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Executive Summary

In order to assess the potential environmental impacts of SECRETed innovative biotechnological value chain for biosurfactants and siderophores production and selected end-use applications, a life cycle assessment (LCA) following ISO 14040/14044 will be undertaken during the project.
The first step in the realization of the LCA is the definition of the goal and scope. This, together with the first definition of the functional units involved in the value chain, and the input data review for the life cycle inventory, are reported in this deliverable.
A literature review has been conducted to provide data for the baseline scenario (synthetic and fossil-based surfactants) which will serve as benchmark against which the environmental impacts, economic performance and social impacts of the new proposed technologies will be compared. It has been seen that most pieces of literature concerning sustainability aspects of surfactants are related to the detergents value chain. Concerning biosurfactants, LCAs on manufacturing processes based on biomass feedstock such as palm oil kernel were found. The biomass-based biosurfactants did not always score positevly on the environment impact assessment, due to the contribution of land use and fertilizers and pesticies consumption. This encourages the pursual of the bacterial route for the manufacturing of biosurfactants.

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1. Introduction

Surfactants are chemical compounds that decrease the interfacial tension between two liquids, a liquid and a gas, or a liquid and a solid. Surfactants may function as emulsifiers, wetting agents, detergents, foaming agents, or dispersants, playing an important role in several industrial fields, and especially in household and industrial cleaning. Additionally, surfactants can organize themselves in complex self-assembled supramolecular structures, such as micelles, liposomes or microemulsions. Thus, they can also be exploited as vehicle or carrier for active ingredients in the cosmetic, nutritional and pharmaceutical industry.
State-of-the-art surfactants are produced from synthetic sources, mainly from the petrochemical or oleochemical sectors, like fatty alcohols. In order to reduce the dependency on fossil resources and the environmental impact, there is an increasing interest in obtaining them from renewable sources. However, market penetration of biosurfactants is still small. This is mainly due to their higher cost compared to chemically derived surfactants, and the limitations in the chemical diversity of molecules and producing microorganisms.
SECRETed will develop novel hybrid molecules with tailor-made properties obtained from the combination of biosynthetic genes of amphiphilic compounds (biosurfactants and siderophores) produced by marine and extremophilic microorganisms. This will expand the chemical diversity and broaden the industrial applications that can be covered with biosurfactants and siderophores.
Indubitably the newly developed products and proceses should have a lower environmental impact than the state of the art. The goal of WP8 includes to quantify and evaluate any effects to the environment caused by the proposed technologies to produce biosurfactants and siderophores. This will be achieved through a Life Cycle Assessment (LCA).

Life cycle assessment is a methodology for assessing environmental impacts associated with all the stages of the life cycle of a commercial product, process, or service. It involves the compilation of a comprehensive inventory of the energy and material inputs and outputs across the value chain, and calculates the resulting emissions to the environment. These emissions are translated to environmental impacts. The final stage is the interpretation step, where the obtained environmental impacts are put into context with the defined goal and scope of the LCA and the assumptions and limitations of the study, in order to draw the main conclusions and recommendations. An LCA may be used to quantitively compare different products or processes that serve the same function, and/or to detect the environmental hot-spots across the value chain, in order to optimize and improve the environmental profile of the product or process under study.
Life cycle stages of products, processes or services are raw material extraction and processing, manufacturing, distribution, use, and end-of-life treatment. An LCA may cover from raw material extraction to any of the intermediate life cycle stages (cradle-to-gate), between several intermediate life cycle stages (gate-to-gate), from raw material extraction to final disposal (cradle-to-grave), or from raw material extraction to the recycling of the final product (cradle-to-cradle).

In order to ensure the quality, transparency and comparability of LCAs, the methodology has been standardized by the International Organization for Standardization (ISO) through ISO 14040 and ISO 14044.

The present deliverable covers the fist stage of the SECRETed LCA, namely the goal and scope definition, and presents a first review of available databases and a preliminary compilation of the Life Cycle Inventory (LCI) material inputs, as well as presents a literature review on LCAs on relevant technologies.

2. Literature review

A review of scientific and technical literature on target compounds and processes was carried out. This activity aims to establish a baseline for the Sustainability Assessment, identifying some related existing materials, production routes and final uses, and their environmental and economic performance.

Establishing a baseline will allow the BLUE SYNERGY team to compare the compounds and processes with state-of-the-art counterparts (mainly synthetic and fossil-based materials), supporting and addressing of the following project expected impacts:

- CO_2 Emissions (<1% of fossil counterparts), Increasing Carbon Efficiency and Reducing Footprint (GWP).
- Use of side and waste streams as inputs (Inventory Analysis).
- Reduced production costs in relation to benchmarking alternatives (Economic Performance).
- Social benefits "highly qualified jobs" (average expected contribution 1-2%) (Working Conditions, Health and Safety, etc.).

This baseline is useful not only for the general environmental and economic performance comparison, but to compare with the project sustainability expectations.

The key words for the literature search included surfactants and biosufractants, together with sustainability, LCA and LCC. It was found that most literature focused on the application for detergents, since is the most extended application of surfactants.

Specific sustainability information related with the LCA and LCC methodology was identified, gathering information from the early to the late stage of the assessment. Related topics as eco-design, toxicity analysis, circular analysis, etc. were included in some cases. The literature data base accounts with 91 documents distributed in 3 types of analysis.

Table 1. Compiled literatura data base

Type of Analysis	Number of documents
Life Cycle Assessment	31
Life Cycle Costing	1
Process / Manufacturing Route Assessment	64
Grand Total	96

2.1. Analysis of life cycle assessment on surfactants and biosurfactants

From the obtained literature, the papers directly contributing to the execution of the LCA of baseline surfactants currently used in the SECRETed value chain and candidates for replacement (see 4.1 and Table 7) will be summarized first.

The work by Schowanek et. al [1] presents cradle-to-gate life cycle inventories (LCIs) for the production of a series of common surfactants used in European detergents and personal care products, compiled in the frame of ERASAM project with the cooperation and data of 14 major companies. This includes alcohol ethoxylates with different ethylene oxide units, which could be used in the modeling of the polysorbate 80 and polyethylenesorbitan monolaureate currently used in encapsulants manufactured by the project partners (see Table 7), directly or as proxies. In this regard, the work by Subramanian & Golden [2] provides a systematic process for the selection of proxies using expert guidance and quantification of their uncertainty for anionic and non-ionic surfactants which may be used in the project, since given its novelty, data gaps are expected.

The environmental impact of Sodium Lauryl Sulphate (SLES) containing 3 mol of ethylene oxide (EO) was evaluated by Nogeira et. al [3] using the life cycle thinking approach. The proposed assessment included a baseline scenario and four individual alternatives aiming at improving its environmental performance, including the production of the mentioned compound using bio-based sources such as palm kernel oil. One of these alternative included the production of the surfactant from synthetic lauryl alcohol. Specifically this alternative comprised the replacement of Lauryl Alcohol obtained from the processing of palm kernel oil extracted from palms cultivated in Malaysia and Indonesia by a synthetic congener derived from olefins and ethylene produced from petroleum. The synthetic lauryl alcohol could be directly used as an input in the ethoxylation stage where it would combine with ethylene oxide to produce ethoxylated lauryl alcohol containing 3 mol of EO, obeying the same conditions established for the Baseline Scenario for obtaining SLES 3EO. The data related to synthetic lauryl alcohol processing were essentially secondary and obtained from the Ecoinvent database. In this case study the reference flow used was the production of 1.0 ton of Sodium Lauryl Sulphate containing 3 mol of ethylene oxide (SLES 3EO) and the LCA technique was applied under a 'cradle-to-gate' approach. The Global Warming Potential for this fossil based alternative was 1.48 t CO_2eq/1.0 ton of surfactant produced and the production of the synthetic lauryl alcohol contributes with approximately 0.7 t CO_2eq/RF, giving a fist value for the calculation of the emissions to be saved by the SECRETed value chain. The primary energy demand was also assessed obtaining for this alternative a result of 50.79 GJ/RF.

The work by López de Lapuente et. al [4] quantified the environmental impacts associated with the life cycle of an enzymatic multipurpose cleaner, which included Ethoxylated Alcohol surfactant from petrochemical origin. It proposes its replacement by Ethoxylated Alcohol from Palm Kernel Oil as an eco-design solution. In this work the system boundaries were cradle-to-grave including all the value chain levels, raw materials extraction, production, packaging, transport, distribution, use and end-of-life. The functional unit was 1 kg of detergent in its container, and the used methods were the OpenLCA software using Ecoinvent 3.7 data set.

With this replacement, the environmental impacts are only reduced in the fossil fuel depletion category (by 7%), while they increase by 4–16% in 5 of the analysed categories, as shown in Table 2. This is because the LCA impacts of bio-based products are highly dependent on parameters such as forest management, fertilizer and herbicides use and on operational practices.

Table 2. Comparison between selected impact of Ethoxylated Alcohol from oleochemical origin and from petrochemical origin, data from [4]

INDICATOR	PC	PKO	% difference
Global Warming Potential (x10^{-2} kg CO_2-eq)	76.19	79.09	4%
Eutrophication Potential (x10^{-4} kg PO_4^{-3}-eq)	15.51	17.11	10%
Photochemical Ozone Creation Potential (x10^{-5} kg C_2H_4 -eq)	18.32	21.32	16%
Water scarcity footprint (10^{-2} m^{-3} -eq)	53.55	55.65	4%
Abiotic Depletion Potential Fossil Fuels (MJ)	13.72	12.72	-7%

PC: Ethoxylated Alcohol from petrochemical origin. **PKO**: Ethoxylated Alcohol from Palm Kernel Oil.

This is consistent with the work by Shah et al. [5], who conducted a cradle-to-gate life cycle assessment of the production fatty alcohols from petrochemical origin and from palm kernel oil. They report an overall lower average greenhouse gas (GHG) emissions when the petrochemical source is used, arising from the land use change for palm plantation, and end life treatment of the palm oil wastewater and empty fruit bunches.

These results reveal the large opportunities of the SECRETed solutions, which will not imply the use of land and raw materials consumed for crops growth and their associated environmental impacts.

Some recent efforts have been conducted to quantify the environmental impacts of biosurfactant production from bacteria.
The work by Hu et. [6] al reports a dynamic life cycle assessment for the microbial production of biosurfactants, in particular sophorolipids (SL). The work compares the environmental impacts of the production of SLs using different types of feedstock and separation techniques in order to identify hot-spots and guide design optimization towards sustainable solutions. It is concluded that SLs produced from organic waste (food waste) in lab-scale batch fermentation coupled with in-situ seperation technique are highly attractive, due to the high yield, and expected to be environmentally friendly and sustainable upon scale-up. No comparison with fossil-based surfactants is provided.
The production of sophorolipids through microbes, in particular Starmerella bombicola was the focus of the work by Baccile et. al [7]. Interestingly, it reports that 90% of the impact related to the manufacturing phase is caused by the fermentation, specifically by the use of

rapeseed oil (47%) and glucose (41%), while only 7% is derived from electricity. Again the plant biomass production is the responsible for a significant part of the environmental impact.

A comparison with state-of-the-art alternatives including alkylbenzene sulfonate, fatty alcohol, fatty alcohol sulfate, esterquat, acetylated sSL-COOH, ethoxylated alcohol and soap was also undertaken, using end-point indicators. It was found that concerning damage to ecosystems, all candidates presented similar results, with alkylbenzenesulfonate scoring significantly better, which interestingly is the only completely fossil derived product under consideration. Optimization of the conversion efficiency and of the glucose/rapeseed oil ratio holds the most important improvement potential.

Aru et. al [8] presents an LCA on the microbial production of biosurfactants using oil waste. The identified hotspot is the energy consumption of the process. Therefore, the use of renewable energy to power the production process is proposed as strategy to minimize the impact. For the case were the target application is soil bioremediation, the direct growth of the bacteria in the polluted soil is proposed.

Schonhoff et. al [9] present a very complete LCA study of the production of two bio-surfactants obtained from bacteria, rhamnolipids (RLs) and mannosylerythritol lipids (MELs). The study identifies hot-spots for the production of both biosurfactants, and compares their environmental impact at pilot (112.5 l) and industrial (5000 l) production scales. Additionally, it compares their environmental impact with those from conventional oleo-/petrochemical surfactants C10−13 linear alkylbenzene sulfonic acid, cocamide diethanolamine and C8−18 alkyl amidopropyl betaine. The work reveals that the RL production has a higher environmental impact impact, at both production scales considered, due to the significantly lower specific yield coefficient. The substrate used appeared not to cause a significant difference in the environmental impact. Concerning the effect of production scale, it was found that the environmental impact of the industrial-scale processes investigated are 9.7% (RL) and 17.9% (MEL) lower than those of the pilot-scale results, highlighting the importance of this aspect. As for the benchmark with comertial surfactants, the production of both biosurfactants present higher environmental impact than the commertial counterparts, though the impacts of MELS are considered of a similar order of magnitude than the conventional surfactants by the authors, and with room for optimization, while it is seen difficult that the RL production can reach competitive results. Recommendations to reduce the environmental impact of biosurfactants include the treatment of organic wastes (recuse/recycling) and the development of a demand oriented aeration concept for the fermentation process. But most importantly, it is seen that increasing the yield would have the highest impact-saving potential, given its linear dependence with the environmental impacts. These findings are relevant for the SECRETed project.

Other pieces of identified literature provide relevant information on assessment methodology, data quality and data quality assessment.

A study on the environmental impacts from the production of surfactant alkylbenzene sulfonates (LAS) reports the differences in results obtained with data from LAS manufactured in Malaysia and LAS data available in Ecoinvent database [10]. The functional unit used by the authors was defined as the mass of the surfactant (1 kg of surfactant), LAS used in Malaysia is either imported from China or manufactured locally in Malaysia. However, linear alkyl

benzene (LAB) used as raw material in the production of LAS is imported from China. The system boundary for LAS covers the whole production of LAS in Malaysia including transportation of LAB from China. The inventory for the production of LAS was compiled from the foreground data obtained from LAS manufacturer in Malaysia. However, the initial data was completed using the Ecoinvent database.
The impact assessment from LAS production shows that the production of LAS in Malaysia has a greater impact on resources than LAS from Ecoinvent database. However, LAS manufactured in Malaysia has lower impacts on the human health and ecosystem quality compared to the LAS from the Ecoinvent database. Weighting results for the comparison between LAS produced in Malaysia and LAS in Ecoinvent database show that both have highest impact on the depletion of fossil fuels compared to the other impacts with 0.263 Pt and 0.257 Pt respectively.

The work by Pant et. al [11] compares the effect of the chosen life cycle impact assessment method (LCIA) for aquatic ecotoxicity on the product environmental risk assessment of a detergent. The authors found that the LCIA method used can change the result about which detergent type is preferable concerning the impact category aquatic ecotoxicity. This highlights the importance of developing and selecting robust and validated impact assessment methods.

Further, it has been found that the life cycle assessments of surfactants typically includes the manufacturing of the end products (i.e detergents), and not only of the surfactants [4], [12], [13]. This supports the inclusion of the complete value chain within the scope of the SECRETed LCA, this is, from the production of the biosurfactants to manufacturing of the end products, as described in section 3.2

2.2. Analysis of techno-economic assessment of surfactants.

The process of documenting, centralising and analysing scientific information also focused on information that could support the Life Cycle Cost analysis.
Since there is an enormous lack of information on this issue in the literature only one paper was selected and analysed. This work by Liu et. al [14] introduces the techno-economic analysis of a furfural surfactant from wheat straw feedstock. The work shows how the production of the surfactant is carried out on a novel formic acid pretreatment-based (Formiline) wheat straw biorefinery, specifically expanding its supply chain to include processing furfural to multiple products such as butadiene, surfactants, jet fuel, and lubricants.
Results indicate that the Formiline process is economically feasible with positive annual cash flow though capital cost is increased after indexing and emission reduction costs are added.
Table 3 presents the cost/yr of capital cost and operating cost. Further, annual incomes are presented. Incomes shows that the surfactant precursor (Furfural) is the most profitable of the production' lines, and the annual cash flow demonstrates the economic feasibility.

Table 3: Capital cost of the Formiline process and the related income for Furfural as surfactant precursor, data from [14].

Items	Formiline process
Cost (USD/yr)	
Capital cost (15-year depreciation)	−1.30E + 07
Operating cost	−4.71E + 07
Income (USD/yr)	
Ethanol	2.58E + 07
Furfural	3.76E + 07
Lignin	1.72E + 07
Tax (USD/yr)	3.08E + 06
Annual cash flow (USD/yr, 15 years)	1.74E + 07

Furfural expanded Supply Chain SC2 (surfactants), become more profitable than Formiline baseline (only furfural production). This is mainly depending on the sales prices of products, which vary in ranges, for furfural between 360 and 740 USD/t, and for surfactants between 2500–2800 USD/t.
The furfural supply chain expansion SC2 (Surfactants) Net Present Value at end of life of the plant (year 30) is 103,000,000 USD, better than Formiline baseline 93,800,000 USD, the Net present value (NPV) is a financial metric that seeks to capture the total value of a potential investment opportunity. The idea behind NPV is to project all of the future cash inflows and outflows associated with an investment, discount all those future cash flows to the present day, and then add them together. The resulting number after adding all the positive and negative cash flows together is the investment's NPV. A positive NPV means that, after accounting for the time value of money, investors will make money if they proceed with the investment.

2.3. Conclusions from the literature review

The presented literature review has provided the following outcomes:

- The assessments identified in the literature usually evaluate the surfactants as a part of a product or process (i.e. detergents) and not as an end product. This supports the inclusion of the complete value chain, including the manufacturing of the end-products, in the SECRETed sustainability assessments.
- The environmental comparisons between fossil-based surfactants and biobased surfactants consider biosurfactants obtained from plant biomass like palm. The environmental impact of these biosurfactants has not been found better than that of fossil-based surfactants, mainly due to land use change for the crops production and fertilizer and herbicides consumption. This sustains the interest of the production of biosurfactants from bacteria as a sustainable alternative to fossil-based surfactants.
- The review has provided relevant data, LCI and references for the modeling of commercial fossil-based surfactants.

- Deviations in the results have been found in the literature, related to data quality and impact assessment method used. This highlights the relevance and need for data quality assessment and sensitivity analysis, and the selection of robust and scientifically accepted impact assessment methods, which will be taken into account for the execution of the SECRETed LCA.
- Bacterial yield and the fermentation step appear critical towards the biosurfactant production environmental impacts.
- Life Cycle Costing papers related to the surfactants and biosurfactants have not been found, highlighting the existing knowledge gap and relevance of including this aspect in the sustainability assessments of SECRETed.

3. LCA Goal and Scope

3.1. Goal Definition

The goal of this LCA is to evaluate the potential environmental impacts of the SECRETed biotechnological value chain for the production of biosurfactants and siderophores and their later use in the manufacturing of final products, in order to identify environmental hotspots as to improve and optimize the process design, as well as to compare the environmental impact with that of the state of the art of surfactants and siderophores.
The target audience is the SECRETed project consortium and the European Commission as funding agent, as well as the scientific community.

3.2. Scope Definition

The LCA will be undertaken following ISO 14040 [15], [16] and ISO 14044 [16].
The complete value chain includes raw material extraction, materials manufacturing by upstream suppliers, the manufacturing of biosurfactants and siderophores, the manufacturing of the final products (encapsulated products including oregano essential oil and RNAi drugs), the use phase by the consumers, and the end of life. The complete value chain is schematically represented in Figure 1.
The use phase of the different end-products is direct human consumption, as cosmetics, nutricional supplements or pharmaceuticals.
While it is anticipated that the biosurfactants will be biodegradable, this is not confirmed nor is the study of their biodegradability included in the scope of the project. Therefore, the system boundaries for the LCA will be from raw material extraction to the manufacturing of the final products, being so from cradle to gate. The system boundaries are represented by the doted lines in Figure 1. These system boundaries will be kept the same for the life cycle costing and social life cycle assessment to be conducted during the project (tasks 8.2 and 8.3), for the sake of consistency.
All material inputs and outputs, as well as energy consumption of each unit process will be included in the analysis. Consumption of auxiliary systems and general infrastructure (i.e building climatization, raw materials storage equipment, PCs) are out of the scope of the LCA.

The manufacturing of the equipment (i.e fermenters, agitators etc) required are out of the scope of the LCA.

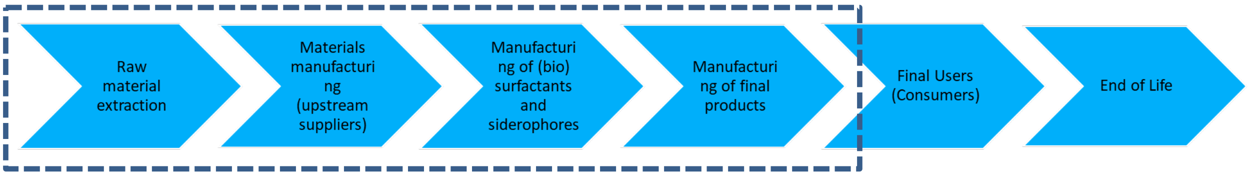

Figure 1. Value chain of the SECRETed technology and products. The doted line represents the scope of the life cycle assessment.

Many biosurfactants with different properties will be obtained from the multiple bacterial strains. There final products considered in the project, include their use in the encapsulants manufacturing of oregano oil, Coenzyme Q_{10} (CoQ_{10}) and RNAi drugs, as well as their use in anti-tumor and antibiotic applications. For these two last end products, the use of siderophores could be part of the drug delivery system, or of a new drug. Since the research to answer this is out of the scope of the project, they will not be included in the LCA.

Therefore three different LCAs will be conducted in parallel: cradle to gate LCA of the biosurfactant for oregano oil encapsulation (LCA1), cradle to gate LCA of the biosurfactant for siRNA encapsulation value chain (LCA2) and cradle to gate LCA of the biosurfactant for CoQ10 encapsulation (LCA3). The scope of each, and the related unit process breakdown, is shown in Figure 2, Figure 3 and Figure 4 respectively. The formulation of the encapsulant will be adapted to the substance to be encapsulated, leading to different manufacturing unit processes. Foreground processes are represented in dark blue and background processes in pale blue. Waste streams are not represented in the diagrams for ease of visualization.

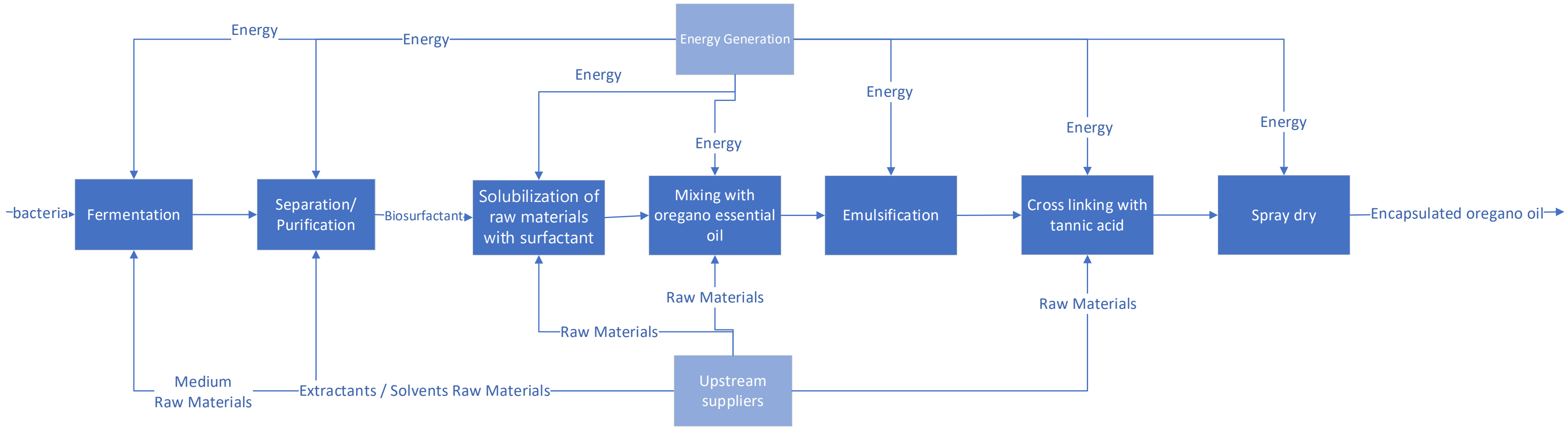

Figure 2. Scope and functional units of LCA1 – encapsulants for oregano oil value chain.

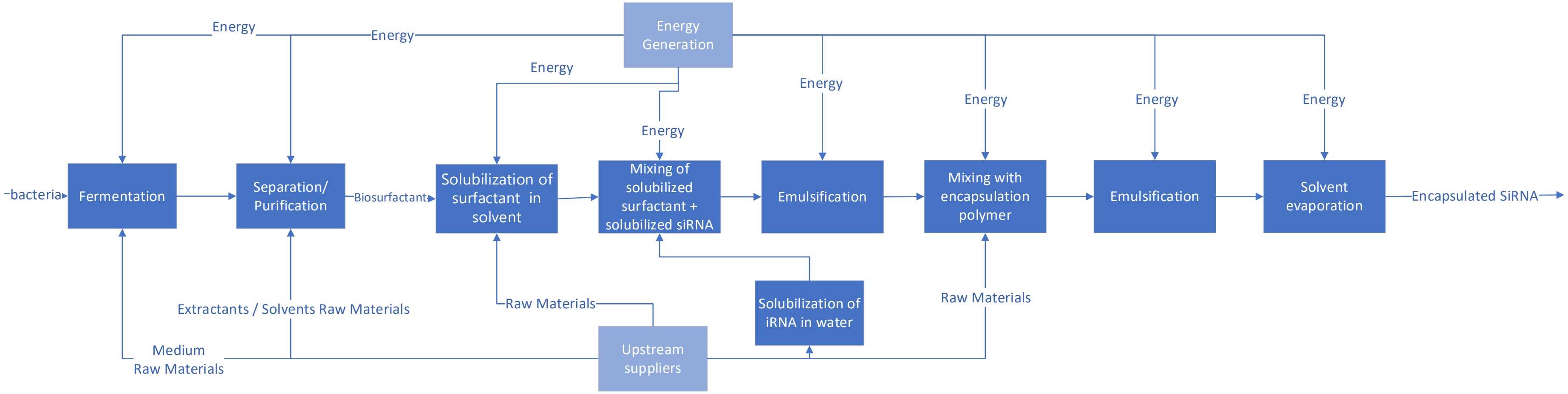

Figure 3. Scope and functional units of LCA2 – encapsulants for siRNA value chain

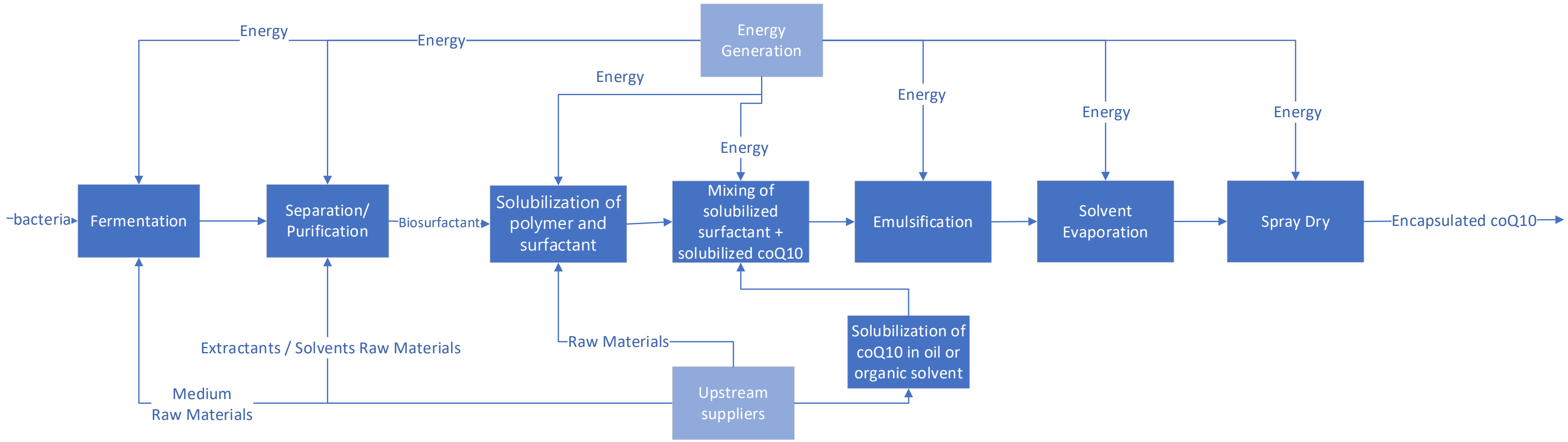

Figure 4. Scope and functional units of LCA3 – encapsulants for coQ_{10} value chain

The functional unit for LCA 1 is the encapsulation of 400 mg of oregano essential oil.
The functional until for LCA 2 is the encapsulation of 2 mg of siRNA drug.
The functional until for LCA 3 is the encapsulation of 500 mg of CoQ.
The reference flow selected is 1 kg of purified biosurfactant for the two cases.

The Impact Assessment Method selected is ReCiPe 2016 Midpoint [17]. This method includes 18 midpoint indicators: climate change, ozone depletion, ionizing radiation, fine particulate matter formation, photochemical oxidant formation: ecosystem quality, photochemical oxidant formation: human health, terrestrial acidification, freshwater eutrophication, human toxicity: cancer, human toxicity: non-cancer, terrestrial ecotoxicity, freshwater ecotoxicity, marine ecotoxicity, land use, water use, mineral resource scarcity, and fossil resource scarcity. Data from foreground processes will be obtained from the relevant project partners based on laboratory and pilot scale manufacturing procedures. Data from background processes will be obtained from Ecoinvent 3.8 database [18] and Agrifootprint database [19] version 6.
The LCA will be conducted using SimaPro 9.4.0.2 software.

4. Baseline Selection

4.1. For LCA1: encapsulants manufacturing of oregano essential oil.

Sphera Encapsulation S.r.l. is an innovative start-up and the first Italian company dedicated 100% to research and development in the field of encapsulation. In WP7, SE will evaluate the possibility to use the identified bio-surfactants in different encapsulation approaches in order to demonstrate the feasibility and efficacy of the processes in different industrial sectors. SE is aiming to replace the following commercial surfactants by the SECRETed biosurfactants: Span 80, Span 20, Tween 80, Tween 20 and/or Sodium dodecyl sulfate (also known as sodium lauryl sulfate). These are used in the encapsulation of different products, including oregano oil. These are the benchmark against which the SECRETed biosurfactants will be compared to. As the project and the SECRETed biosurfactants characterization progresses, the above mentioned list will be shortcut by matching technical properties.

4.2. For LCA2: encapsulation of RNAi drug

Sylentis is a Spanish pharmaceutical company, focused on the development of innovative compounds based on RNA interference (siRNA) for the treatment of various diseases. Sylentis is exploring together with SE the encapsulation of novel RNAi drugs. In this case, the baseline is siRNA encapsulated with a commercial transfection agent (jet Optimus) and encapsulants based on PLGA, PVA, PGPR and PEG. The raw materials required for the commercial transfection agent are obtained from the patents.

The following scenarios under development, which will be compared with the baseline, are:

- Sphera encapsulant containing nanoparticles + biosurfactants.
- Sphera encapsulant containing nanoparticles + biosurfactants + siderophores.

Depending on the technical results obtained in WP7 the successful scenarios will be included in the LCA2.

4.3. For LCA3: encapsulation of coQ_{10}

The baseline for this case is equivalent to that of LCA1, where SE is aiming to replace the following commercial surfactants by the SECRETed biosurfactants: Span 80, Span 20, Tween 80, Tween 20 and/or Sodium dodecyl sulfate (also known as sodium lauryl sulfate), which are used in the encapsulation of different products, including coQ_{10}. These are the benchmark against which the SECRETed biosurfactants will be compared to. As the project and the SECRETed biosurfactants characterization progresses, the above mentioned list will be shortcutted by matching technical properties.

5. Assumptions

For the raw material extraction and up-stream suppliers' manufacturing, it is assumed that only raw materials from the global market will be used.
For the geographic location of the SECRETed manufacturing plant, Europe will be assumed and the average European mix selected for the energy supply. For the geographic location of the encapsulants manufacturing, Italy will be selected since it is the location of Sphera Encapsulation partner.
The list of assumptions may change as the project and LCA progresses and will be regularly updated.

6. Limitations

Data from foreground processes are based on lab and pilot scale processes. Deviations between the LCA results of this project and the results of large-scale manufacturing processes may occur due to process scale up and optimized plant efficiency [20]. The environmental impacts obtained for pilot processes would be overestimated.

7. Life Cycle Inventory and Database Review

Though the work in WP 2-7 is ongoing, a preliminary Life Cycle Inventory (LCI) of the raw materials required for the different unit processes (fermentation, separation, end product manufacturing) has been compiled, as well as the raw materials for the benchmark products. At this stage the LCI is qualitative, since the required amounts of each material flow are under research.

This LCI has been cross checked with the Ecoinvent 3.8 and Agri-footprint 6.0 data bases to confirm the availability of data to feed the background processes, as well as to identify data gaps where further sources need to be checked.
This LCI is preliminary and captures the current state of project development, and will be adjusted as the project progresses.

Table 4: Inputs for Unit Process Fermentation

Material Input	Availability in Databases
Glucose	yes, in Ecoinvent 3.8
Glycerol	yes, in Ecoinvent 3.8
$(NH_4)2SO_4$	yes, in Ecoinvent 3.8
$(NH_4)Cl$	yes, in Ecoinvent 3.8
Na_2HPO_4	yes, in Ecoinvent 3.8
KH_2PO_4	No, needs to be obtained from literature
$Na_2EDTA.2H_2O$	use EDTA as proxy, in Ecoinvent 3.8
$ZnSO_4.7H_2O$	yes, in Ecoinvent 3.8
$CoCl_2.6H_2O$	use stoichometric quantities of $CoCO_3$ and HCl, in Ecoinvent 3.8
$MnCl_2.4H_2O$	use stoichometric quantities of MnO_2 and HCl, in Ecoinvent 3.8
H_3BO_3	yes, in Ecoinvent 3.8
$Na_2MoO_4.2H_2O$	use stoichometric quantities of MoO_3 and NaOH, in Ecoinvent 3.8
$FeSO_4.7H_2O$	yes, in Ecoinvent 3.8
$CuSO_4.5H_2O$	yes, in Ecoinvent 3.8
$MgSO_4.7H_2O$	yes, in Ecoinvent 3.8
$CaCl_2.2H_2O$	yes, in Ecoinvent 3.8
Spectinomycin dihydrochloride pentahydrate	No, needs to be obtained from literature
Toluic acid	use benzoic acid as proxy, in Ecoinvent 3.8
Tryptone	use co-product lactose as proxy, in Agri-footprint data base
Yeast extract	use fodder yeast as proxy, in Agri-footprint data base
Tryptic soy broth	use soybean meal as proxy, in Agri-footprint data base
Bacto-peptone	use generic enzymes, in Ecoinvent data base
Tris Base	use diethanolamine as proxy, in Ecoinvent data base
KCl	yes, in Ecoinvent data base
Dextrose	use glucose, in Ecoinvent data base
Soluble starch	yes (from maize, potato, wheat and pea available Agri-footprint data base)
Soy peptone	use soybean meal as proxy, in Agri-footprint data base
Soy bean flour	yes (soy bean meal) in Agri-footprint data base

NaCl	yes, in Ecoinvent data base
$NaSO_4$	yes, in Ecoinvent data base
$CaCO_3$	yes, in Ecoinvent data base
Mannitol	use glucose as proxy, in Ecoinvent data base
Malt extract	use fodder yeast as proxy, in Agri-foodprint data base

Table 5: Inputs for Unit Process Separation & Purification

Material Input	Availability in Databases
etyl acetate	yes, in Ecoinvent 3.8
methanol	yes, in Ecoinvent 3.8
acetone	yes, in Ecoinvent 3.8
ethanol	yes, in Ecoinvent 3.8
resin XSD4/XAD7	use of PS as proxy, in Ecoinvent 3.8

Table 6: Inputs for Unit Process Encapsulants Manufacturing

Material Input	Availability in Databases
whey protein isolate	Whey, evaporated 50% dry mass, in Agri-foodprint database
pea protein isolate	yes, in Ecoinvent 3.8
gum arabic	No, needs to be obtained from literature
PVA	vinyl acetate, in Ecoinvent 3.8
PLGA	polylactice granulate, in Ecoinvent 3.8
maltodextrin DE 19	potato starch, in Ecoinvent 3.8
ethyl acetate	Yes, in Ecoinvent 3.8

Table 7: Inputs for Baseline Encapsulants Manufacturing (state-of-the-art surfactants)

Material Input	Availability in Databases
Sodium lauryl sulfate	fatty alcohol sulfate, in Ecoinvent 3.8
Polysorbate 80	non-ionic surfactants using ethylene oxide, in Ecoinvent 3.8
Polyethylenesorbitan monolaurate	non-ionic surfactants using ethylene oxide, in Ecoinvent 3.8
Polyglycerol polyricinoleate	use estequiometric mixture of glycerol and fatty acids, in Ecoinvent 3.8
Sorbitan monolaurate	Fatty acids methyl ester, in Ecoinvent 3.8
Sorbitane monooleate	Fatty acids methyl ester, in Ecoinvent 3.8
poly(lactic-co-glycolic acid)	Use lactic acid, in Ecoinvent 3.8

Polyvinyl acetate	vinyl acetate, in Ecoinvent 3.8
Polyethylene glycol	No, obtain from literature

Table 8: Inputs for Baseline siRNA encapsulation (commercial transfection agent)

Material Input	Availability in Databases
Amphiphilic cationic molecule	Alkylbenzene sulfonate to be used as proxy, in Ecoinvent 3.8

8. Conclusions

This deliverable presents the Goal and Scope, selected baselines, functional units definition and preliminar LCI compilation and data base review for the life cycle assessment of the SECRETed value chain and selected end-products. As the project and execution of the project progresses, these will be iteratively reviewed and updated, as per ISO 14040/14044, and included in future deliverables D8.2 and D8.3.

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