- Potential Jobs Created = (WH each input * G stock available)/FTE
- Gstock: t/year
- FTE (Full-time equivalent): h/year for all sectors
- WH input = f*Y (h)
- Y: cost from inventory for all the inputs (€)
- f = S*$(I\text{-}A)^{-1}$
- S: direct working h/€
- $(I\text{-}A)^{-1}$: Input-Output tables for Spanish economy

Regarding the evaluation of categories and social topics included in specific S-LCA methodologies and standards, the impact assessment method will be based on a scale-based approach to identify social risks or hotspots. The selected social topics will be assessed individually and no weighting will be applied to obtain a single score result. Every social topic result will be presented in terms of risks and scale levels. The scales levels are defined differently from (Goedkoop, M.J.; de Beer, I.M; Harmens, 2020) to (Maister et al., 2020). In both cases the highest risk corresponds to red colour and green corresponds to lowest risk.

In the methodology developed by Goedkoop et al. the scale levels go from -2 (highest risk and red colour) to +2 (green colour and lowest risk) (see Table 4). To identify the scale level, performance indicators need to be defined based on data collected from stakeholders and from secondary data sources. Several performance indicators can be used to identify the scale level. Some performance indicators are defined on quantitative approach, defining minimum or maximum values to fulfil the criteria, and other performance indicators are based on qualitative justifications.

Table 5. Scale reference impact assessment method. Health and safety of users.

Stakeholder group / category	Social topic	Scale level description	Performance indicator	Score
Users	Health and Safety	There is solid science-based evidence that normal use of the product can contribute very significantly to a better health and safety AND the product or service is marketed and managed in such a way that it does reach the most vulnerable groups who would benefit most from this product and service.	The evidence must contain two parts: • Scientific evidence or opinions from independent experts or independent organisations that are specialised in this area, confirming the product has properties that can significantly improve the health and safety of users • Opinions from independent experts who confirm that the product indeed is marketed and managed in such a way that it reaches the most vulnerable groups In a B2B situation a description of the efforts to design components and/or support the design of the final product that contributes to this achievement.	+2
		The company has a dossier or other evidence that shows how the product or service has been successfully designed to create a maximum contribution to health and safety of the user and that the recommended use of the product contributes to a better health and safety for the intended users.	A dossier or evidence that contains elements such as: • The company has assessed how the product can optimise or harm the health and safety of the user; for instance, through reduction of salt, saturated fats or calories, or significantly improved ergonomics. • The product developers have a verifiable audit trail on the efforts and decisions to optimise the health and safety of the user. In a B2B situation a description of the efforts to design components and/or support the design of the final product that contributes to this achievement	+1
		The normal use product and the way it is marketed and managed does not have any significant detrimental effect on the health and safety of the user.	Absence of verifiable claims by authorities, consumer organisations and user groups that there is a significant detrimental health and safety impact (for B2B and B2C situations). Reports from authoritative sources that confirm there is no or a negligible health impact, in the way the product is used (for B2B and B2C situations)	0
		The normal use of the product has negative health or safety impacts, but the producer has developed a corrective action plan to improve the	Verifiable information that the health and safety issue is recognised by the company and that the product and the way it is managed and marketed is being improved with a clear and credible timeline	-1

		product and to influence the way the product is used in order to significantly reduce the negative impacts.	In a B2B context: verifiable information that the health and safety issue is recognised and that the component or ingredient and the way it is applied is being improved with a clear and credible timeline.	
		Any use of the product has direct negative health or safety impacts on short or long term.	Reports from consumer organisations, NGOs, watchdogs and authorities that describe the negative impacts The product does not conform to the legal requirements and is not approved by the authorities.	-2

In conclusion, each social topic will be assessed individually and no aggregation or weighting of results will be performed, due to low robustness of methods and lack use of this approach by the industry stakeholders who tested the methodology developed by The Roundtable for Product Social Metrics. Each social topic result will represent a risk (higher or lower) according to the criteria described by the methodology in which the indicator was obtained from.

5 Interpretation of results

An individual interpretation will be performed and the final conclusions will interconnect the results of the three assessments.

5.1.1 LCA

The environmental impact results will be interpreted throughout a hotspot analysis. The **hotspot analysis** is a methodology to interpret the LCA results according to the PEF Guide. It aims to identify the most relevant impact categories, stages, processes and elementary flows of the life cycle of a product or activity. The definition of most relevant relies on the 80% criteria, i.e., the most relevant impact categories, stages, processes and elementary flows are those which contribute to the greatest 80% of the normalized and weighed impacts. The following steps must be followed to do a hotspot analysis:

1) First, characterized results are calculated by classification and using characterization factors to obtain the results for each impact category.
2) The categories related to toxicity impacts are excluded due to the low robustness of their characterization factors.
3) The remaining impact categories results are normalized to the average global person emissions for each impact category (EF method normalization factors).
4) Then, the impacts are weighted using the weighting impacts provided by the European Commission (EF method), converting all the results into one common unit (points).
5) The results are sorted from greatest to lowest and the greatest values are summed until the greatest 80% of the impacts is achieved. The impact categories which results are part of this 80%, are considered as most relevant impact categories.
6) The same methodology is used to identify the most relevant stages for each most relevant impact category and the most relevant processes and elementary flows.
   In this study, the most relevant elementary flows will not be identified due to the final application of this LCA. The stakeholders involved and parties interested in this LCA do not have influence on the

elementary flows although they have it on the processes, that is why the hotspot analysis identify the most relevant impact categories, stages and processes.

5.1.2 LCC

A similar criterion than the established for the LCA will be used for the economic analysis. The same threshold of 80% will be used to identify the most relevant costs, i.e., the types of cost with highest contribution within the whole-time framework of the assessment.

In addition, the feasibility of the processes can be evaluated in terms of NPV and Internal Rate of Return (IRR).

The results of LCOP will be interpreted comparing them with current competitors' price in the market.

Also, sensitivity analysis on certain parameters with higher uncertainty will be performed to evaluate different scenarios.

5.1.3 S-LCA

Job creation and job retention potential will be interpreted considering the amount of feedstock available and the potential production with the developed extraction processes. Also, the hotspot analysis results performed with SHDB and by literature review will be assessed using a hotspot analysis perspective, as used for LCA and LCC.

Regarding the impacts in categories from specific S-LCA methodologies, the results will be interpreted in function of the quality of data. A data quality assessment will be performed according to the criteria defined by UNEP (see Table 6).

Table 6. Data quality assessment criteria and score description (Benoît Norris et al., 2020).

Score	1	2	3	4	5
Reliability of the source(s)	Statistical study, or verified data from primary data collection from several sources	Verified data from primary data collection from one single source or non-verified data from primary sources, or data from recognized secondary sources	Non-verified data partly based on assumptions or data from non-recognized sources	Qualified estimate (e.g. by expert)	Non-qualified estimate or unknown origin
Completeness conformance	Complete data for country-specific sector/ country	Representative selection of country-specific sector / country	Non-representative selection, low bias	Non-representative selection, unknown bias	Single data point / completeness unknown
Temporal conformance	Less than 1 year of difference to the time period of the dataset	Less than 2 years of difference to the time period of the dataset	Less than 3 years of difference to the time period of the dataset	Less than 5 years of difference to the time period of the dataset	Age of data unknown or data with more than 5 years of difference to the time period of the dataset

Geographical conformance	Data from same geography (country)	Country with similar conditions or average of countries with slightly different conditions	Average of countries with different conditions, geography under study included, with large share, or country with slightly different conditions	Average of countries with different conditions, geography under study included, with small share, or not included	Data from unknown or distinctly different regions
Further technical conformance	Data from same technology (sector)	Data from similar sector, e.g. within the same sector hierarchy, or average of sectors with similar technology	Data from slightly different sector, or average of different sectors, sector under study included, with large share	Average of different sectors, sector under study included, with small share, or not included	Data with unknown technology / sector or from distinctly different sector

A score will be obtained for every data collected by doing the average of all criteria. Subsequently, the average score among all the results for all data used will serve as reference to estimate the quality of results for every social topic.

Finally, all the conclusions from LCA, LCC and S-LCA will be interpreted together. All the hotspots will be compared to identify the origin of sources and provide recommendations to avoid burden shifting among categories and pillars of sustainability. This means that no decision to improve the environmental performance should compromise the social or economic performance of the process in the upscaling.

6 ECO2DES TOOL

The process will be evaluated using the tool developed in CONTACTICA by an Industrial PhD program financed by the Community of Madrid (Spain) in 2017 (García-Casas, M. et al. 2020). The LCA, LCC and S-LCA methodologies previously described will be embedded into the tool, which will link them with the virtual plant simulation of the UP4HEALTH process. Then, a multi-objective optimization problem will be defined and resolved using genetic algorithms to optimize technical, economic, environmental and social indicators.

6.1 Introduction.

Industry is a key sector to achieve worldwide sustainability with a prosperous society, with a modern, resource-efficient and competitive economy; and where there are no net emissions of greenhouse gases (European Commission, 2019). Therefore, new value chains must be studied and developed, as well as, the current ones must be optimized in terms of sustainable key performance indicators. However, during the development of new innovative processes, there are no industrial data that can support any life cycle assessment, LCA, or life cycle cost, LCC, analysis, which gives rise to numerous trial-and-error phases during technology upscaling, exorbitantly increasing time-to-market and costs, while achieving solutions that may not be optimized or, even, feasible in sustainable terms.

Predictive models and process simulations, however, are able to compute, through physicochemical relationships, the behaviour of that technology under development at industrial scale and formulate scenarios for environmental or cost optimization. Even so, process simulation, LCA and LCC methodologies are well structured and there are many options of commercial software specialized in these areas. Nowadays, at the best of our knowledge, there is no current research combining them in a holistic way for their application in the economic and environmental optimization of any industrial design of process under research and/or development. With this premise, the **eco2des** framework was born. It is an object-oriented Python framework for sustainability-based optimization of industrial processes. The tool takes advantage of the full feature set of Python, such as its facilities for fast prototyping and the several available libraries for data processing, data analysis, scientific computing and data visualization. **Eco2des** is a descriptive tool, which documents life cycle inventories and characterizes them through their environmental impact and associated costs. It is a predictive tool, since it uses as inputs physicochemical models for process simulation in the research phase; and adaptive, since it automates process design selections based on multi-objective optimization algorithms. As a result, the framework is able to take a process simulation, such an aspen plus file (Figure 1), linking it with a LCA and a LCC models and optimize its sustainable objectives changing operational variables, topology or supply chain decisions.

Figure 4. eco2des concept

6.2 Process modelling design and plantwide simulation methodology.

The aim of this task is to generate feasible and industrially realistic basis, information/data to optimize the UP4HEALTH concept before scaling it up to a real plant. Figure 5 shows the principal process steps: In green, the olive oil production process is represented. This process is already implemented and optimized in ISANATUR plant so it is considered out of scope for the optimization task of this project and, therefore, it will not be modelled. Then, in dark orange, it is represented the supercritical carbon dioxide extraction of polyphenols rich fibres and essential oils from the residue of the olive oil production process. This step has room for optimizing its integration into the main process from a sustainable point of view, so it will be explicitly modelled. Finally, in blue, the main steps of the enzymatic hydrolysis of lignocellulose residue are shown. This process will be modelled and implemented into eco2des, as well.

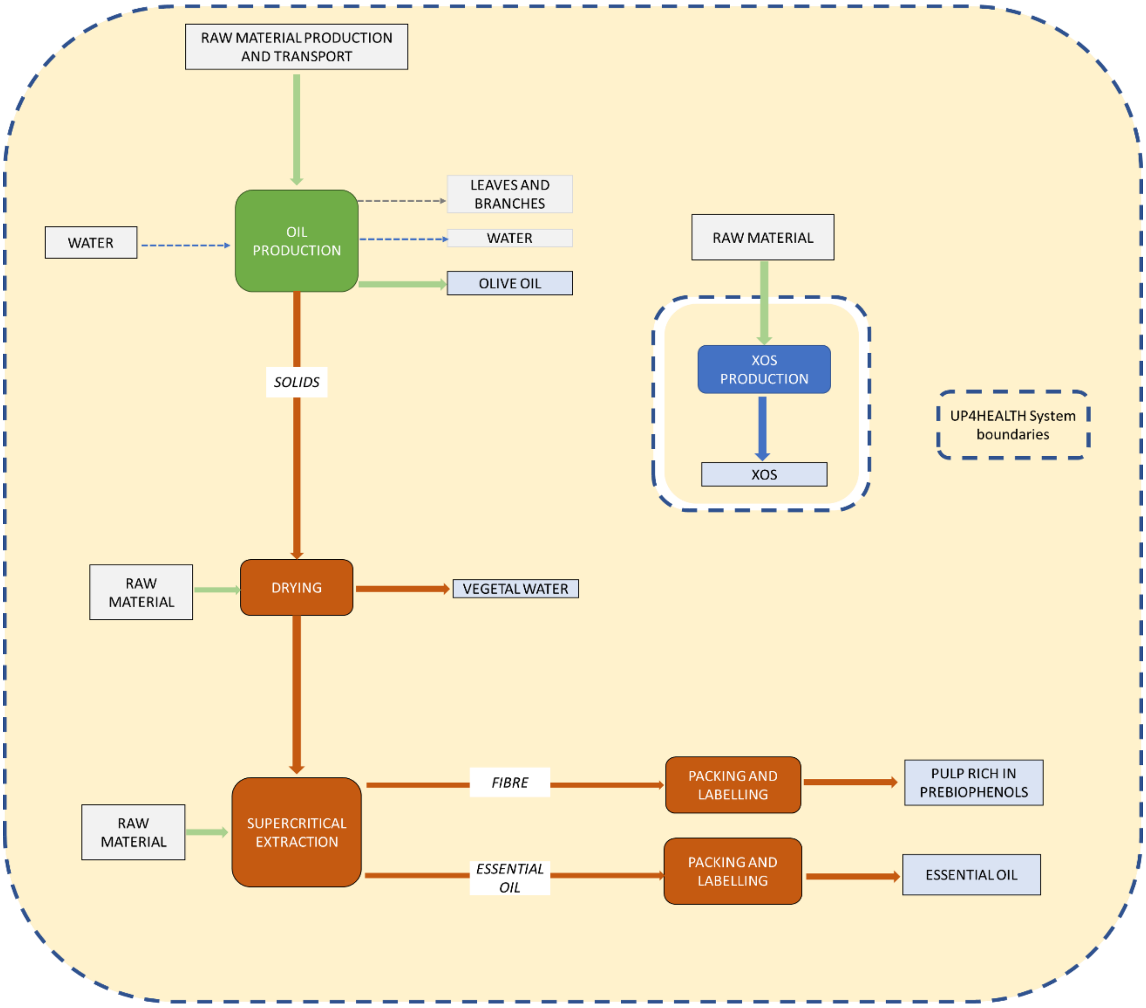

Figure 5. UP4HEALTH functional ingredients production steps

The process steps will be explicitly modelled and considered in the simulation by CONTACTICA. For each of the steps a first-principles based predictive model will be selected to simulate the physical, chemical and biological phenomena taking place. Moreover, when necessary, machine learning techniques will be applied to develop predictive regression models.

For supercritical extraction two models' approach will be taken into account and validated against experimental data from the ISANATUR plant. On the one hand, a thermodynamic phase equilibrium model will be developed. This model will have as key parameters the pressure, temperature and solvent to feed mass ratio. For this purpose, the Stryjek–Vera Peng–Robinson equation of state as a thermodynamic model for the experimental bubble pressures and vapor compositions will be used to represent the phase equilibria behaviour of the multicomponent oil-type material and carbon dioxide mixture; predicting the steady-state efficiency of the extraction. On the other hand, in order to take into account the interaction between the solute and the solid matrix, the Sovova's extension of Lack's plug-flow model (Sovova, 1994) will be developed for this particular case. This way, the effects of pressure, temperature, extractor capacity and superficial velocity on the extraction rate of essential oils will be evaluated in the extraction curves behaviour.

For enzymatic hydrolysis, a kinetic approach will be used to model the xylooligosacharides (XOS) production under different enzyme dosages, temperatures, pressures and residence times. A modified Angarita et al.

(2015) model will be developed including enzyme adsorption, xylose and XOS formation, end-product inhibition and substrate reactivity. The model will be validated with experimental data from the ISANATUR process.

Finally, these models will be implemented in a plant wide simulation built in Aspen Plus software, in which downstream processes will be also considered to perform mass and energy balances according to target scale-up capacity. The simulation will provide inventory data in different scales to perform subsequent LCSA studies and to solve multi-objective optimization problems.

6.3 Life Cycle Sustainability Assessment methodology.

In order to preserve the harmony between LCSA of reference systems, simulated processes and real plant analysis, the LCSA methodology implemented in **eco2des** will be analogue to that described below Section 6.3.1. The data used for simulation and optimization will be collected from partners using data collected in templates found in Annex 1: LCI templates.

6.3.1 Multi-objective optimization methodology.

First, sustainable key performance indicators (S-KPI) will be defined as objectives of the optimization problem:

- Environmental objective: Those shown in Table 1 normalized and weighted into a single score following the PEF methodology.
- Economic objective: Net present value of the UP4HEALTH bio-process.

Social objectives will not take into account due to a lack of a robust and standardized methodology. Therefore, the LCSA interpretation and hot-spots detection from previous analysis is considered enough to assess and optimize the social performance of UP4HEALTH value chain.

After the definition of the optimization objectives, key operational and value chain variables will be identified carrying out sensitivity analysis in the virtual plant and value chain models developed. Then, their boundaries and principal constraints will be defined.

For solving multi-objective optimization problems finding reasonable solutions, **eco2des** offers a set of different genetic algorithms. In this case study, multi-objective evolutionary algorithm with decomposition, MOEA/D, (Zhang and Li, 2007) and non-dominated sorting genetic algorithm II, NSGA-II, (Deb et al., 2002) will be used to find the Pareto front of the problem, in which a set of solutions will be presented. Between them, that which better fulfils the KPIs of the call will be selected as optimal solution to be tested and scaled-up in real plants.

7 References

Benoît, C., Mazijn, B., United Nations Environment Programme., CIRAIG., Interuniversity Research Centre for the Life Cycle of Producs, P. and S., & Canadian Electronic Library. (2013). *Guidelines for social life cycle assessment of products*.

J.D. Angarita, R.B.A. Souza, A.J.G. Cruz, E.C. Biscaia, A.R. Secchi, Kinetic modeling for enzymatic hydrolysis of pretreated sugarcane straw, Biochemical Engineering Journal, Volume 104, 2015, Pages 10-19, ISSN 1369-703X, https://doi.org/10.1016/j.bej.2015.05.021.

Benoît Norris, C., Traverso, M., Neugebauer, S., Ekene, E., Schaubroeck, T., Russo Garrido, S., Berger, M., Valdivia, S., Lehmann, A., Finkbeiner, M., Arcese, G., & UNEP. (2020). Guidelines for Social Life Cycle Assessment of Products. *Management*, *15*(2), 104. Retrieved from http://www.unep.fr/shared/publications/pdf/DTIx1164xPA-guidelines_sLCA.pdf

Deb, K., Pratap, A., Agarwal, S., Meyarivan, T., 2002. A fast and elitist multiobjective genetic algorithm: NSGA-II. IEEE Trans. Evol. Comput. 6, 182–197. https://doi.org/10.1109/4235.996017

European Commission, 2019. Communication from the commission to the European parliament, the European council, the council, the European economic and social committee and the committee of the regions the European green deal, com/2019/640 final.

García Casas M., Dufour Andía J., Galvez Martos J., (2020) ECO2DES: Python Framework for the Eco-Design of Industrial Processes, Computer Aided Chemical Engineering, Elsevier, Volume 48, 2020, Pages 1987-1992, ISSN 1570-7946, ISBN 9780128233771, https://doi.org/10.1016/B978-0-12-823377-1.50332-3.

Goedkoop, M.J.; de Beer, I.M; Harmens, R. . P. S. D. M. A. F. A. L. H. D. I. D. V. A. M. E. M.-F. C. A. I. R. U. S. M. H. M. C. T. A. J.-F. V. A. W. (2020). *Handbook for Product Social Impact Assessment*. *5th editio*.

ISO. (2006a). *14040 Environmental management — Life cycle assessment — Principles and framework*.

ISO. (2006b). *Iso 14044 Environmental Management. Life Cycle Assessment. Requirements and Guidelines. 3*(571), 16. Retrieved from http://tienda.icontec.org/brief/NTC-ISO14044.pdf

Kloepffer, W. (2008). Life cycle sustainability assessment of products. In International Journal of Life Cycle Assessment (Vol. 13, Issue 2). doi: 10.1065/lca2008.02.376

Maister, K., Di Noi, C., Ciroth, A., & Srocka, M. (2020). *PSILCA v.3*.

H. Sovova´, Rate of the vegetable oil extraction with supercritical CO2 — I. Modelling of extraction curves, Chem. Eng. Sci. 49 (1994) 409.

Swarr, T. E., Hunkeler, D., Klöpffer, W., Pesonen, H. L., Ciroth, A., Brent, A. C., & Pagan, R. (2011). Environmental life-cycle costing: A code of practice. *International Journal of Life Cycle Assessment*, *16*(5), 389–391. doi: 10.1007/s11367-011-0287-5

United Nations Environmental Program (UNEP). (2011). *Towards a Life Cycle Sustainability Assessment*. doi: DTI/1412/PA

Zampori, L., & Pant, R. (2019). Suggestions for updating the Product Environmental Footprint (PEF) method. In JRC Technical Repports. doi: 10.2760/424613

Zhang, Q., Li, H., 2007. MOEA/D: A Multiobjective Evolutionary Algorithm Based on Decomposition. IEEE Trans. Evol. Comput. 11, 712–731. https://doi.org/10.1109/TEVC.2007.892759

8 Annex 1: LCI templates

Table A 1. Data collection template for LCA, LCC and S-LCA.

Stage	Input	Quantity	Unit	Cost (€/UNIT)	Output	Quantity	Unit	Cost OUTPUT (€/UNIT)	CAPEX (€)	Number of workers	Cost of workers (€/h)	Comments
OliveOil production	Electricity		kWh		Water To WWTP		L					
	Olives		Kg		Olive Oil		L					
	Water		L		Solids to drying		kg					
XOS Production	Raw material		kg		XOS		kg					
	Electricity		kWh		Water To WWTP		kg					
	Water		L		Solid waste		kg					
Drying	Solid humid biomass		kg		Vegetal Water		L					
	Electricity		kWh		Pulp		kg					
Supercritical FLUID EXTRACTION	Fluid		Kg/L		Essential Oil		kg					
	Pulp				Phenol Rich Pulp		kg					
	Electricity		kWh									

Olive husk (SCE)

Oil content		kg/kg
Moisture		kg/kg

Apparent density		kg/m3
Average particle diameter		m

Free fatty acids		kg/kg
Tocopherols		kg/kg
Physterols		kg/kg
Squalene		kg/kg
Triglycerides		kg/kg

Carbon dioxide (SCE)

Purity		kg/kg

Black liqour composition (EH)

Monosaccharides	Rhamnose		g/L
	Arabinose		g/L
	Galactose		g/L
	Glucose		g/L
	Xylose		g/L
XOS	Xylobiose		g/L
	Xylotriose		g/L
	Xylotetraose		g/L
	Xylopentaose		g/L
	Xylohexaose		g/L
Polysaccharides			g/L
Lignin			g/L

Figure A 1 LCI template for Eco2Desraw material characterization

Table A 2. Supercritical extraction with carbon dioxide template.

Run	Initial conditions		Results		Extract composition (kg/kg)				
	q (kgkg-1s-1)	U (ms-1)	t (min)	e (kgkg-1)	Free fatty acids	Tocopherols	Physterols	Squalene	Triglycerides
p =		Mpa							
T =		K							
p =		Mpa							
T =		K							

Where q is the specific flow rate, U is the solvent superficial velocity, t is the residence time,
e is the yield measured as extract mass per solute mass

Table A 3. Enzymatic hydrolysis template.

Run	Initial conditions			Extract composition (g/L)											
	E (IU/L)	pH	t (min)	Rhamnose	Arabinose	Galactose	Glucose	Xylose	Xylobiose	Xylotriose	Xylotetraose	Xylopentaose	Xylohexaose	Polysaccharides	Lignin
p = T =		Mpa K													
p = T =		Mpa K													

Where E is the enzyme dosage

and t the residence time