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DOCTORAL DISSERTATION

A techno-sustainability assessment framework: indicator selection and integrated method for sustainability analysis of biobased chemicals

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vito

“It is important to replace the language from ‘good is forward-and-up’ to ‘good is in-balance’ between human needs and the earthly limits of the Earth.”

Kate Raworth on Doughnut Economics (2017)

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SUMMARY

The emerging biobased industry has the potential to tackle some of the sustainability challenges the chemical industry must endure. However, the use of biomass as a feedstock does not imply that technologies and product value chains are always sustainable. Sustainability impacts need to be evaluated and monitored to highlight the advantages and pitfalls of different biobased routes over the product life cycle. This dissertation aims to develop a framework for sustainability assessment, specifically for biobased chemicals, while accounting for technological as well as economic, environmental, and social aspects in an integrated approach.

First, a review of the state-of-the-art sustainability indicators for biobased chemicals was conducted and a gap analysis was performed to identify indicator development needs. The results show that existing sets of indicators lack a holistic view on sustainability. There is a clear hierarchy present within the sustainability domains (i.e., environmental, economic, and social) with a preference for certain environmental indicators and ignorance towards social aspects. The existing sets lack focus and are not adapted to case-specific characteristics of biobased chemicals. The review study shows that the need exists to elaborate and enhance a standardized and comprehensive list of sustainability indicators for biobased chemicals.

To fill this gap, a Delphi study was performed to select sustainability indicators specifically for biobased chemical value chain assessment, and to reach consensus among experts on prioritization of these indicators. Stakeholders were selected from three core groups: the private, public, and academic sector. Best-worst scaling (BWS) was performed to gather data on a prioritization of sustainability indicators per respondent. Next, a multi-criteria decision analysis (MCDA) was applied to compare the individual rankings of the respondents and develop a consensus ranking among the experts. Greenhouse gas (GHG) emissions, market potential and acceptance of biobased materials are deemed the most crucial indicators for respectively environmental, economic, and social sustainability. Expert consensus was found positive in all three domains, with the strongest consensus measured for environmental sustainability.

Next, the practicability of the defined indicator set from the Delphi study was evaluated. An integrated techno-sustainability assessment (TSA) framework was developed, which combines environmental, economic, and social analyses to evaluate the impacts over the life cycle of biobased chemicals. TSA integrates technological and country-specific data with environmental characterization factors, economic values, and social data. Decision makers should be able to assess sustainability from a low technology readiness level (TRL) by identifying potential hurdles and opportunities. A MCDA integrates the sustainability indicators expressed in different units, taking into account stochastic and flexible method options. A stochastic, hierarchical outranking approach for sustainable decision-making was proposed with the aim to structure decisions between different alternative scenarios and to make sustainable choices at low TRL. The developed integrated TSA framework was applied to a case for which the sustainability of a production and harvesting plant of microalgae-based food colorants was assessed. Four possible microalgae scenarios were defined comparing two different red microalgae feedstocks, *Porphyridium* and *Dunaliella salina*, and two algae cultivation systems, an open pond and a photobioreactor. The integrated TSA results of the microalgae case showed that cultivating *Porphyridium* in open pond technology and *Dunaliella Salina* in a photobioreactor, are superior to the other assessed scenarios, given the assumptions made.

The novel integrated techno-sustainability assessment framework developed in this dissertation is the first to focus on a combination of methods for (i) a comprehensive indicator selection, (ii) a dynamic integration of sustainability dimensions in one assessment, and (iii) a multi-criteria decision making tool allowing for data uncertainty. The aim of the integrated TSA is to gain insights in the sustainability performance of technologies, products, and value chains. Integrated TSA enables to assess sustainability already in early development stages, to guide research and development, and to support sustainable investment decisions. The most and least preferred scenarios can be selected and better-informed choices between alternatives can be made by evaluating environmental, economic, and social sustainability impacts in one holistic framework.

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(E)TEA	(Environmental) techno-economic assessment
(I)LUC	(Indirect) land use change
AFD	Abiotic fossil depletion
AHP	Analytic Hierarchy Process
AURORA	Aggregating uni-criterion rankings into one ranking
BIBD	Balanced Incomplete Block Designs
BWS	Best-worst scaling
CBC	Choice Based Conjoint
CED	Cumulative energy demand
CP	Capital productivity
EAP	Environment action programme
EC	Energy cost
EF	E-factor
EHSI	Environment, health and safety index
EMSC	Environment, health, and safety management system compliance
EoL	End-of-life
Eq.	Equivalent
EU	European Union
EW	Equal weights
FAO	Food and Agriculture Organization
FEC	Fossil energy consumption
FEP/MEP	Freshwater/marine eutrophication potential
FETP/METP/TETP	Freshwater/terrestrial/marine ecotoxicity potential
FWP	Fair wage potential
GHG	Greenhouse gas (emissions)
GRI	Global Reporting Initiative
GWP	Global warming potential
HB	Hierarchical Bayes
$HTP_{c/nc}$	human toxicity potential cancer/non-cancer
ILO	International Labour Organization
IPCC	Intergovernmental Panel on Climate Change
ISO	International Organization for Standardization
LCA	Life cycle assessment
LCSA	Life cycle sustainability assessment
LUP	Land use potential
M&E	Mass and energy
MACBETH	Measuring Attractiveness by a Categorical Based Evaluation Technique
MCDA	Multi-criteria decision analysis
MLI	Mass loss index

MSP	Minimum selling price
NPV	Net present value
OECD	Organisation of Economic Co-operation and Development
OP	Open pond
ORNL	Oak Ridge National Laboratory
PBR	Photobioreactor
PCI	Process innovation
PDI	Product innovation
PEF	Product Environmental Footprint
PFD	Process flow diagram
PROMETHEE	Preference Ranking Organization METHod for Enrichment Evaluation
PT	Product transparency
R&D	Research and development
RA	Risk aspects
REACH	Registration, Evaluation and Authorization of Chemicals
REW	Rank exponent weights
RMC	Raw materials costs
ROCW	Rank-order centroid weights
RoHS	Restriction on Hazardous Substances
RQ	Research question
SC	Scenario
SEC	Specific energy consumption
SETAC	Society of Environmental Toxicology and Chemistry
SMAA	Stochastic multi-attribute analysis
SRW	Stochastic random weights
TRL	Technology readiness level
TSA	Techno-sustainability assessment
UN	United Nations
UNEP	United Nations Environment Programme
WCED	World Commission on Environment and Development
WCP	Water consumption potential
WoS	Web of Science
Yr	Year

CHAPTER 1

Introduction

1. Sustainability and the bioeconomy

The concept of "sustainability" is widely used, but its scope and operationalization is still a subject to debate. Many attempts have been undertaken to limit its ambiguity by publishing definitions, tools, methods, and frameworks to define and measure sustainability (Glavič & Lukman, 2007). A widespread definition on sustainable development was formulated in 1987 by the WCED in the Brundtland report: "development that meets the needs of the present without compromising the ability of future generations to meet their own needs" (World Commission on Environment and Development, 1987). In 2002 on the World Summit on Sustainable Development, the United Nations introduced the three dimensions concept for sustainable development, which embraces economic development, social development, and environmental protection (UN, 2002).

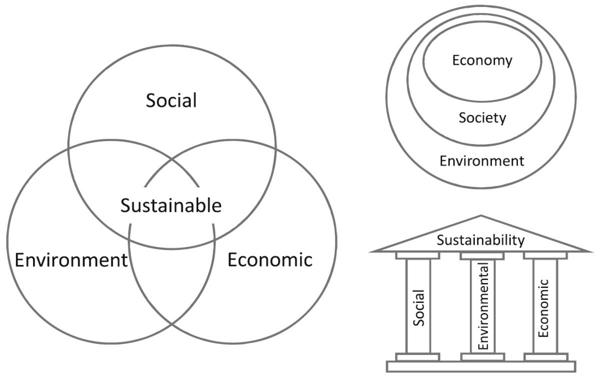

Figure 1. Different representations of sustainability dimensions: environment, economic, and social (Purvis et al., 2019).

These dimensions of sustainability can be approached and visualized in multiple ways: as three intersecting circles, as literal 'pillars', or as concentric circles (Figure 1) (Purvis, Mao, & Robinson, 2019). The 2030 Agenda for Sustainable Development declares the commitment to "achieve sustainable development in its three dimensions — economic, social, and environmental — in a balanced and integrated manner" (United Nations, 2015). However, to date, there is no consensus on the exact content of these three dimensions, nor their evaluation in practice. In addition, a distinction can be made between strong sustainability and weak sustainability (Neumayer, 2010). Strong sustainability argues that certain natural resources are limited and irreplaceable and must be conserved, while weak sustainability supports substitutability between both natural and manufactured capital (Barinaga-Rementeria & Etxano, 2020). The support of strong versus weak sustainability influences the way sustainability is defined and assessed.

Policy makers on a regional, national, or supranational level publish strategic documents, guidelines, and directives, with sustainability as one of their main priorities. An example is the Europe 2020 strategy, which will soon reach its deadline. This strategy was adopted in 2010 and focused on smart, sustainable, and inclusive growth of Europe, and the expansion of a sustainable social market economy. Some key targets that were covered in the Europe 2020 strategy were the reduction of greenhouse gas (GHG) emissions, the use of more renewable energy, an increase in energy efficiency, fewer risks of poverty, and increased employment. All these aspects are part of this wider concept of sustainability in an environmental, economic, or social way and, as such, should be part of the assessment of sustainability. A more recent global action plan was launched by the Club of Rome in 2019. This book titled "Sustainable action – overcoming the barriers" offers guidance for concrete actions that need to be taken given the ambitious targets set by the 2030 Agenda and the Paris Agreement (Berg, 2019). Specifically for the EU, a recent growth strategy called "the European Green Deal" was set out by the European Commission, which aims to transform the EU into a "fair and prosperous society, with a modern, resource-efficient, and competitive economy" (European Commission, 2019). Next to governmental policies and environmental legislations, bottom-up incentives to stimulate sustainability are also coming from customer's demand and growing societal environmental awareness (Leal-Millán, Peris-Ortiz, & Leal-Rodríguez, 2018). As a consequence, companies are challenged to adopt new strategies, products, and technologies with a focus on (more) sustainability.

Achieving sustainability is inevitably linked to the introduction of new innovative technologies and products, with preferably lower environmental impacts and social and economic gains. Within a world of population growth and increasing GHG emissions, the bioeconomy is getting more and more attention by offering the opportunity to reconcile economic growth with environmentally responsible actions and promising a low carbon economy with new jobs (Eickhout, 2012). Boosting the bioeconomy is also a cornerstone of the 2020 strategy (Fritsche & Iriarte, 2014). Therefore, the Bioeconomy Strategy was formulated by the European Commission in 2012 as a guide for research and innovation agendas (European Commission, 2012). In 2018, an update of this bioeconomy strategy was published, which responds better to recent policy priorities (European Commission, 2018). New or improved industrial processes need to be built for the conversion of biomass into a variety of energy applications and other products. However, the use of organic matter (i.e., biomass) for food, feed, biobased products, and bioenergy could also lead to negative impacts such as land use changes because of deforestation and poor farming practices, or additional water use. That is why these impacts concerning sustainability should be measured and monitored, preferably already within the development phase of new biobased technologies. A comprehensive assessment framework is needed to evaluate the sustainability impacts of biobased products.

This dissertation is dedicated to the development of an integrated techno-sustainability assessment (TSA) framework with a focus on emerging technologies within the biobased economy. A comprehensive indicator selection and an integrated method for sustainability analysis will be proposed, specifically for the assessment of biobased chemicals. The aim is to provide a framework to assess technologies already in early development stages and, through its application, boost a sustainable economy which is viable, bearable, and equitable. In the next paragraphs, the topic of this dissertation will be further explained and the major concepts are defined. Hereafter, the problem identification will be summarized and the research questions (RQs) that are answered in this PhD thesis are described.

2. Sustainability assessment of biobased chemicals

2.1 Biobased chemicals

Green chemistry is defined as “the design of chemical products and processes that reduce or eliminate the use and generation of hazardous substances” (Mulvihill, Beach, Zimmerman, & Anastas, 2011). Twelve principles of **green chemistry** were defined, which should guide technology development within chemistry (Anastas, Paul T; Warner, 1998) (Figure 2). One of these principles is the use of renewable feedstocks, which could drive the chemical industry towards the application of **biobased chemicals** (Anastas, Paul T; Warner, 1998). These biobased chemicals could potentially also adhere to other principles such as degradability, pollution prevention, and safer products. Turnover of the EU biobased chemical- and plastic industry already reached 60 billion euros in 2017 according to the 2020 BBI consortium press release from NOVA Institute (Bio-based Industries Consortium, 2020). However, biobased chemicals still occupy only a small share of 4 percent of the total volume of chemicals within the EU[1] (RoadToBio consortium, 2019).

Figure 2. Twelve principles of green chemistry by Anastas and Warner in 1998.

There are many chemicals which can be produced from biomass (J. C. Philp, Ritchie, & Allan, 2013). In this dissertation, a case study is selected that concerns the use of **microalgae as biobased feedstock**. Microalgae have received significant interest as a biofuel feedstock, but the large investment costs prevent the "fuel only" option to be economically viable, to date (Zhu, 2015). However, microalgae also include high-value products that can be used in the food, feed, and pharmaceutical industry (Raja, Hemaiswarya, Kumar, Sridhar, & Rengasamy, 2008). An example is the availability of pigments in algae, such as blue colored

[1] Taking into account the product categories: surfactants, paints and coatings, man-made fibers, cosmetics, plastics/polymers, lubricants, adhesives, solvents, and agrochemicals.

phycocyanin from *Spirulina,* or red pigments like phycoerythrin from *Porphyridium* and β-carotene from *Dunaliella salina* algae. In this dissertation, a microalgae case growing *Porphyridium* and *Dunaliella salina* algae in different open and closed cultivation systems, specifically for the production of red pigments as food colorants, is further assessed and used as a case study.

The use of sustainability assessment within the biobased economy is extensively addressed in academic literature and scientific projects. These assessments started with sustainability analysis on the management of natural resources, such as forest management, and low value biomass applications, such as bioenergy and biofuels (Fritsche & Iriarte, 2014). However, guidance on sustainability assessment specifically for biobased chemicals seems to be lacking and is usually limited to unconnected environmental or economic assessments. The environmental impact of a (biobased) technology is usually assessed separately from its economic value. As a consequence, results are difficult to compare due to evaluations at different TRLs, with different system boundaries (Thomassen, Van Dael, Van Passel, & You, 2019).

2.2 Sustainability indicators

Assessment tools to measure sustainability of various technologies and products, can broadly be divided into three categories: monetary, biophysical, and indicator-based tools (A. Gasparatos & Scolobig, 2012). In this dissertation, an indicator-based method is developed as it is the most flexible to quantify a range of economic, social, and environmental impacts, complying with the three sustainability dimensions (A. Gasparatos & Scolobig, 2012). An indicator-based sustainability assessment seeks to identify a range of indicators to measure sustainability performance (Juwana, Muttil, & Perera, 2012). Biophysical and monetary indicators can be added to ensure interlinkages with technological aspects. Indicator-based methods include a range of value-laden methodological choices, which should be clearly addressed and justified while assessing sustainability (A. Gasparatos & Scolobig, 2012).

Indicators are used to assess and evaluate performances, to provide trends on improvements, and warnings on declining trends. This way, indicators provide information to decision makers to formulate strategies and communicate achievements to stakeholders (Lundin, 2003). However, an extensive indicator selection is often lacking when performing sustainability analysis. ‘Popular’ indicators, such as global warming potential (GWP) or net present value (NPV), are naturally considered by most assessments without consulting stakeholders or performing a comprehensive literature review for the inclusion of other relevant impacts. In addition, sustainability analysis is case-specific and indicator sets should be defined accordingly. An example is the construction of criteria and indicators specifically for sustainable woodfuels by the Food and Agriculture Organization of the UN (FAO) (*Criteria and indicators for sustainable woodfuels*, 2010). An indicator set specifically designed for the assessment of biobased chemicals, including all three sustainability dimensions, did not yet exist.

When developing sets of indicators, a thorough understanding of the market and policy environment is necessary. Two approaches for indicator selection exist: a literature review or a participatory approach (Mascarenhas, Nunes, & Ramos, 2015). Design validation of the indicators can be increased by using expert judgements for their selection (Bockstaller & Girardin, 2003). **Expert involvement** could aid the selection of indicators combined with a prioritization exercise to determine the relative importance of each (Kurka & Blackwood, 2013). A stakeholder meeting with experts from the industry, academics, and governmental bodies, could be carried out by means of a Delphi method, “a method used to obtain the most reliable consensus of opinion of a group of experts by a series of intensive questionnaires interspersed with controlled feedback” (Dalkey & Helmer, 1962). A Delphi study is known to have a flexible design and is always compiled in multiple rounds, until consensus among the experts is reached (Okoli & Pawlowski, 2004). In this dissertation, a Delphi study will be used for the selection of sustainability indicators, using expert opinion, for the assessment of biobased chemicals.

2.3 Sustainability assessment

When indicators are selected, a mathematical analysis and impact calculations at product level can be initiated. Any sustainability analysis starts by collecting relevant **technological** data concerning the processes of the value chain. A process flow diagram (PFD) and the corresponding mass and energy (M&E) flows should be mapped. The nature of the data and level of detail is highly depending on the technology readiness level (TRL) of the considered technology, ranging from an initial idea situated at TRL 1 or 2, to a proven and mature technology at TRL 9 (Mankins, 2009) (Figure 3). Emerging biobased technologies are often situated at low TRL (from TRL 4 to TRL 6), meaning that secondary data from literature, computer models, and lab scale results can be the only available information sources. However, this data entails a lot of uncertainty and many process operations and parameters change while scaling up. Furthermore, one should avoid approaching a technology without considering its up- and downstream value chain activities. A life cycle view should be supported during the technological analysis and subsequent sustainability assessment.

	TRL 1	TRL 2	TRL 3	TRL 4
	Basic principles	Technology/ application concept	Proof of concept	Laboratory testing of protoype
TRL 5	**TRL 6**	**TRL 7**	**TRL 8**	**TRL 9**
Laboratory testing of integrated system	Prototype verified	Pilot system	Commercial design	Full scale

Figure 3. An overview of technology readiness levels (TRLs) (Mankins, 2009).

Life cycle analysis, or LCA, is a globally recognized method to perform an **environmental** analysis over the entire life cycle of a product. It is a methodology, formally described in the ISO 14040 guidelines, which estimates potential environmental impacts in different categories based on life cycle inventory collected. Many environmental indicator sets were defined to use within LCA, such as the widely applied ReCiPe indicators (M.A.J. Huijbregts et al., 2017). The ReCiPe set includes seventeen midpoint categories (including eutrophication, ozone depletion, human toxicity, etc.) and three corresponding endpoint categories: human health, ecosystem quality, and resource scarcity. Next to ReCiPe, other impact assessments methodologies are available such as TRACI 2.1 and CML-IA. There are four basic steps necessary to perform an LCA: (1) definition of goal and objective, (2) inventory analysis, (3) impact assessment, and (4) interpretation. The techno-sustainability assessment framework developed in this dissertation aims to be compliant with these four steps.

Economic sustainability aims to produce viable and profitable products and services. A common way to assess the economics while taking into account technological feasibility, is the techno-economic assessment (TEA) methodology (Kuppens et al., 2015). Financial indicators, such as NPV or payback period, are quantified in a dynamic way, and a sensitivity analysis facilitates the interpretation of the results. The latter step identifies the most influential parameters and provides decision makers with lots of information concerning their technologies and products. Thomassen et al. (2018) elaborated on the TEA by adding LCA concepts to the assessment. Their method is called the 'environmental techno-economic assessment' (ETEA) for which an integration between the economic and environmental dimensions of sustainability was implemented (Thomassen, Van Dael, & Van Passel, 2018). A recent review by Wunderlich et al. (2020) focused on different types of integration of TEA and LCA (Wunderlich, Armstrong, Buchner, Styring, & Schomäcker, 2020). They advised adapting a certain type of integration to the goal of the study, which can be to (i) reveal hotspots, (ii) benchmark technologies, or (iii) select the preferred process options. These goals depend on the stakeholders involved being academics, policy makers, or technology managers. A broad framework for different types of integration was proposed, but is difficult to apply at low TRLs, where data uncertainty and availability are very pronounced.

The **social** dimension completes the three-pillar system of sustainability and is often approached by social life cycle assessment. A Life Cycle Initiative supporting social LCA was set up by UNEP and SETAC who developed the "Methodological sheets for sub-categories in social life cycle assessment" in 2013 (UNEP SETAC, 2013). They proposed indicators for different stakeholder groups, such as workers and local communities. Metrics were proposed to measure the indicators, but they remain mostly qualitative or semi-quantitative. For a specific analysis, the proposed indicators are only applicable when a full-scale company at high TRL is assessed, using company reports or interviews. More generic analysis requires country or sector data, and might be more relevant for sustainability assessments at low TRL. However, compared to the economic and environmental dimension of sustainability, social sustainability is usually neglected. As a result, the social dimension is the least conceptually developed of the three dimensions (Cuthill, 2010). Social impacts are known to be added in a qualitative and rather simplified way due to the lack of knowledge and the high level of subjectivity present within this sustainability dimension.

The previous paragraphs describe the three sustainability dimensions and the methods used for their assessments. The UNEP/SETAC Life Cycle Initiative proposed a life cycle sustainability assessment (LCSA) approach that addresses all three sustainability dimensions in one assessment and aids decision-making (Valdivia et al., 2013). This approach has been applied in fields such as, for example, renewable energy, circular economy, and biobased economy (Fauzi, Lavoie, Sorelli, Heidari, & Amor, 2019). Fauzi et al. (2019) conducted a review study with 114 publications discussing and applying LCSA. However, it remains a challenge to enable stakeholder involvement and to apply the LCSA approach to technologies and products at low TRL. A clear harmonization of the three sustainability dimensions is still missing and further practical and technical recommendations on methods within LCSA are required (Fauzi et al., 2019). Also, current LCSA applications have mostly focused on ex-post assessment of full-scale technologies, while the LCSA approach could be valuable for assessments in early development stages as well (Cucurachi, Giesen, & Guinée, 2018). Ex-ante LCSA assessment could explore future opportunities by assessing a range of possible scenarios, and linking process data directly with the three dimensions of sustainability. Finally, a set of indicators is still missing including aspects from the three sustainability dimensions (Valdivia et al., 2013).

2.4 Multi-criteria decision analysis (MCDA)

An **integrated indicator-based analysis** should enable practitioners to draw conclusions on the technology’s full sustainability in a balanced and holistic way. Multi-criteria decision analysis (MCDA) is a well-known and commonly used technique which is able to consider conflicting, multidimensional, and incommensurable effects of the sustainability concept (Bulckaen, Keseru, & Macharis, 2016). MCDA on itself is already considered as a form of integrated sustainability evaluation (Wang, Jing, Zhang, & Zhao, 2009). The selected indicators should be scored and receive weights that reflect the relative importance within the decision context (Inotai et al., 2018). Many MCDA methods exist, such as the Analytic Hierarchy Process (AHP) or the Preference Ranking Organization METHod for Enrichment Evaluation (PROMETHEE). However, it is important that these methods fit the decision problem. Even within these generally applied MCDA methods, many different methodological choices need to be made concerning preference structures, accepted weights, and aggregation techniques. These choices are often made prior to the analysis, instead of comparing multiple options to encounter methodological uncertainty (Opon & Henry, 2020).

3. Problem identification

Technologies at an early stage of development should be assessed on their environmental, economic, and social sustainability performance. It is important that these three dimensions are balanced within sustainability assessments of entire product value chains. Sustainability evaluations are already being performed using LCA, TEA, and (social) LCA, focusing on the total life cycle of a product. However, existing indicators and methods to measure sustainability as a whole, are still insufficient. Three major concerns exist:

(1) While sustainability as a concept encompasses three dimensions (environment, economic, and social), existing sets of indicators often lack information on the economic and social aspects (Fritsche & Iriarte, 2014). Especially the social aspects have often been neglected as they are difficult to quantify and potentially subjective (Rafiaani et al., 2018). In addition, environmental impact assessments of bioeconomy value chains are also incipient and usually limited to a few indicators (Cristóbal, Matos, Aurambout, Manfredi, & Kavalov, 2016).

(2) Sectoral characteristics for high-value applications, such as biobased chemicals, should be included in sustainability assessments. General indicators can be used as guidance for the development of sustainability indicators for biobased products, but should be adapted to case-specific characteristics (Fritsche & Iriarte, 2014).

(3) When all three sustainability dimensions are included, they are mostly addressed separately while sustainability should be assessed holistically

by integrating various concerns (Singh, Murty, Gupta, & Dikshit, 2009). LCSA offers such an approach, but the combination of multiple assessment methods in one framework and the application on technologies at low TRL, remains a challenge. An integration of different indicators and metrics is needed to seek comprehensive and multidisciplinary thinking (Singh et al., 2009). This way, decision makers would be able to make choices based on a complete sustainability assessment, including all dimensions, in early development stages.

The aim of this dissertation is to develop a novel framework to assess emerging technologies on their relative environmental, social, and economic sustainability. Early sustainability assessments of technologies, products, and their entire value chain can guide decision makers towards making sustainable, better-informed choices. An integrated techno-sustainability assessment (TSA) framework will be implemented, including a comprehensive indicator selection within all sustainability domains and a flexible tool for decision-making. An integrated TSA can be used for policy recommendations and impact assessments by academics, governmental bodies, and industries. Different steps were undertaken to develop the integrated TSA framework and the separate research questions (RQs) are further explained below.

4. Research questions

RQ 1. Which indicators are available in current scientific literature for the sustainability assessment of biobased chemicals?

In the second chapter, a review of the state-of-the-art sustainability indicators, specifically for biobased chemicals, is conducted, and a corresponding gap analysis is performed. Environmental indicators, as well as social and economic indicators were analyzed and classified, and research gaps were defined. The review discloses the lack of a holistic view concerning sustainability, with often incomplete and unspecific sets of indicators used in assessments. The need for a comprehensive indicator selection is highlighted, which was the starting point for the second research question.

RQ 2. Which indicators are needed and preferred for the sustainability assessment of biobased chemicals?

In the third chapter, a Delphi study in combination with a MCDA outranking method investigates expert consensus concerning indicators needed and preferred for a sustainability analysis of biobased chemicals in Europe. The experts are consulted by means of the Delphi survey method with an open and closed question round. Sustainability indicators were selected and the stakeholders' priorities were assessed. A final consensus ranking can be developed based on the survey data and the use of a MCDA. The rank correlation coefficient Kendall's τ measures how well a candidate consensus ranking fits an expert's ranking (De Keyser & Springael, 2009; Kendall, 1938). A full ranking of sustainability indicators is composed, comprising environmental as well as economic and social indicators, specifically for biobased chemicals.

RQ 3. How can sustainability indicators be quantified for the assessment of emerging biobased technologies?

In the fourth chapter, the selected indicators from chapter 3 need to be quantified in order to check the practicability of the defined, survey-based indicator set. An integrated techno-sustainability assessment (TSA) framework is first proposed, in which technological and country-specific data are integrated with environmental characterization factors, economic values, and social data. The developed framework is applied to a case where microalgae are used as feedstock for the production of biobased chemicals. The developed integrated TSA method consists of six major steps including: (1) the definition of goal and scope, (2) indicator selection, (3) the development of a PFD and M&E balance, (4) environmental, economic, and social analysis, (5) uncertainty and sensitivity analysis and (6) final decision-making using MCDA. The first five steps are discussed in chapter 4. The last step provides an answer to RQ 4 and will be further elaborated in chapter 5.

RQ 4. How can sustainability indicators be integrated in order to make decisions?

In the fifth chapter, the sustainability indicators that were selected and quantified for the microalgae case are integrated to enable decision-making by various stakeholders. MCDA is added to the TSA framework to tackle data uncertainty and enable comparison when indicators are expressed in different units. A hierarchical, stochastic outranking approach is developed and applied to the present microalgae case. Flexible method options concerning preference schemes and weights are added, which provide a check for robustness of the integrated results. The final step of the integrated TSA framework should enable decision makers to assess the relative sustainability of their technologies, and make adequate choices concerning research and development (R&D) targets and key processes.

Figure 4 shows how the separate research questions contribute to the development of the integrated TSA framework. Chapters 2, 3, 4, and 5 of this PhD thesis will handle each of these research steps in detail. The dashed arrow going back from Step 6 to Step 1 indicates the iterative character of a TSA. An emerging technology should be assessed continuously while moving higher on the TRL scale.

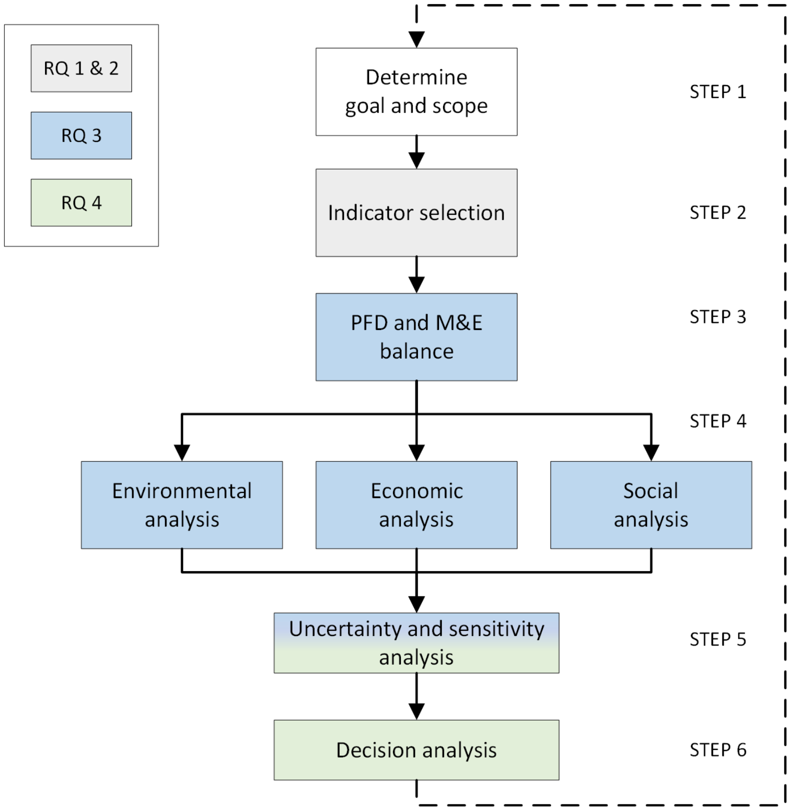

Figure 4. Summary of the research questions within the integrated techno-sustainability assessment (TSA) framework. RQ = research question, PFD = process flow diagram, and M&E = mass and energy.

CHAPTER 2

A review of sustainability indicators for biobased chemicals

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ABSTRACT

Companies dealing with chemical products have to cope with large amounts of waste and environmental risk due to the use and production of toxic substances. Against this background, increasing attention is being paid to "green chemistry" and the translation of this concept into biobased chemicals. Given the multitude of economic, environmental, and social impacts that the production and use of biobased chemicals have on sustainability, assessment approaches need to be developed that allow for measurement and comparison of these impacts. To evaluate sustainability in the context of policy and decision-making, indicators are generally accepted means. However, sustainability indicators currently predominantly exist for low-value applications in the bioeconomy, like bioenergy and biofuels. In this chapter, a review of the state-of-the-art sustainability indicators for biobased chemicals is conducted and a gap analysis is performed to identify indicator development needs. Based on the analysis, a clear hierarchy within the concept of sustainability is found, where the environmental aspect dominates over economic and social indicators. All one-dimensional indicator sets account for environmental impacts (19 out of 38), whereas two-dimensional sets complement the environmental issues with economic indicators (13 out of 38). Moreover, even the sets encompassing all three sustainability dimensions (6 out of 38) do not account for the dynamics and interlinkages between the environment, economy, and society. Using results from the literature review, an indicator list is presented that captures all indicators currently used within sustainability assessment of biobased chemicals. Finally, a framework is proposed for future indicator selection using a stakeholder survey to obtain a prioritized list of sustainability indicators for biobased chemicals.

1. Introduction

The chemical industry must cope with large amounts of waste and environmental risk due to the use and production of toxic substances. About 60 percent of chemicals are hazardous to human health or the environment in the EU (Goldenman et al., 2017). Chemicals made from biomass could potentially reduce these risks and be more sustainable compared to their fossil-based counterparts.

Biobased chemicals belong to the biobased economy, where organic matter (i.e., biomass) is converted into materials and energy. Biomass as a feedstock offers opportunities to deal with increasing prices of fossil feedstocks and their decreasing availability (Sillanpää & Ncibi, 2017). The focus in the biobased economy is currently shifting from bioenergy and biofuels to the production of high-value biobased products, including biobased chemicals (Fritsche & Iriarte, 2014). Biobased products are products wholly or partly derived from biomass, such as plants, trees or animals, with the biomass potentially undergoing physical, chemical or biological treatment (European Committee for standardization, 2014).

The emerging biobased economy is often associated with increased sustainability (Pfau, Hagens, Dankbaar, & Smits, 2014). However, the use of biomass can also lead to negative consequences, for example, by driving up food prices through increased competition for land and resources, or by increasing greenhouse gas (GHG) emissions through land use change (Baskar, Baskar, & Dhillon, 2012; Lange, 2011). To ensure that biobased products become or remain more sustainable than their fossil fuel based counterparts, a systematic and interdisciplinary assessment approach is needed (Pfau et al., 2014). The current trend is to move away from multidisciplinarity towards transdisciplinarity and holism, where adequate sustainability evaluations account for the interactions and interdependencies across the different sustainability themes (Sala, Ciuffo, & Nijkamp, 2015). Criteria and indicators can be used as flexible and user-friendly techniques to evaluate and integrate environmental, economic, and social impacts. Sustainability indicators are needed to translate sustainability into a practical set of measures and are frequently used for policy- and decision-making (Sala et al., 2015; Singh et al., 2009; Tanzil & Beloff, 2006).

International attempts to provide and stimulate sustainability within the general bioeconomy started with the development of criteria and indicators for sustainable forest management (Fritsche & Iriarte, 2014). These first environmental assessments were designed as a result of the concerns about tropical deforestation. Later, sustainability frameworks for biofuels and bioenergy followed (Fritsche & Iriarte, 2014). More general sustainability frameworks were constructed through initiatives and projects like UNEP-SETAC (2009), the Global-

Bio-Pact (2012), ORNL (2013) and BioSTEP (2016). As sustainability assessment became more popular, a significant variety of mostly environmental stand-alone indicators were developed, like the cumulative energy demand (CED) and the E-factor (Mark A J Huijbregts et al., 2006; Roger Arthur Sheldon, Arends, & Hanefeld, 2007). Nevertheless, one indicator can never capture all aspects of sustainability.

Researchers are concerned with the development of indicators and frameworks for the assessment of sustainability. Singh et al. (2012) and Ruiz-Mercado et al. (2012) compiled an overview of indicators and indices for generic sustainability assessment of chemical processes and concluded that most assessments only evaluate one aspect of sustainability (Ruiz-Mercado, Smith, & Gonzalez, 2012; Singh et al., 2009). They argued that by using the indicators complementarily, interlinkages and dynamics between the different aspects of sustainability have been missed. Seuring and Müller (2008), Lozano (2012), Tang and Zhou (2012), Seuring (2013), and Aktin and Gergin (2016) agreed with these concerns regarding inadequate sustainable management (Aktin & Gergin, 2016; Lozano, 2012; Seuring, 2013; Seuring & Müller, 2008; Tang & Zhou, 2012). If we narrow the broader sustainability scope down to a focus on biobased chemicals, no full overview or discussion of sustainability indicators currently exists.

The aim of chapter 2 is to review existing indicator sets, to classify the different indicators, and to define the gaps in sustainability assessments, specifically for biobased chemicals. While assessing the sustainability of biobased chemicals, all indicators covering the full value chain from cradle to cradle should be considered (Iriarte & Fritsche, 2015). A state-of-the-art review like this one is a crucial step towards a generalized set of indicators that can be used to assess and evaluate performances, and to provide information on improvements or declining trends. These indicators should be uniform within the field of biochemistry, since they will provide information to decision makers on formulating strategies and communicate achievements to stakeholders (Bosch, van de Pol, & Philp, 2015; Lundin & Morrison, 2002). If more stakeholders use the same set of metrics, efforts involving data collection and the time required to assess the products will be reduced as a result of experience and knowledge sharing (Patel et al., 2013).

Moreover, a standardized set of sustainability indicators enables comparisons between biobased chemicals and facilitates policy recommendations. This dissertation focuses on biobased chemicals, taking into account the specific chemical- and biological characteristics of the products. Although some indicators can be used in all process industries, sector-specific indicators are often required to address specific features of each industrial sector (Saurat, Ritthoff, & Smith, 2015).

The next section explains the method used to perform an adequate review of the current biobased chemistry indicators landscape. Existing indicators are defined, classified and the gaps in current literature are determined. The results are covered in the third section of this chapter, followed by an extensive discussion and conclusion.

2. Method

The review study is based on a systematic literature search, considering articles published up to and including 2017, using Boolean logic on ISI Web of Science (WoS) (Figure 5). The initial query: 'biobased chemicals' AND 'sustainability indicators', yielded 130 results. Related search terms containing 'green chemistry', 'sustainability metrics' and 'sustainable decision making', enriched the dataset and were added as a necessary extension for the review. At this stage, 26 papers were considered relevant to include in this review study. Finally, additional queries based on the separate sustainability dimensions were included ('environmental sustainability', 'economic sustainability' and 'social sustainability'), and resulted in 12 extra papers for the final dataset. In total 38 papers were selected and further reviewed.

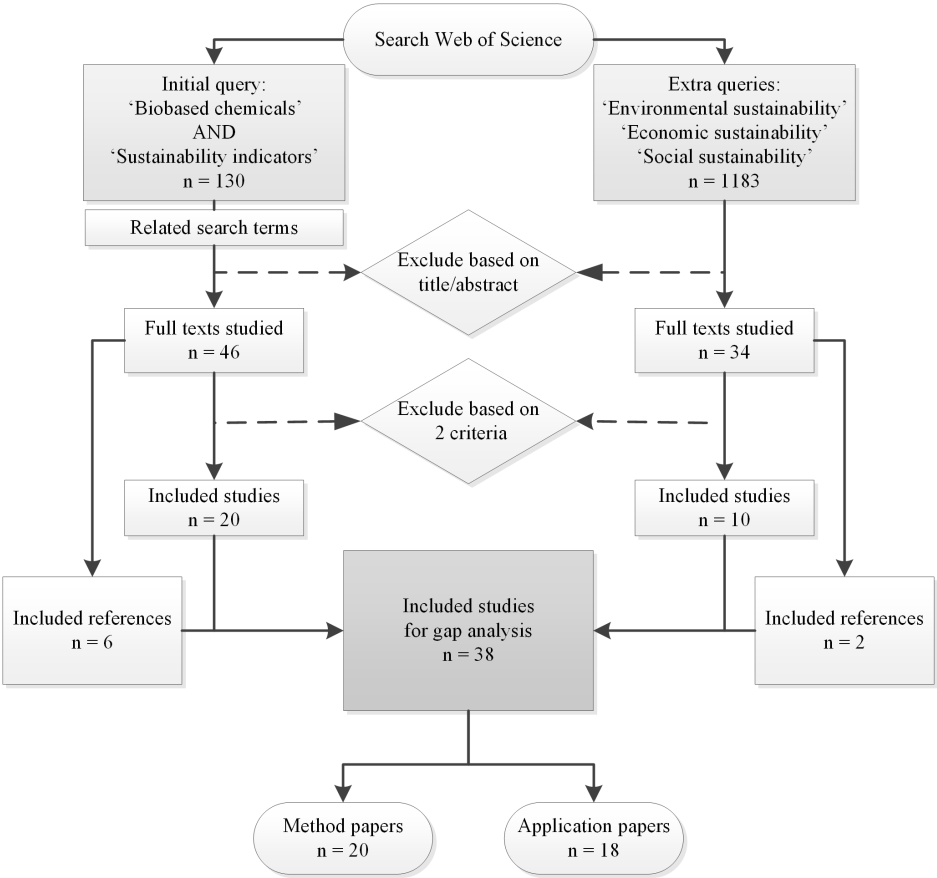

Figure 5. Flowchart of article search and selection for review analysis.

The decision for inclusion of articles was based on two criteria: (1) the focus on 'sets' of indicators instead of stand-alone indicators, and (2) enclosing sets which assess only on product- and/or activity level. First, the included articles were selected based on the use of sets of indicators aiming for a sustainability evaluation of a biobased chemical. Research about stand-alone indicators was left out of the initial dataset, but articles about these stand-alone indicators were often necessary to clarify and complete the output of this analysis. Also, research articles about indicators used in the broader bioeconomy or chemical industry were not necessarily included, only if applied to a biobased chemical case study or considered relevant by other biobased chemical research applications. Second, the included indicator sets were all developed for assessment on the product level of the chemical. Research that explored sustainable development more broadly, like on a company- or country-level, was excluded from the dataset.

The 38 papers that were included in this review analysis are provided in Appendix A1. A distinction is made between 'method papers' and 'application papers'. The method papers provide new sets of indicators developed to evaluate the sustainability of biobased chemicals. The application papers apply (part of) the sets described in the method papers to business-cases within the biobased chemical industry.

The studies included for the gap analysis were analysed according to (i) the inclusion of different sustainability pillars (i.e., environment, economy, and society), (ii) their focus (i.e., general sustainability, general biomass, chemicals and biobased chemicals), (iii) the overlap between indicators (derived from description and formula), and (iv) interlinkages between the sustainability domains. Based on the results of this review, an indicator list is presented that captures all indicators currently used in scientific literature for sustainability assessments of biobased chemicals (Appendix A2). The indicators found during the review process were classified within the corresponding sustainability domain and assigned to a sustainability criterion.

3. Results

The included pool of articles consists of 20 method papers and 18 application papers. 14 method papers also provide a concise biobased chemical application case within the same article. The earliest article that developed a set of sustainability indicators, specifically for biobased chemicals, dates from 2002, four years after the introduction of the 'green chemistry' concept by Anastas and Warner (1998) (Anastas, Paul T; Warner, 1998) (Figure 6). Between 2004 and 2007, no relevant publications were found. From 2010 onwards, the first actual applications of the method articles emerged.

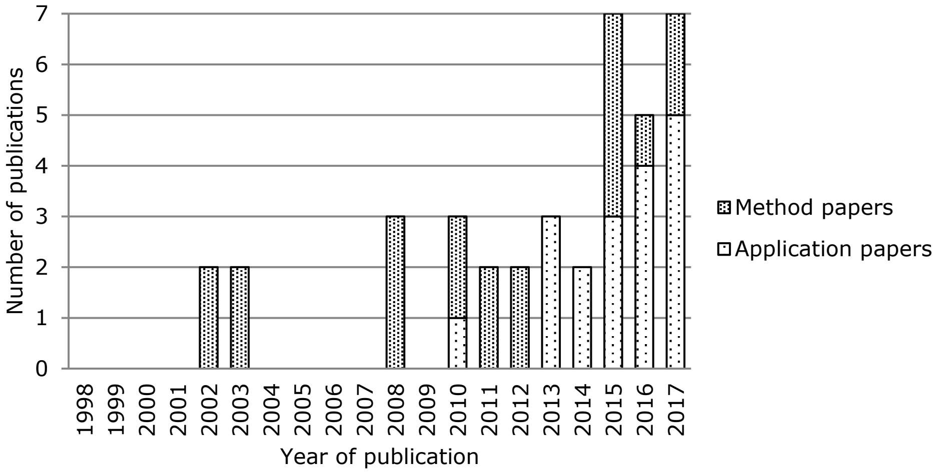

Figure 6. Number of included publications 1998-2017 (38 papers).

Often, indicators are closely related or overlap when examining their descriptions or formula. For example, the fossil energy consumption (FEC) is calculated based on the CED of raw materials and the CED of utilities, and material efficiency is often based on the E-factor. Some sustainability schemes provide a detailed description of the measurement along with a specific formula. Other sets provide only limited documentation and leave room for interpretation. This illustrates that no clear, widespread definition of an 'indicator' is used. Some of the developed indicators tend to be highly specific, like a metric, whereas others stay more vague, like a criterion. One 'criterion' can enclose several indicators, which can be quantitative or qualitative. 'Indicators' are more specific when compared to criteria, and can indicate a trend over time. The difference between a 'metric' and an 'indicator' is more difficult to explicitly define. Tanzil et al. (2006) confirmed the interchangeability between metrics and indicators and specifed metrics as only referring to quantitative measures, whereas indicators can also encompass qualitative descriptions (Tanzil & Beloff, 2006). In this dissertation, the approach of Tanzil et al. (2006) in which indicators can be both quantitative and qualitative, is followed.

When screening the pool of indicators, a differentiation was made between the indicators that are explicitly available (referred to as 'available indicators'), and indicators that are constituents of these explicit indicators (referred to as ‘constituent indicators’). Indicators were marked as ’available’ when explicitly described as part of the proposed framework developed or used in the paper. Indicators were marked as ‘constituent indicators’ when the indicator is described or used in formulas to calculate the explicit indicator. For example, the ‘reduction of baseline emissions’ is an available indicator in the framework of Sacramento-Rivero (2012), which is calculated using the constituent indicators global warming potential, ozone depletion, photo-oxidant formation, eutrophication, toxicities and acidification (Sacramento-Rivero, 2012) (Figure 7). Eutrophication itself is composed of the constituents freshwater-, terrestrial- and marine eutrophication. The aim of making the distinction between available and constituent indicators is to prevent overlooking indicators that are involved in the indicator set as a constituent. For instance, the cost of raw materials is only cited in four different sets as a separate economic indicator, while accounting for the involvement within other indicators, the cost of raw materials is present in 15 papers.

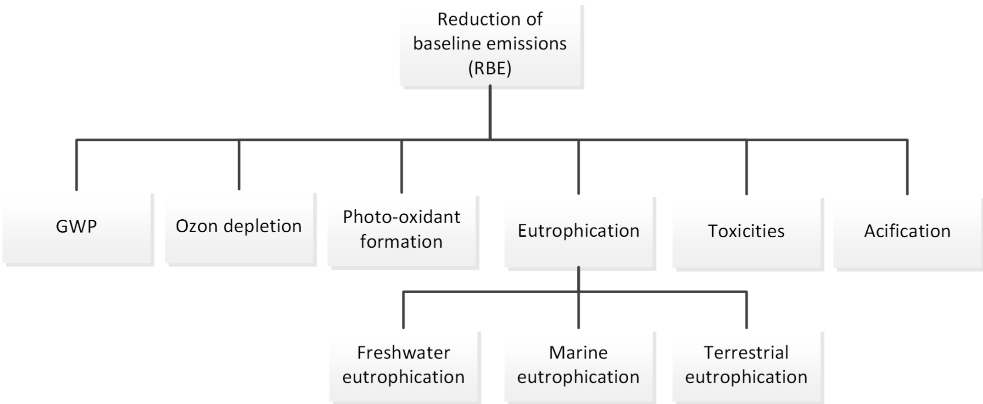

Figure 7. Example of interlinkages between indicators (Saurat et al., 2015).

Overall, 85 different indicators were proposed or used, with 49 indicators reflecting a variety of environmental impacts, 23 indicators reflecting economic impacts, and 13 indicators reflecting social impacts. The results of the review point to an asymmetry of indicators with a dominating position for the environmental impact categories. Moreover, it is rather exceptional that sets of indicators, evaluating biobased chemicals, include all three sustainability pillars. Only 4 out of 20 sets developed in method papers explicitly tackled all three sustainability dimensions, whereas nine of the method papers only assessed the environment.

On top, even if all three pillars are mentioned, the environmental dimension represented the majority of indicators in all papers. This lack of comprehensive and complete sets of indicators is even more explicit when the existing case studies were examined (i.e., the application papers). For the biobased chemical application papers, 10 out of 18 of the included papers only evaluate the environmental aspects. On top, these application papers often applied generic indicator sets like ReCiPe or CML2 Baseline 2000, where the specific characteristics of biobased products, like renewability, were not taken into account (Bare, 2002; Nguyen, Kikuchi, Noda, & Hirao, 2015). Over time, there was no trend noticed as for the inclusion of all three sustainability domains. The first authors that explicitly dealt with economic and social impacts within biobased chemistry were Sugiyama et al. (2008), who introduced a combination of net present value (NPV) and the 'environment, health and safety index (EHSI)' within their assessment. In 2016 and 2017, there were no publications including social impacts, except for some including human toxicity as an environmental indicator.

Based on the reviewed indicators, 10 main criteria were defined for biobased chemicals that combined serve the sustainability goal (Table 1). The different indicators were assigned to these main criteria. Note that some composite indicators were difficult to assign to a certain criterion. Therefore, additional categories, next to these 10 main criteria, are described as 'indices'. In the next paragraphs more details are provided about the different criteria and the corresponding indicators.

3.1 Environmental indicators

The selected sustainability assessments provide 49 different environmental indicators (Appendix A2). Frequently used indicators like eutrophication, acidification, and global warming appear already in the first publications included in this review study (Bare, 2002; Guinee, 2002; M.A.J. Huijbregts et al., 2017). No significant change in focus within environmental sustainability is found. The final list, including all existing indicators, is divided into four different categories, based on the criteria: (i) climate mitigation, (ii) clean and efficient energy, (iii) resource management, and (iv) ecosystem care.

Table 1. Main sustainability criteria derived from current use in literature.

	Criterion	Description
Environment	Climate mitigation	Mitigating global climate change by reducing greenhouse gas emissions emitted by transport, chemical processes, etc.
	Clean and efficient energy use	Controlling and reducing energy requirements and using renewable and cleaner energy technologies
	Resource management	Managing land use, raw materials, process materials and water resources in an efficient, eco-friendly, and economic way
	Ecosystem care	Preventing degradation of natural ecosystem and ecosystem services due to air pollution, eutrophication, ecotoxicity, and waste disposal
	Indices	Composite indicators
Economy	Low costs	Securing a profitable chemical product by efficient low cost management
	Value creation	Securing a profitable chemical product by creating value
	Risk management	Identifying and managing risks to control financial losses due to unfortunate events linked to biobased chemicals
Society	Health	Securing public health by avoiding toxic chemicals
	Safety	Securing a safe (working) environment by identifying risks related to the production of a biobased chemical
	Social care	Promoting a sustainable society for all stakeholders by making a contribution through employment, food security, quality of life, etc.
	Indices	Composite indicators

Climate change is widely included as an impact category when assessing the environmental performance. 32 out of 38 publications consider climate change as a constituent indicator, which makes it the number one used indicator in biobased chemical sustainability assessment. Nguyen et al. (2015) described 'greenhouse gas (GHG) emissions' as "all sources of CO_2, CH_4 and N_2O released from the production process, less any amount of CO_2 absorbed by the biobased feedstock during growth" (Nguyen et al., 2015). GHG emissions operate as a useful indicator for climate change because the atmospheric concentrations of CO_2, CH_4 and N_2O

have been claimed in several IPCC reports to be the dominant cause of global warming (IPCC, 2014). Often, the emissions are expressed in CO_2 equivalents in reference to their GWP, which measures the impact of greenhouse gasses on climate change by combining radiative forcing and the atmospheric lifetime of a gas molecule (Scheutz, Kjeldsen, & Gentil, 2009).

Another environmental criterion considers the energy use in the life cycle. A widely-used indicator to measure energy use is the 'cumulative energy demand' (CED), involved as a constituent indicator in 28 out of 38 publications. CED is defined as the total direct energy use throughout the entire life cycle (Nguyen et al., 2015). Huijbregts et al. (2010) found that CED serves as a relevant screening indicator for environmental performance (Mark A J Huijbregts et al., 2006). Sometimes, only part of the total energy demand is used to evaluate the impact of energy use, like the 'fossil energy consumption' (FEC) or the 'CED of raw materials' (Cespi, Passarini, Vassura, & Cavani, 2016). Some indicator sets include the energy consumption indirectly in their assessment by including indicators like abiotic depletion potential which includes 'mineral- and fossil resource depletion' (Guinee, 2002). In this analysis five different energy-indicators were found, although they are strongly interconnected.

A third criterion covers the management and availability of resources. A key feature of biochemical products is the use of biomass as a renewable feedstock. These indicators, focusing on this characteristic of renewability, are rarely included in biobased chemical sustainability assessments. Tabone et al. (2010) created indicators like 'renewable resources', 'design products for recycle', and 'design biodegradable products', in which chemicals based on biomass can possibly gain advantage over their fossil-based counterparts (Tabone, Cregg, Beckman, & Landis, 2010). Another indicator that is often highly related with the use of biomass, but has a rather negative impact, is the much-discussed 'land use' indicator which encompasses the exploitation of land as a limited and vulnerable resource. The rising human population, together with competition between forestry, agriculture, infrastructure, and nature, are exerting pressure on productive land (Mattila, Helin, & Antikainen, 2012). Land use is included in half of the existing indicator sets (as a constituent indicator). Debate exists on how to measure the various effects of land use. In literature, a distinction is made between ‘land use’, referring to land occupation, and ‘land use change’, referring to land transformation (Mattila et al., 2012). A thorough evaluation of the environmental effect of land use needs to take into account both occupation and transformation of land. For example, the ReCiPe method includes land transformation, occupation, and relaxation to calculate the full land use impact (M.A.J. Huijbregts et al., 2017). Because the land use indicator is often not well specified, different definitions of ‘land use’ are used interchangeably. Sheldon et al. (2015) defined land use as the amount of good agricultural soil required to produce 1 ton of product (in mass), whereas Bare et al. (2003) and Uhlman et al. (2010) highlighted the resulting ecosystem damage (Bare, 2002; Roger A. Sheldon & Sanders, 2015; Uhlman & Saling, 2010). It is important to state a difference between the midpoint and endpoint indicators concerning land use. Midpoint indicators measure the amount of land taken, while an end-point approach looks at the impact of the land use, which is concerned with biodiversity loss and ecosystem services. In this analysis, we divide the land-use category in ‘occupation and transformation’ indicators (17 out of 38 as a constituent indicator), including the midpoint indicators, and ‘ecosystem damage’ indicators (5 out of 38 as a constituent indicator), including the endpoint effects. Only two indicator sets mention the inclusion of ‘indirect land use change’ (ILUC), which covers the greenhouse gas emissions caused by land use change. By ignoring the ILUC, the extra carbon emissions that arise as e.g. farmers convert forest to cropland are not taken into account, and incorrect conclusions might be drawn (Searchinger et al., 2008).

Next to the ecosystem damage caused by land use, other types of pollution and degradation need to be taken into account. The main themes within the fourth ecosystem care criterion are: air pollution, eutrophication, ecotoxicity, and waste generation. Popular indicators arise within these themes, like ‘acidification’ (21 out of 38), ‘photo-oxidant formation’ (18 out of 38), ‘marine eutrophication’ (20 out of 38) or ‘freshwater eutrophication’ (22 out of 38), all as constituent indicators. The ‘E-factor’, which accounts for the actual amount of waste in the process, initially broached the problem of waste generation in the chemical industry and is still involved in four method papers (Roger Arthur Sheldon et al., 2007). Existing indicator sets also propose some new metrics to quantify the undesired products to stimulate waste reduction and the use of biodegradable products, like the 'mass loss index' (MLI) (Sugiyama, Fischer, Hungerbühler, & Hirao, 2008).

3.2 Economic indicators

The economic sustainability dimension is represented by 23 different indicators minimizing costs, maximizing value and managing the risks in the entire life cycle of the biobased chemical (Appendix A2). The most frequently used indicator, and also starting point of most sustainability assessments, is the 'costs of raw materials'. All indicator sets including the economic dimension account for these raw material costs as a constituent indicator, mostly comprised in profitability indicators like 'economic constraint', 'economic index' or investment value indicators like 'net present value' (NPV) or 'minimum selling price' (MSP). Although the listed economic indicators use mostly cost-related measures, 14 of the indicator sets tackling economic impacts additionally try to estimate the profitability or calculate the investment value. The other five indicator sets only calculate the costs related to the biobased chemical value chain. It may be argued that ignoring selling prices and revenues will not correctly reflect the economic value of the product, especially for high-value products like biobased chemicals.

When translating the economic measurements into umbrella themes, the indicators can be distributed over the different life cycle categories (i.e., feedstock, transportation, production, end of life, etc.). The feedstock category receives most attention in the existing indicator sets, mostly to compare production and transportation costs of traditional feedstock for chemicals with the biomass used for the creation of green chemicals.

3.3 Social indicators

Sustainability assessments of biobased chemicals including the social dimension are limited. In this review, social consequences (such as 'workplace accidents', 'social investment', 'human health', etc.) are often included in the evaluation as the additional impacts that have to be calculated with caution. Effects of biobased products and processes on society are difficult to quantify, and few research has dealt with this facet of sustainability.

The review analysis shows 13 different indicators evaluating the social sustainability of biobased chemicals (Appendix A2). Health and safety indicators represent the gross of the social domain in the existing sets. To be more precise, only one measurement does not include health or safety aspects, which is the 'social investment' indicator, representing the contribution to employment and philanthropic developments (Sacramento-Rivero, 2012). 'Human toxicity', accounting for the impact of toxic substances on human environment, is by far the most included social indicator currently existing for the assessment of biobased chemicals. Human toxicity is included in all three-dimensional indicator sets present in this review study. Most publications consider human toxicity as an environmental indicator instead of a social indicator. In this analysis 'human toxicity' was moved to the social dimension to account for its direct effect on human health and safety, which is also done in European projects like BioSTEP (2016) (Hasenheit, Gerdes, Kiresiewa, & Beekman, 2016).

When comparing the 13 indicators with broader social sustainability assessments like UNEP-SETAC (2009), the Global-Bio-Pact (2012), ORNL (2013) and BioSTEP (2016), the existing biobased chemical indicator sets are missing some up-front social indicators. The existing sets neglect topics like product transparency, employment, working conditions, land access, quality of life, etc. A widely discussed topic within the biobased economy is the competition of biomass products with food (Koizumi, 2014). With demand for food increasing and climate change impacting agricultural yields, the impacts of the biobased economy on food security and prices raise concerns (Souza, Victoria, Joly, & Verdade, 2015). Previous studies on the impact of bioenergy and -fuels have shown that there is no significant impact on food availability and that it can even improve food production systems when good governance is in place (Lynd & Woods, 2011; Souza et al., 2015). However, policy makers should stimulate good governance and should facilitate synergies between the different biomass uses (Kline et al., 2017).

3.4 Indices

Finally, indices were found in the literature that represent relationships within a sustainability dimension or between different sustainability dimensions. In the analysis, five indices were classified into the environmental dimension and three indices were classified into the social dimension. Most of the indices are composed of intra-discipline indicators like the 'environmental impact of raw materials' that consists of GWP and CED of feedstock (de Assis et al., 2018a). Only two indices represent an interdisciplinary relationship between two or more sustainability dimensions: the 'environment, health and safety index' (EHSI) and 'the environment, health, and safety management system compliance' (EMSC), both integrating environmental and social impacts (Patel et al., 2012). The lack of these interdisciplinary indices points to the availability of multidisciplinary indicator sets without accounting for sufficient integration.

4. Discussion

The review analysis performed in this chapter found that 19 out of 38 included indicator sets consider only one sustainability dimension, 13 included two sustainability dimensions and another 6 emphasized all three dimensions. Environmental impacts were included in all of the sustainability sets, economic impacts in half of the included sets and the social impacts in 6 sets (Figure 8) (left axis). A close relationship was found between the number of dimensions included and the content of the sustainability indicators. Analyzing the proportion of indicators used in biobased chemical assessment, again the environmental indicators predominate (Figure 8) (right axis). A hierarchy of sustainability dimensions was found. If an assessment includes one sustainability dimension (1D), only the environmental impacts were considered. When two dimensions (2D) are included, economic and environmental issues were estimated. The social dimension only appears whenever environmental and economic aspects were also included in the indicator set (3D).

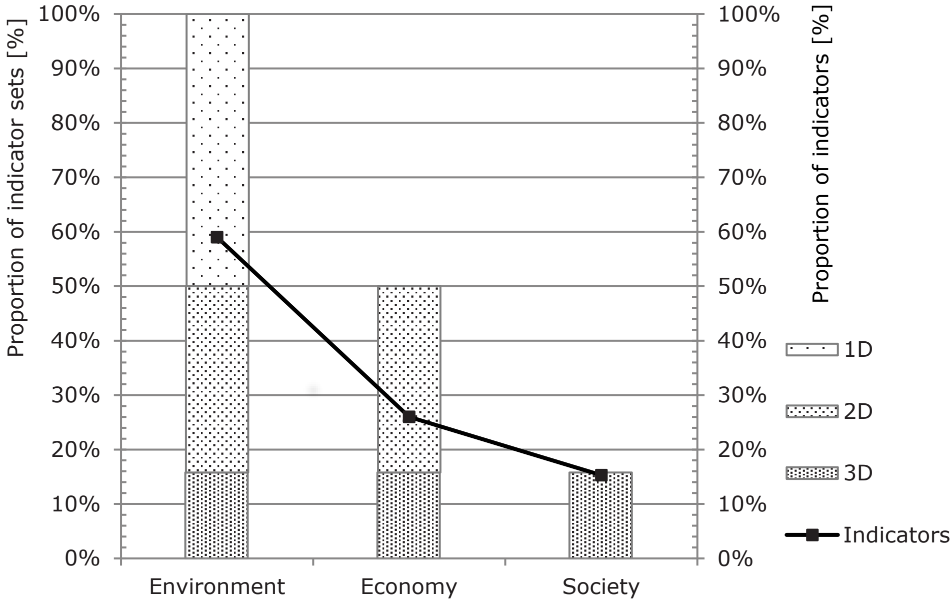

Figure 8. Sustainability dimensions included in assessments of biobased chemicals (in %).

Considering the 12 most-used indicators for biobased chemical sustainability, environmental indicators clearly predominate the ranking (Figure 9). The popularity of environmental assessments and indicator development can be explained by environmental policy that has been growing over the past decades. The 7th environment action programme (EAP) sets a long-term direction for the EU towards a better environment in 2050, enhancing objectives like conserving natural capital, resource-efficiency, and safeguarding environmental pressures (European Commission, 2014). To evaluate such policies, indicators are needed that are often part of a Life Cycle Assessment (LCA) which looks at the environmental impact of a product considering the entire process flow, from raw materials to disposal and recycling. LCA is considered the best framework for assessing potential environmental impacts of products by the European Commission (Commission of the European Communities, 2001). LCA is widely applied in practice, and is also included in European legislation like the Product Environmental Footprint method (PEF) (Lehmann, Finkbeiner, Broadbent, & Balzer, 2015). However, the challenge remains to define a relevant set of indicators and include all components of sustainable development (A Azapagic, Millington, & Collett, 2006). The fixation on environment is in stark contrast with the poor inclusion of social indicators (Rafiaani et al., 2018). Most assessments justify this lack of social consequences by addressing its subjectivity and pointing to the lack of current scientific research related to the topic of social sustainability.

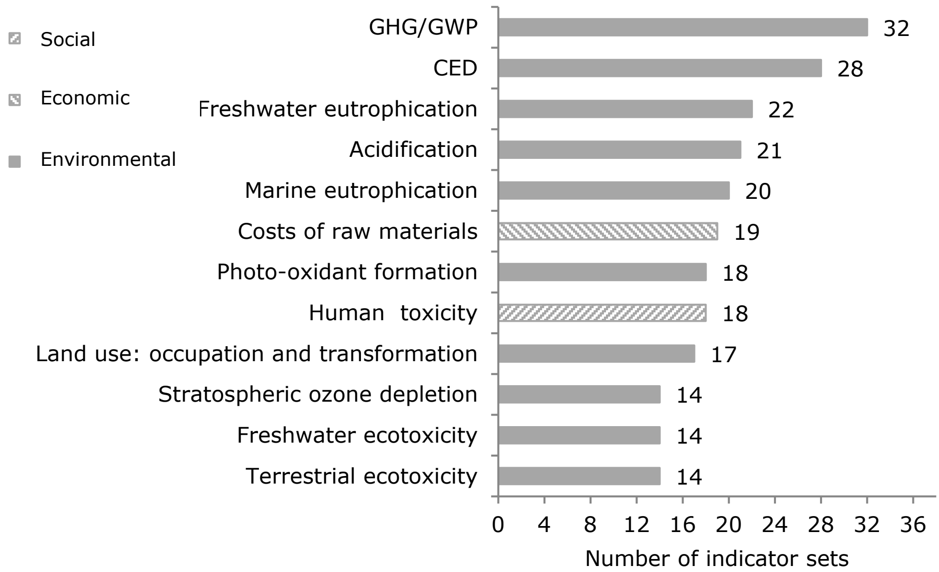

Figure 9. Top 12 sustainability indicators used in biobased chemical sustainability assessments.

The review study shows that many indicators were still divided into the classic three-pillar sustainability dimensions (i.e., environment, economy and society). Some articles provided other classification schemes as well. For example, Sacramento-Rivero (2012) grouped indicators into five categories (i.e., feedstock, process, products, environment and corporate) and Tabone et al. (2010) established a link between indicators and the green chemistry principles (Sacramento-Rivero, 2012; Tabone et al., 2010). Multidisciplinarity within sustainability research is accepted, and the importance of all three sustainability fields is recognized. Nevertheless, a multidisciplinary approach might lead to a conflict between the three fields of study, where the aspects of sustainability become conflicting rather than potentially complementary (Gibson, 2006). Moving to interdisciplinarity or transdisciplinarity can provide a solution by incorporating insights from the different fields, and generating integration between the sustainability domains (Pfau et al., 2014).

There is no consensus on a set of indicators for biobased chemical assessment and gaps, mostly concerning the assessment of economic and social impacts, are present in current literature. To move towards a comprehensive and well-accepted list of indicators for the industry, government, and academics, a first framework is proposed in Figure 10. This framework was developed based on the results of this chapter and the performed review already encloses the starting point of the framework by defining goal and scope and constructing a comprehensive list of indicators. Next, the developed list of indicators (Appendix A2) can be used as an input to consult stakeholders from the public sector as well as academics and the industry on regional, national, or international level, depending on the scope. Such a stakeholder survey can be constructed by using the Delphi method, which gathers feedback from different stakeholders to deal with the complexity of the topic of sustainability (Okoli & Pawlowski, 2004). A balance between effective, implementable, and fit-for-purpose indicators on the one hand and comprehensive indicators on the other hand should be maintained to stimulate sustainability assessment in practice. In a third step, a multi-criteria analysis should be applied to rank and select indicators based on a range of different criteria like cost-effective data collection and robustness. Some indicators might need to be left out or replaced by more feasible alternatives, for example, because of the lack of data. The final step of the framework consists of a proof-of-concept with a sensitivity analysis to evaluate the practicability of the indicator set. As a result, a weighted set of indicators can be derived for use in a standardized sustainability assessment.

The inclusion of social indicators together with environmental and economic indicators means that qualitative and (semi-) quantitative indicators need to be integrated in an assessment framework. In addition, every biobased chemical has different properties and cultural values differ per region, making it difficult to create a general biobased chemical assessment tool. If future research can overcome these challenges, policy makers can adopt an adequate set of indicators and use it as an evaluation tool for biobased products. Sustainable products can be offered to society and awareness about and acceptance of sustainable products can be increased. The indicators can be used to identify promising experimental and emerging products and sustainability barriers can be identified and addressed from the beginning.

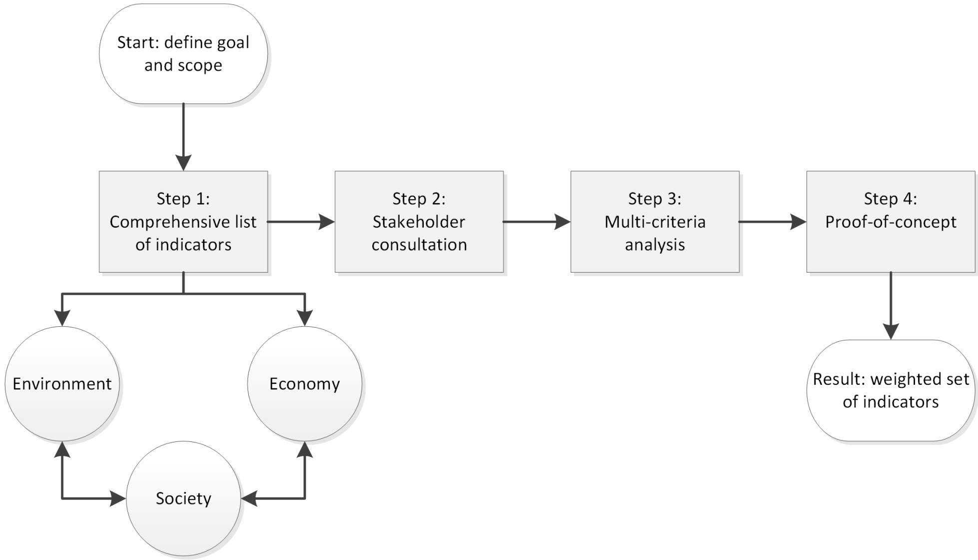

Figure 10. Constructing an indicator set to assess sustainability: a framework.

5. Conclusion

Chapter 2 reviewed sets of sustainability indicators for the biobased chemistry to classify sustainability indicators and elucidate research gaps and future research needs. Sustainability considerations have become increasingly important over time as is reflected by an increasing rate of publications pertaining to the topic. For the existing body of literature, it was found that many existing sets of indicators (1) lack a holistic view on sustainability, (2) are incomplete and/or, (3) lack focus, potentially concerning the applicability on biobased chemicals. First, most indicators remain one-dimensional and can therefore be categorized into a specific sustainability dimension, without accounting for the interlinkages between the sustainability dimensions. Second, a balanced inclusion of environmental as well as social and economic indicators remains a critical challenge in sustainability research and evaluations. An environmental evaluation is incomplete if only GHG emissions are measured and comprehensive economic evaluation has to include measures of profitability in addition to cost or revenue measures. Furthermore, the subjectivity and location-specific characteristics of social indicators are difficult to overcome when creating a complete sustainability set. Including all three sustainability domains requires combining quantitative and qualitative indicators into one integrated analysis. Finally, so far, biobased chemical case studies rely on the use of indicators of more generic assessment frameworks, with no adaptation to specific characteristics of the biobased chemical products.

No generally accepted set of indicators has been developed yet for sustainability assessment of biobased chemicals. Sustainability indicator sets do exist, yet not on a mature and complete level. To pursue and enable adequate decision- and policy making, the need exists to elaborate and enhance a standardized and comprehensive list of indicators. These indicators can be selected by following the proposed framework (Figure 10), starting from the list of indicators constructed in this review study. The next chapter follows up on this framework to create a set of sustainability indicators specifically for biobased chemicals. If companies, academics and governmental bodies assess their activities by applying the same indicators, consistent evaluations and comparisons between biobased chemicals will become possible.

CHAPTER 3

Sustainability indicators for biobased chemicals: a Delphi study using multi-criteria decision analysis

Parts of this chapter have been published in:
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ABSTRACT

Biobased chemistry has gained interest and has the potential to tackle some of the sustainability challenges the chemical industry must endure. Sustainability impacts need to be evaluated and monitored to highlight the advantages and pitfalls of different biobased routes over the entire product life cycle. Chapter 3 aims for an expert consensus concerning indicators needed and preferred for sustainability analysis of biobased chemicals in Europe. Experts are consulted by means of a Delphi method with stakeholders selected from three core groups: the private, public, and academic sector. Best-worst scaling (BWS) is performed to gather data on the prioritization of the sustainability indicators per respondent. Afterwards, multi-criteria decision analysis (MCDA) is used to develop a consensus ranking among the experts. The results show that *GHG emissions*, *market potential* and *acceptance of biobased materials* are deemed the most crucial indicators for respectively environmental, economic, and social sustainability. Expert consensus is positive in all three sustainability domains, with the strongest consensus measured for environmental sustainability showing a median Kendall's τ of 0.63 (with τ ranging from -1 to 1) and the weakest consensus found within social sustainability showing a median Kendall's τ of 0.51. The next chapters should apply the ranked indicators on a specific case study to evaluate the practicability of the defined indicator set.

1. Introduction

As population is growing and fossil resources are shrinking, more attention is paid to building and maintaining a sustainable global economy. The desire of countries to reduce fossil fuel import dependency, stimulate regional and rural development, mitigate climate change, and promote circularity, has driven the 'start' of the transition towards a biobased economy (Chiu, Ashton, Moreau, & Tseng, 2018; Jong, Higson, Walsh, & Wellisch, 2011; Ranta, Aarikka-Stenroos, Ritala, & Mäkinen, 2018). However, this transition to an economy based on renewable resources is expected to have many setbacks and obstacles on a technical and political level (J. Philp, 2017). As was mentioned in the previous chapter, a biobased economy does not guarantee an increase in environmental, economic, and social sustainability. While biobased technologies and products can potentially decrease greenhouse gas emissions (GHG) and reduce ecotoxicity, it can also trigger adverse effects like e.g. land use change (LUC), soil degradation and pollution of water resources (Gawel & Ludwig, 2011; Pursula, Aho, Rönnlund, & Päällysaho, 2018). It is important to assess these sustainability impacts of biobased products and steer technologies towards sustainable development, while still being at a low technology readiness level (TRL).

Within the biobased economy, (social) LCA and TEA are most often developed for biofuels and bioenergy (Fritsche & Iriarte, 2014). However, biobased chemicals can potentially be sold at a higher selling price which creates more opportunities within the biobased and chemical industries (Fritsche & Iriarte, 2014; Wu, Long, Zhang, Reed, & Maravelias, 2018). Within the European bioeconomy, the highest levels of labor productivity were achieved in the manufacturing of biobased chemicals, pharmaceuticals, plastics and rubber (Ronzon, Piotrowski, M'Barek, & Carus, 2017). The corresponding biobased feedstock encompasses agricultural crops, dedicated energy crops and trees, agriculture and forestry residues, aquatic plants, and animal and municipal waste (Roger A. Sheldon, 2011). A large amount of chemicals can be produced from biomass like many platform chemicals, amino acids, vitamins, polymers and industrial enzymes (J. C. Philp et al., 2013).

Next to economic opportunities, there is also an environmental justification to explore the market of biobased chemicals. The introduction of biobased chemistry can potentially reduce the number of toxic chemicals being produced and so benefit human and environmental health. The production of chemicals in the European Union reached 319.5 million tonnes in 2016, with approximately 63 percent of these chemicals being hazardous to human health (Eurostat, 2017b). The implementation of stringent regulatory frameworks, like REACH (Registration, Evaluation and Authorization of Chemicals) and RoHS (Restriction on Hazardous Substances), has driven the industry to look for less toxic substitutes, including biobased chemicals. Other potential sustainability benefits include the reduction of GHG emissions, biodegradability, employment opportunities, local production, etc. A thorough sustainability analysis and comparison with the fossil-based counterpart is necessary to draw proper conclusions and invest in the most sustainable alternative. The entire product life cycle of a biobased chemical should be taken into account in such an analysis, to correctly estimate the sustainability impacts of technologies and products. Figure 11 shows the simplified life cycle of a biobased chemical from raw material extraction to possible end-of-life options.

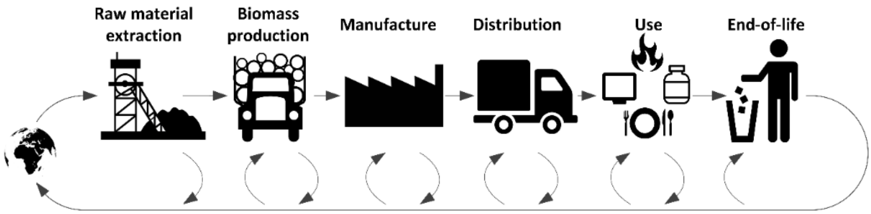

Figure 11. Total life cycle of a biobased product (Thomassen, 2018).

Many definitions and assumptions about the concept of 'sustainability' do exist. However, putting this definition into practice has been a challenge for decades as it leaves room for many interpretations (Bennich & Belyazid, 2017). As a result, practitioners of sustainability analysis currently use different sustainability indicators which leads to a lack of harmonization (J. Philp, 2017). An in-depth analysis on the criteria, indicators, and remaining gaps within sustainability evaluations of biobased chemicals was performed in chapter 2 of this dissertation. The review shows that a complete and comprehensive indicator framework for the evaluation of sustainable biobased chemicals does not exist. The previous chapter concluded that the existing indicator sets are often incomplete, lack a holistic view on sustainability, and require more focus on the applicability for biobased chemicals (Van Schoubroeck, Van Dael, Van Passel, & Malina, 2018). There is a lack of inclusion of social and economic impact categories, and most assessments stay one-dimensional using a limited set of environmental indicators (J. Philp, 2017; Van Schoubroeck et al., 2018).

The study performed in this chapter will be the first to develop a complete and balanced set of indicators to perform sustainability evaluation, specifically for biobased chemicals. A consensus ranking can lay the foundation for the harmonization of sustainability analysis within the field of biochemistry. Industrial, governmental and academic stakeholders will be able to identify promising and emerging products and factor in sustainability considerations for funding and procurement decisions. By assessing environmental, as well as social and economic aspects, sustainability barriers can be identified and addressed starting from a low TRL. This shortens the time-to-market of new sustainable biobased products and facilitates their implementation. Entailing this full sustainability analysis enables industries and policy makers to bring sustainable biobased chemicals to the society and foster the biobased economy as a whole. Furthermore, this chapter contributes to the development of a mixed-method using qualitative (i.e., Delphi) and quantitative (i.e., MCDA) tools, which can deal with many attributes (i.e., sustainability indicators) in an ordinal way.

Chapter 3 is structured as follows: section 2 provides an overview of the different research steps and methods. In section 3, the research outcomes are quantitatively described, compared and a final consensus sustainability ranking is proposed. Section 4 further discusses the results and limitations of this study, and provides suggestions for future research. Section 5 concludes the chapter.

2. Method

The research goal requires a methodological approach which (1) collects and interprets information about sustainability indicators on the one hand, and (2) ranks the indicators based on their relevance on the other hand. Therefore, a Delphi study was combined with a multi-criteria decision analysis (MCDA) to fully address the research question. Previous research at the Engineer Research and Development Center shows that the combination of these methods can resolve research designs which involve decision-making under situations of high complexity and uncertainty (De Carvalho, Marques, & Netto, 2017; B. Trump, Cummings, Kuzma, & Linkov, 2018; B. D. Trump et al., 2018). A Delphi survey is an iterative group facilitation methodology, designed to transform opinion into group consensus (Hasson, Keeney, & McKenna, 2000). The Delphi method is pooling the talents of experts to reach consensus based on structured feedback (P. T. Chang, Huang, & Lin, 2000). Using group feedback from the previous round, the researcher develops a next round of questions for the respondents (Okoli & Pawlowski, 2004). Delphi techniques are useful for indicator selection of complex sustainability issues (Benitez-Capistros, Hugé, & Koedam, 2014; Hai et al., 2014; Mapar et al., 2017). This qualitative survey method contributes to a higher efficiency of quantitative techniques, such as MCDA (De Carvalho et al., 2017; Kendall, 1970). A combination of Delphi and MCDA is already widely applied in the topic of sustainability (Chiu et al., 2018; De Feo, De Gisi, De Vita, & Notarnicola, 2018; Zhao & Li, 2016).

Within this chapter, a two-round Delphi survey is conducted with an open and closed question round to select and prioritize sustainability indicators for the evaluation of biobased chemicals. The questionnaires were created in Qualtrics Software (© 2018 Qualtrics ®) and distributed by e-mail to experts. A full version of the questionnaire can be provided by the authors upon request (Van Schoubroeck, Springael, Van Dael, Malina, & Van Passel, 2019). Participants were selected based on their expertise in sustainability and biobased chemistry. The experts were divided into the following three core groups: private sector (industrial companies), public sector (administrations, certification and labelling bodies and non-governmental organizations), and academic sector (universities and research institutes). Literature recommends at least 10 experts, which are anonymous to each other, for a Delphi panel to be able to reach consensus based on group dynamics (Okoli & Pawlowski, 2004). In total, 246 potential experts in Europe were contacted for this study.

2.1 First Delphi round

In the first Delphi round, open questions were asked to brainstorm and gather data for the creation of a list of sustainability indicators. Respondents were asked which indicators they think are important when performing an environmental, economic, or social sustainability analysis of a biobased chemical. In total, the responses of 71 experts were included for analysis (response rate: 29 percent), with 39.44 percent of the experts working in industry, 39.44 percent of the experts working in academics, and 21.13 percent of the experts working in the public sector. The respondents were located in twelve different countries in Europe, most of which holding a doctoral degree (64.99 percent). The experts' answers were analyzed by open coding, using the NVivo software for qualitative data analysis (NVivo, 2015; Strauss & Corbin, 1998). Open coding is defined as the "analytical process through which concepts are identified and their properties and dimensions are discovered in the data" (Strauss & Corbin, 1998). The outcome of this qualitative analysis was merged with the results of the literature review performed in chapter 2, and resulted in a comprehensive list of indicators which was used as input for the second Delphi round.

2.2 Second Delphi round

”The objective of MCDA is the study of decision problems in which several points of view must be taken into consideration” (Roy & Vincke, 1981). As the decision problem in this particular study entails more than nine attributes (i.e., indicators) per sustainability dimension, the use of certain MCDA methods, such as AHP (Analytic Hierarchy Process) or MACBETH (Measuring Attractiveness by a Categorical Based Evaluation Technique) are not appropriate for this study (Bana e Costa & Chagas, 2004; Saaty & Ozdemir, 2003). Data collection is time consuming and complex when many attributes are involved, and the selection of an appropriate MCDA has to be adapted to this specific multi-attribute situation. The utilization of an object-case best-worst scaling (BWS) exercise was therefore selected as a fitting question format for the second Delphi round. Finn and Louviere introduced BWS in 1992 as an alternative for the use of rating scales in questionnaires (Flynn & Marley, 2014). BWS is a cost-efficient way of obtaining more information from the experts (Finn & Louviere, 1992; Flynn & Marley, 2014). BWS provokes discrimination and avoids using a rating scale by asking the experts to indicate the ‘best’ and ‘worst’ item from a set of attributes (J. A. Lee, Soutar, & Louviere, 2008). In this study, the BWS method is used to measure the preference scores from a list of sustainability indicators by using experts opinion. Afterwards the survey data is used to compose a ranking per respondent, which provides the input needed to perform a specific MCDA approach called AURORA (i.e., aggregating uni-criterion rankings into one ranking) (De Keyser & Springael, 2009). The AURORA method merges and compares the experts’ rankings, respecting its ordinal character (De Keyser & Springael, 2009; Keune, Springael, & Keyser, 2013).

Sawtooth’s SSI Web platform (© 2018 Sawtooth Software ®) is used to build Balanced Incomplete Block Designs (BIBD) for the BWS exercise. Three different questionnaire versions were created, each containing three separate block designs for the environmental, social, and economic aspects of sustainability. Every questionnaire design contains 25 questions, with 6 attributes shown per question. The design algorithm is comparable with those of a Choice Based Conjoint (CBC) and is created based on one- and two-way frequencies, positional balance, and connectivity (Sawtooth Software, 2013). The three questionnaire versions are assigned randomly to the different respondents. In total, 47 respondents filled out the 25 BWS exercises. Only the experts that responded to the first Delphi survey were contacted again for the second Delphi round (response rate: 66 percent).

Hierarchical Bayes (HB) regression is performed using Sawtooth Software to estimate preference scores for each respondent. HB is a "data borrowing" technique, stabilizing part-worth estimates for each individual by means of borrowing information from other respondents within the same data set (Orme & Baker, 2000). Potential rankings were developed by applying three different methods to compare and improve potential rankings: (1) HB average ranking, (2) HB frequency ranking, and (3) HB AURORA ranking. The first two methods, average ranking and frequency ranking, can be conducted using the Sawtooth Software. Afterwards, a specific Branch-and-Bound algorithm was written in C++ to apply the MCDA-method, AURORA. AURORA requires pairwise comparisons between the respondents and a ranking of the alternatives per respondent. Based on the HB preference scores, a ranking per respondent is first computed. The higher the preference score of a respondent for a certain indicator, the higher the ranking position for that indicator. The rank correlation coefficient of Kendall, referred to as Kendall's τ, is used to measure how well a candidate consensus ranking fits a respondent's ranking (Equation (1)) (De Keyser & Springael, 2009; Kendall, 1938).

$$\text{Kendall's } \tau = \frac{2*(C-D)}{n^2-n} \qquad \text{where} \qquad C + D = \frac{n^2-n}{2} \tag{1}$$

with C = Concordant pairs and D = Discordant pairs

The value of Kendall's τ ranges from -1 to 1, from perfect disagreement to perfect agreement. The median of these correlation coefficients is determined after every iteration and maximized over the set of potential consensus rankings. The pseudocode of the operating principle is provided in Appendix B1. The flowchart of the research steps, including the HB AURORA ranking is shown in Figure 12.

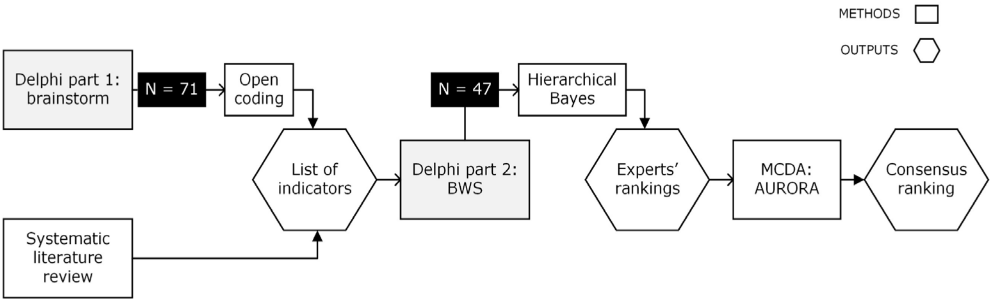

Figure 12. Flowchart research steps of mixed Delphi – MCDA method. HB = Hierarchical Bayes, BWS = best-worst scaling, MCDA = multi-criteria decision analysis.

3. Results

Table 2 represents the outcome of the first Delphi round, created by combining open coding and literature review. In total, 20 environmental attributes, 13 economic attributes and 15 social attributes were selected for further analysis in a second Delphi round. A brief description of these indicators, also provided to the experts in the second questionnaire round, is included in Appendix B2.

Furthermore, in the first Delphi round, the respondents were asked which evaluation tool they preferred to measure sustainability of biobased chemicals: 'a single index', 'multiple indicators', or 'both'. The results of this survey indicated that 56 experts preferred multiple indicators, 14 chose both and only 1 preferred a single index. The experts in favor of multiple indicators pointed out that sustainability is too complex to summarize in one index. Providing a scoreboard with multiple indicators allows for more transparency and visualization of the trade-offs between different sustainability impacts. Aggregation and weighing may mask those trade-offs and present an oversimplification of reality. The reason why some experts have chosen 'both', was mostly due to the communication aspect of an index. It allows easy communication with non-experts, providing a good foundation for first ranking and selection. However, most experts indicated that the index has to be accompanied by separate scores for different stand-alone indicators. A single index allows for direct comparison between biobased alternatives, but similar index-scores might be calculated even when products differ on specific sustainability aspects.

Table 2. Output Delphi round 1: sustainability indicators for biobased chemicals (unranked).

Environmental	**Economic**	**Social**
Abiotic fossil depletion	Capital productivity	Acceptance of biobased chemicals
Abiotic mineral depletion	Energy cost	Child labor
Acidification	Labor productivity	Community support and involvement
Agricultural land occupation	Land productivity	Cultural heritage
Ecotoxicity	Market potential	Discrimination
End of life options	Process innovation	Education and training
Energy efficiency	Product efficiency	Fatal work injuries
Eutrophication	Product innovation	Human toxicity
GHG emissions	Raw materials cost	Income levels
Ionising radiation	Subsidies	Job creation
Management practices in crop production	Technical risks	Product transparency
Natural land transformation	Transportation cost	Security measures
Organic carbon depletion	Waste disposal cost	Social security
Particular matter formation		Working hours
Photo-oxidant formation		Workplace accidents and illnesses
Raw material efficiency		
Soil erosion		
Stratospheric ozone depletion		
Waste generation		

In the second Delphi round, responses of the BWS exercises were analyzed using Hierarchical Bayes with all of the experts reaching a fit-statistic, a Root Likelihood, higher than a minimum of 0.167 (Sawtooth Software, 2009). Tables 3-5 show the results of the analysis of the BWS data. The fifth and the sixth columns entail a counting analysis, showing the proportion an indicator is picked as best and/or worst. Some attributes were never picked 'best' like *photo-oxidant formation*, *ionising radiation,* and *cultural heritage*. *Ionising radiation* had the highest consistency in answers with 60 percent of the experts indicating it as 'least important'.

The fourth columns of Tables 3-5 show the average rescaled utility scores (i.e., preference scores) per sustainability indicator. High importance was given to *GHG emissions*, with an average utility score of 14.40, followed by *raw material efficiency* with 10.27 and *end of life options* with 10.04. Low importance was given to *ionising radiation* and *photo-oxidant formation* with average scores of 0.18 and 0.35. Overall, the average utility scores of the environmental attributes decrease more gradually compared to the economic and social dimension. For the economic dimension, a stable middle section was noticed with utility scores between 8.98 and 8.20 for the attributes *process innovation*, *product innovation*, *energy cost*, *technical risks*, *land productivity,* and *capital productivity*. The highest utility scores were assigned to *market potential* and *raw materials cost* with 18.41 and 15.57. For the social attributes, the indicators having the highest importance are *human toxicity*, *product transparency*, *job creation* and *acceptance of biobased materials*. According to the experts, these four attributes together accounted for 51.11 percent of the total importance in social sustainability. In Appendix B3, the distributions of the average rescaled utility scores per sustainability dimension are shown.

The second columns of Tables 3-5 display the results of the HB average ranking (i.e., the first ranking method), enclosing a ranking based on the average utilities per indicator with the attributes *GHG emissions*, *market potential,* and *human toxicity* ranked first for respectively the environmental, economic, and social dimension. *Ionising radiation*, *waste disposal cost* and *cultural heritage* were ranked last. However, these average utility scores, used to create the average ranking, should be handled with care as they might be affected by extreme values.

In the third columns of Tables 3-5, the HB frequency rankings (i.e., the second ranking method) were constructed based on the frequency an item was placed at a certain rank order. Individual rankings were created using the individual preference scores from the HB analysis. A first example is given in Figure 13, where a pairwise comparison is made between the frequencies of the attributes *subsidies* and *transportation cost* at a certain rank position for the 47 respondents. Although these frequency analyses gave a good first impression of a final consensus ranking and avoids averaging, the distribution of some attributes can also be too dispersed for comparison. A second example, provided in Figure 13, shows the difficulty to compare the frequencies of four selected social indicators. To improve the validity of the final ranking, a model was created based on the HB AURORA method (i.e., the third ranking method) to construct a more reliable consensus ranking.

Table 3. Best-worst scaling results for the environmental dimension.

Indicator	Hierarchical Bayes analysis			Counting analysis	
	Average ranking	Frequency ranking	Rescaled utility score	Best count proportion	Worst count proportion
GHG emissions	1	1	14.3964	0.5750	0.0083
Raw material efficiency	2	2	10.2738	0.3417	0.0417
End of life options	3	3	10.0402	0.3500	0.0833
Ecotoxicity	4	4	7.6652	0.2250	0.0250
Waste generation	5	5	6.7041	0.2417	0.1000
Energy efficiency	6	6	6.4310	0.1667	0.0750
Eutrophication	7	9	5.9786	0.1917	0.0500
Natural land transformation	8	7	5.4493	0.1833	0.1250
Agricultural land occupation	9	8	5.3674	0.1750	0.1417
Abiotic fossil depletion	10	10	5.2322	0.2000	0.1167
Organic carbon depletion	11	12	4.9843	0.1667	0.0417
Water consumption	12	11	3.9648	0.1083	0.1333
Management practices in crop production	13	14	3.6921	0.1500	0.2583
Soil erosion	14	13	2.9394	0.0667	0.1583
Acidification	15	16	2.2364	0.0750	0.1917
Stratospheric ozone depletion	16	18	1.5164	0.0667	0.3167
Particular matter formation	17	17	1.3784	0.0167	0.2333
Abiotic mineral depletion	18	15	1.2158	0.0333	0.2833
photo-oxidant formation	19	19	0.3527	0.0000	0.3500
Ionising radiation	20	20	0.1815	0.0000	0.6000

Table 4. Best-worst scaling results for the economic dimension.

Indicator	Hierarchical Bayes analysis			Counting analysis	
	Average ranking	Frequency ranking	Rescaled utility score	Best count proportion	Worst count proportion
Market potential	1	1	18.4073	0.4574	0.0233
Raw materials cost	2	2	15.5672	0.3250	0.0333
Process innovation	3	4	8.9783	0.2164	0.1194
Product innovation	4	3	8.6059	0.1716	0.0672
Energy cost	5	5	8.6042	0.1667	0.0333
Technical Risks	6	6	8.5811	0.1825	0.0584
Land productivity	7	7	8.5131	0.2417	0.1333
Capital productivity	8	8	8.1990	0.1168	0.1241
Product efficiency	9	9	6.5183	0.1085	0.1085
Subsidies	10	12	3.2001	0.0949	0.4307
Labor productivity	11	11	1.6609	0.0583	0.3167
Transportation cost	12	13	1.6474	0.0310	0.4651
Waste disposal cost	13	10	1.5173	0.0149	0.2388

Table 5. Best-worst scaling results for the social dimension.

Indicator	**Hierarchical Bayes analysis**			**Counting analysis**	
	Average ranking	Frequency ranking	Rescaled utility score	Best count proportion	Worst count proportion
Human toxicity	1	1	13.7164	0.3358	0.0373
Product transparency	2	2	13.3042	0.3167	0.0833
Job creation	3	3	12.2509	0.3723	0.1095
Acceptance of biobased materials	4	4	11.8403	0.3798	0.1628
Fatal work injuries	5	5	7.5035	0.2083	0.1500
Workplace accidents and illnesses	6	6	6.6466	0.1240	0.0775
Community support and involvement	7	7	6.3201	0.1866	0.1343
Income levels	8	8	5.6892	0.0949	0.1241
Education and training	9	9	4.8797	0.0930	0.1705
Child labor	10	15	4.8053	0.0970	0.3284
Social security	11	11	3.9995	0.0917	0.1833
Security measures	12	10	3.8287	0.0917	0.2083
Discrimination	13	12	2.3004	0.0511	0.1533
Working hours	14	13	1.9336	0.0333	0.2500
Cultural heritage	15	14	0.9817	0.0000	0.3500

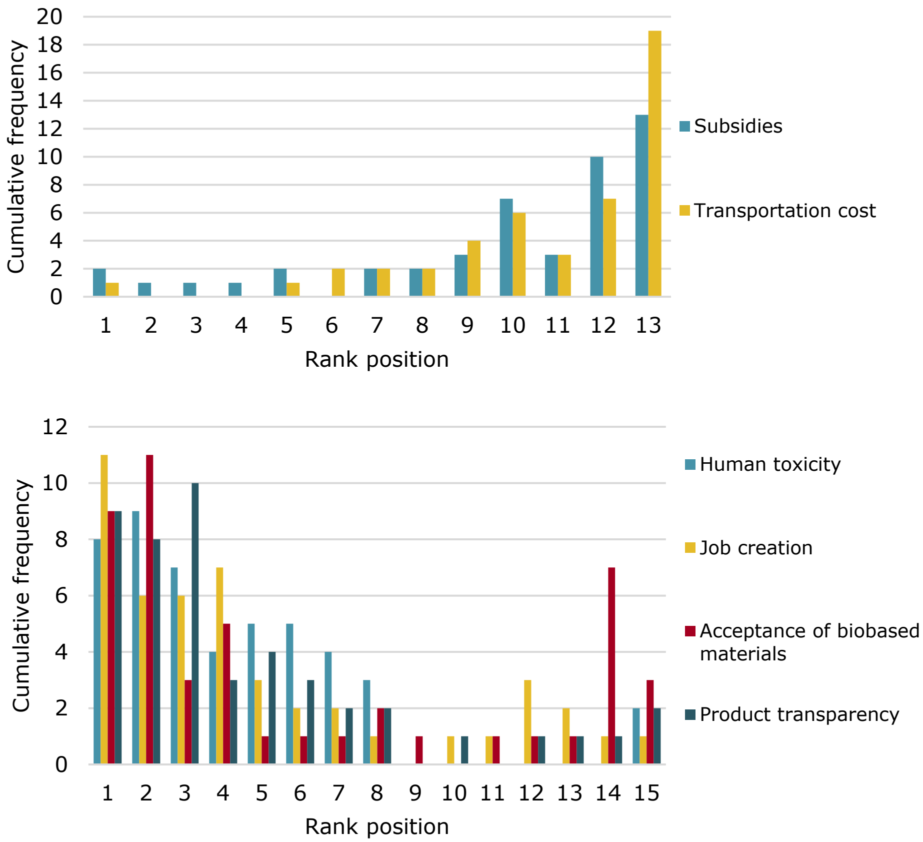

Figure 13. Cumulative frequencies of the rank positions.

For the HB AURORA ranking method, a Branch-and-Bound algorithm was written, using the method of Springael and De Keyser (2009), to determine a prioritization of sustainability indicators per dimension. The median Kendall's τ was maximized to select the best fitting ranking. Multiple optimal solutions were found by running the Branch-and-Bound algorithm per sustainability dimension: 1 optimal solution for the environmental dimension, 23 optimal solutions for the economic dimension, and 974 optimal solutions for the social dimension. An example is given in Figure 14, in which the 23 solutions for the economic dimension are compared. Every optimal solution had the same maximized median Kendall's τ, which is 0.6316 for the environmental sustainability solutions, 0.5641 for the economic sustainability solutions, and 0.5048 for the social sustainability solutions. Intuitively, for the economic dimension, this means that at least 50 percent of the respondents has a rank correlation coefficient of 0.5641 or more with regard to the optimal solution.

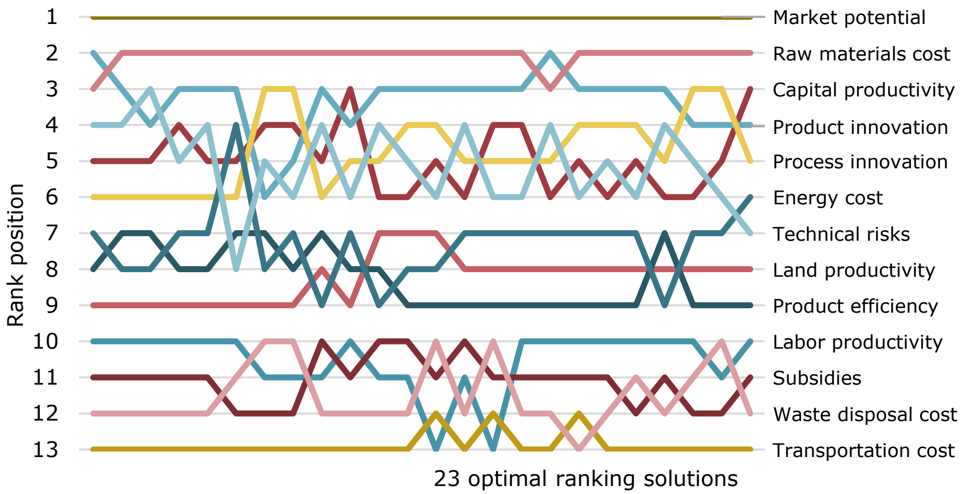

Figure 14. Optimal ranking solutions for the economic dimension (based on HB AURORA).

If the complexity of the decision problem increases, the AURORA algorithm generates a higher amount of optimal solutions with a lower median Kendall's τ, designating a lack of consensus. Table 6 shows the corresponding rank correlation coefficients per decile. Decile 0 includes the decision maker with the lowest Kendall's τ, i.e., the lowest agreement with the optimal solution(s). Decile 10 includes the decision maker with the highest Kendall's τ, i.e., the highest agreement with the optimal solution. If consensus was compared between the three sustainability rankings, it is noted that there was relatively less consensus concerning social sustainability indicators, which is proven in this study by the high amount of optimal solutions (i.e., 974), and the relatively lower median Kendall's τ (i.e., 0.5048). At least 10 percent of the decision makers had a negative correlation and tend to disagree with the optimal ranking solution. Social indicators are difficult to quantify and research is limited compared to economic and environmental assessment studies (Rafiaani et al., 2018). The root problems of social data scarcity and shortage of knowledge should be tackled to increase consensus and improve social sustainability analysis. The sole optimal environmental solution with a Kendall's τ of 0.6316 indicates that more attention in sustainability analysis is being paid to environmental indicators and experts tend to agree on the relative importance of these indicators.

Table 6. Kendall's τ per decile. [a]Environmental; [b]Economic; [c]Social.

	Decile										
	0	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
ENV[a]	0.08	0.24	0.32	0.42	0.50	0.62	0.64	0.66	0.68	0.74	0.92
EC[b]	-0.13	0.23	0.26	0.33	0.46	0.56	0.59	0.62	0.67	0.77	0.82
SOC[c]	-0.16	-0.01	0.14	0.22	0.30	0.51	0.54	0.56	0.64	0.68	0.77

One optimal solution per sustainability dimension was selected based on a frequency analysis. It was counted how many times an indicator received a specific ranking position. The indicator got a final position at the rank number for which its counting frequency was the highest. The AURORA-based rankings, shown in Table 7, were the best-fitting results considering a consensus had to be reached between all the experts. In the next section, the ranking positions of the different indicators will be further discussed.

4. Discussion

The final results of the HB average ranking, HB frequency ranking, and AURORA ranking, are discussed below based on literature and experts' feedback. *GHG emissions* was considered as the most relevant environmental indicator in all three ranking methods. Respondents indicated *GHG emissions* as a widely-accepted indicator with existing, elaborated calculation techniques. However, it is a common mistake to only include *GHG emissions* and generalize these results to make conclusions about environmental sustainability. Second place in the environmental ranking was covered by *raw material efficiency*. In a time with growing scarcity of natural resources, the efficient use of raw materials is crucial for environmental as well as economic sustainability (European Commission, 2012; Mantau et al., 2010). *Raw material efficiency* is directly linked with the *raw*

Table 7. Final consensus rankings of sustainability indicators for the assessment of biobased chemicals (based on HB AURORA).

	Environmental		Economic		Social
1	GHG emissions	1	Market potential	1	Acceptance of biobased materials
2	Raw material efficiency	2	Raw materials cost	2	Product transparency
3	End of life options	3	Product innovation	3	Job creation
4	Ecotoxicity	4	Process innovation	4	Human toxicity
5	Waste generation	5	Technical risks	5	Income levels
6	Energy efficiency	6	Capital productivity	6	Workplace accidents and illnesses
7	Natural land transformation	7	Energy cost	7	Education and training
8	Abiotic fossil depletion	8	Land productivity	8	Community support and involvement
9	Eutrophication	9	Product efficiency	9	Fatal work injuries
10	Agricultural land occupation	10	Labor productivity	10	Security measures
11	Water consumption	11	Subsidies	11	Social security
12	Organic carbon depletion	12	Waste disposal cost	12	Child labor
13	Management practices (crops)	13	Transportation cost	13	Working hours
14	Soil erosion			14	Discrimination
15	Acidification			15	Cultural heritage
16	Particular matter formation				
17	Abiotic mineral depletion				
18	Stratospheric ozone depletion				
19	Photo-oxidant formation				
20	Ionising radiation				

materials cost indicator, also ranked second in the economic sustainability prioritization. *End-of-life options* were ranked third, including the options to recycle, biodegrade or, for example, using biobased waste streams for new products, which offers a solution for the competition with food and feed in the agricultural sector. *Market potential* was ranked first for economic sustainability, which considers product price and output. According to the experts, it gives a first indication if a product is viable compared to their fossil-based counterpart or other technologies and feedstocks. For the social domain, the top 4 indicators were ranked in a different order when the three ranking methods were compared. *Human toxicity* took the lead when using the HB average- and frequency method, but got ranked fourth when applying the HB AURORA-method. Within the chemical sector, 'toxicity' is considered an important topic considering many chemicals are hazardous to human health and/or the environment (Eurostat, 2017a). *Product transparency*, ranked second when applying HB AURORA, is highly related with the communication strategy towards the customers. Disclosing detailed product information avoids greenwashing and builds trust, leading to potential economic advantages in the long run. Finally, *Acceptance of biobased materials* was placed first in the HB AURORA ranking. Public acceptability can pose a major barrier towards new innovative products. The measurement of social acceptance is difficult to define as it relates to many subjective and qualitative aspects. Social acceptance can be defined by sub-indicators like *fear*, *knowledge,* and *perception* (Assefa & Frostell, 2007). Nevertheless, measurement methods are limited and no case studies were found focusing on the acceptance of biobased chemicals (Van Schoubroeck et al., 2018).

Next to the top ranked indicators, it is also valuable to examine the indicators ranked at the bottom. Although respondents selected social sustainability indicators related to working conditions as relevant in the first Delphi round, an explanation given to the relatively low ranking position of *child labor*, *security measures* and *working hours* is the stringent social regulation in Europe. For example, child labor is completely banned in the European Union and might not be relevant to assess in social sustainability analysis when the entire value chain is EU based. The same argumentation is used with the valuation of the indicator *photo-oxidant formation*, better known as 'summer smog', which is perceived by the experts to be a more urgent matter in the metropolitan areas in Asia. However, sustainability assessment is very case-specific and this general prioritization of the indicators does not mean that the attributes ranked low are not relevant in some specific biobased chemical processes. For example, although *ionising radiation* was ranked last in Table 7, it can be a crucial sustainability indicator in certain processes using radioactive materials.

In the following paragraphs, some limitations, challenges and ideas for future research are discussed. First, some methodological concerns are raised. This Delphi study used best-worst scaling, which avoids scaling bias and provokes discrimination (Flynn & Marley, 2014). To avoid lengthy questions, the description of the indicators in the questionnaire was brief and to the point, which is in strong contrast with the complex nature of the research question. In some cases, this might lead to ambiguous questions and misinterpretation of the different sustainability attributes. For that reason, definitions were provided at the start of the survey and a 'comment box' was included in both rounds to encourage respondents to report haziness. A follow-up focus group could improve the validity of the research and gather information for the application of the selected sustainability indicators on a European case study (Morgan & Krueger, 1993). Furthermore, the three ranking methods used in this study (i.e., HB average ranking, HB frequency ranking, and HB AURORA ranking) show large similarities within the rankings, which indicates robustness in the survey results. The top and bottom ranked indicators remained stable and only minor switches between the indicators appeared when changing the ranking method. In this study, the Branch-and-Bound algorithm of the AURORA method does not allow for ties. Such a constraint in the model ensures a clear-cut ranking for decision makers who have to perform assessment with a limited amount of resources. However, allowing for ties could potentially increase consensus and enable clustering of the indicators. Future research could extend the current AURORA algorithm and investigate the effects of allowing ties into the MCDA model (De Keyser & Springael, 2009).

Apart from methodological challenges, follow-up research is necessary to apply and verify the indicators for biobased chemical assessment. Current sustainability evaluations lack an inclusion of social aspects or tend to focus only on *human toxicity* (Van Schoubroeck et al., 2018). To perform a balanced sustainability analysis, the development of measurement methods for social indicators like *acceptance of biobased materials* and *product transparency* are necessary to fill the gap in current literature. Next, the indicators identified by this Delphi study were broadly defined and might include sub-indicators and be quantified in many ways. For example, *eutrophication* can be divided in *marine water*, *freshwater,* or *terrestrial eutrophication*. These subdivisions create more insights and better judgement of sustainability. The performance of a case study can identify the further need for subdivisions and relevant sub-indicators. In addition, when using this prioritized set of sustainability indicators in practice, the challenge remains to include the linkages and interdependencies between the different sustainability indicators and domains. By incorporating the interrelationships between environment, society, and economy, the tradeoffs and win-wins can be discovered (Hacking & Guthrie, 2008).

Finally, this Delphi study developed a general indicator prioritization for European biobased chemicals, but a complete sustainability analysis should include as much information as possible. A prioritization can be useful when resources are limited for example, when data is lacking due to a low TRL or projects in small and medium-sized enterprises (SMEs). In order to adapt this general prioritization to a specific case, an iterative stakeholder process is suggested. Experts should first assess the general guideline and propose changes to confirm if all the crucial indicators are included in the analysis. After a first round of indicator calculations on the specific case study, stakeholders should be consulted again to evaluate the validity and completeness of the first results. The developed, general rankings in this chapter provide a foundation for further harmonization between practitioners of sustainability analysis, focusing on the research field of biobased chemicals.

5. Conclusion

A two-round Delphi study using best-worst scaling exercises resulted in consensus rankings of sustainability indicators, specifically developed for biobased chemicals. The expert elicitation process was performed with stakeholders from the private, public, and academic sector. The final rankings represent how experts elaborate on the concept of sustainability within biobased chemistry, and offers a prioritization of indicators to practitioners of sustainability analysis within Europe. Three different methods were used to develop a ranking of the sustainability attributes: (1) Hierarchical Bayes average preference ranking, (2) Hierarchical Bayes frequency ranking, and (3) Hierarchical Bayes AURORA ranking. The different methodologies and outcomes were compared and the third, MCDA, method was chosen as the most appropriate ranking, providing the most information on the level of consensus. The third method used a Branch-and-Bound algorithm to create a final consensus ranking of indicators. Consensus was measured by the median Kendall's τ and proved to be positive within all three sustainability domains. The strongest consensus was measured for the environmental sustainability ranking with a median Kendall's τ of 0.6316. The weakest consensus was found for the social sustainability ranking with a median Kendall's τ of 0.5048.

The experts indicated *GHG emissions*, *market potential,* and *acceptance of biobased materials* as the most crucial indicators for environmental, economic, and social sustainability. In literature, a significant lack of social aspects was noticed within sustainability analysis of biobased chemicals. By using the results of the MCDA performed in this study, priorities can be established for the inclusion and measurement of social aspects. Furthermore, a prioritization of indicators is useful to assign weights or select attributes when resources like time, data, and money are limited or unavailable. However, reducing the amount of indicators is always a risk and makes the analysis less comprehensive and complete. Key in performing sustainability analysis is being transparent about the indicator specifications and limitations of the study. Experts therefore preferred multiple sustainability indicators over one single index.

Finally, these ranked sets of sustainability indicators provide general guidelines for indicator selection in biobased chemistry, but the relevance of different (sub)indicators might differ from case to case. In the next chapter, the indicators are applied to a specific case study in order to verify and extend a full sustainability analysis. Assessing the sustainability of biobased chemicals is an essential step towards a sustainable biobased economy with environmental, economic, and social benefits over product life cycles.

CHAPTER 4

Techno-sustainability assessment (TSA) framework for biobased chemicals: a microalgae case

In collaboration with G. Thomassen (UAntwerp), S. Van Passel (UAntwerp), R. Malina (UHasselt), & M. Van Dael (VITO, UHasselt). Part of this research was funded by NORTH-WEST EUROPE INTERREG, grant number NWE 639 as part of the IDEA project (Implementation and development of economic viable algae-based value chains in North-West Europe).

ABSTRACT

In order to ensure sustainable new products and technologies, biobased value chains need to be assessed already from a low technology readiness level (TRL). To this end, a techno-sustainability assessment (TSA) framework is developed. The TSA combines environmental, economic as well as social analyses to evaluate the sustainability of biobased chemicals. TSA integrates technological and country-specific data with environmental characterization factors, economic values, and social data. The developed framework is applied to a biobased chemical case for which a production and harvesting plant of microalgae-based food colorants is assessed. Four possible scenarios are defined comparing two different red microalgae and two algae cultivation systems. The TSA framework combines methods for comprehensive indicator selection and quantification for technology assessment already from a low TRL, and identifies potential hurdles and opportunities to support sustainable investment decisions. The next chapter (i.e., chapter 5) handles further integration and interpretation of the results by adding a multi-criteria decision analysis (MCDA) to the TSA framework to tackle data uncertainty and enable scenario comparison if indicators are expressed in different units.

1. Introduction

The question on how to appropriately assess sustainability has a broad scope for interpretation; the literature and scientific reports have made many attempts to provide answers. Entities such as countries and industries strive for sustainability, and multiple evaluation methods have emerged to measure sustainability performance. A variety of disciplines and dimensions should be integrated to capture interactions between human and natural systems (Capellán-Pérez et al., 2020). Sikdar et al. (2017) stated that experts believe "sustainability can nurture the economic advancement, environment stewardship, and societal well-being by steering technology development to assure continual improvement in resource utilization" (Sikdar, Sengupta, & Mukherjee, 2017).

Classically, sustainability can be divided into environmental, economic, and social aspects. Assessment methods have been developed accordingly, such as TEA for economic sustainability, LCA for environmental sustainability, and social LCA for social sustainability. A variety of studies have explored and reviewed these existing sustainability methods and their integration (Buytaert et al., 2011; Rafiaani et al., 2018; Thomassen, Van Dael, Van Passel, et al., 2019). As was explained in the introductory chapter of this dissertation, TEA is an evaluation method where a technological assessment is integrated with an economic assessment (Thomassen, Van Dael, Van Passel, et al., 2019). At low TRL, TEA can identify potential economic hurdles and at higher TRL it provides information on the economic feasibility of the assessed processes (Thomassen et al., 2018). The total life cycle environmental impacts were added in the environmental TEA (ETEA) to include environmental sustainability using LCA concepts (Thomassen, Van Dael, Van Passel, et al., 2019). Finally, social aspects can be added which consider impacts on local communities, workers, and consumers (Rafiaani et al., 2018). However, social assessment is often subjective and difficult to quantify. As a result, the social dimension is rarely added in practice within sustainability analyses for new technologies (Rafiaani et al., 2018; Van Schoubroeck et al., 2018). Economic, environmental, and social assessments are especially interesting to apply in early-stage technology development, as more flexibility is still available to adapt the technology (Thomassen, Van Dael, Van Passel, et al., 2019).

The introductory chapter introduced the life cycle sustainability assessment (LCSA) approach, which combines all three sustainability domains. Within the LCSA approach, diligent indicator selection is critical (Wulf et al., 2018). The literature review in chapter 2 showed that this indicator selection is usually limited to a few well-known indicators, such as global warming and human toxicity, without the inclusion of stakeholder consultation or case-specific characteristics of the assessed value chain (Van Schoubroeck et al., 2018). Accordingly, a method for comprehensive indicator selection was developed in chapter 3, specifically for the assessment of biobased chemicals. Consensus was reached among relevant stakeholders on a prioritization of these indicators (Van Schoubroeck et al., 2019).

Even if one properly selects relevant indicators from all sustainability dimensions, the challenge remains to quantify the selected indicators in an integrated way, and add them to the sustainability assessment methods. The aim of chapter 4 is to develop and apply an overarching framework that conducts a full techno-sustainability assessment (TSA) in early development stages in which all three dimensions of sustainability are integrated. A TSA includes a comprehensive indicator selection and measures the environmental, economic, and social impacts for a specific product or technology and their entire value chain. In the next section, the TSA method is first explained. Chapters 2 and 3 of this dissertation contributed to an important step within this TSA framework which will be further explained in the 'method' section. The 'results' section will further elaborate on the TSA framework applied to a specific case concerning microalgae as feedstock for biobased colorants. Four different scenarios are defined in which technical, environmental, economic, and social data are gathered and used to assess relevant impact categories and compare the alternative scenarios. Finally, the developed method is discussed, future opportunities are disclosed, and final conclusions are drawn in the last section of this chapter.

2. Method

TSA builds further on the ETEA method developed by Thomassen et al. (2018), where environmental and techno-economic aspects were integrated (Thomassen et al., 2018; Thomassen, Van Dael, Van Passel, et al., 2019). The TSA framework consists of six steps (Figure 15):

1. The first step determines the goal and scope and consequently defines different scenarios. This includes a market study where market actors, prices, and volumes of the considered products are defined (Thomassen et al., 2018). System boundaries need to be determined that clearly state the unit processes included within the scope of the study. In addition, the functional unit is defined, which should be consistent throughout the analysis.

2. In the second step, environmental, social, and economic indicators pertaining to the scenarios are selected based on a literature review and

expert opinion. The review performed in chapter 2 and the Delphi study from chapter 3 can be consulted for a comprehensive indicator selection.

3. Once the different scenarios are known and the indicators have been specified, a third step is to gather technological information and construct a process flow diagram (PFD) and a mass and energy (M&E) balance. Data are gathered using lab results, computer models, literature, and supplier information to model the product value chain.

4. In the fourth step, the actual sustainability analysis is performed and the selected indicators are measured per scenario and compared relative to the other scenarios. These indicator quantifications should be linked to the mass and energy balance as much as possible so that technological changes are immediately reflected in the indicator results.

5. In the fifth step, the dynamically quantified indicators can be further interpreted with the aid of an uncertainty and sensitivity analysis that identifies the crucial connections between the indicators and the input data. Identifying the most influential parameters within the analyzed system helps decision makers in further technology development. A feedback loop returns from Step 5 to Step 3 providing the option to adjust process parameters based on the sensitivity results.

6. The uncertainty and sensitivity analysis in Step 5 provides input for a final interpretation step. Here, one evaluates which scenarios perform best or worst based on an entire pool of sustainability indicators measured. A stochastic, hierarchical outranking approach can be followed to integrate all sustainability indicators and help decision makers identify the most and least sustainable scenarios. This last step will be further explained in chapter 5 and is outside the scope of the present chapter. Whenever the sixth step is included, the framework is referred to as the 'integrated techno-sustainability assessment' framework. A final feedback loop returns from Step 6 to Step 1, which clarifies that the framework presents an iterative process that should be repeated when moving to higher TRLs.

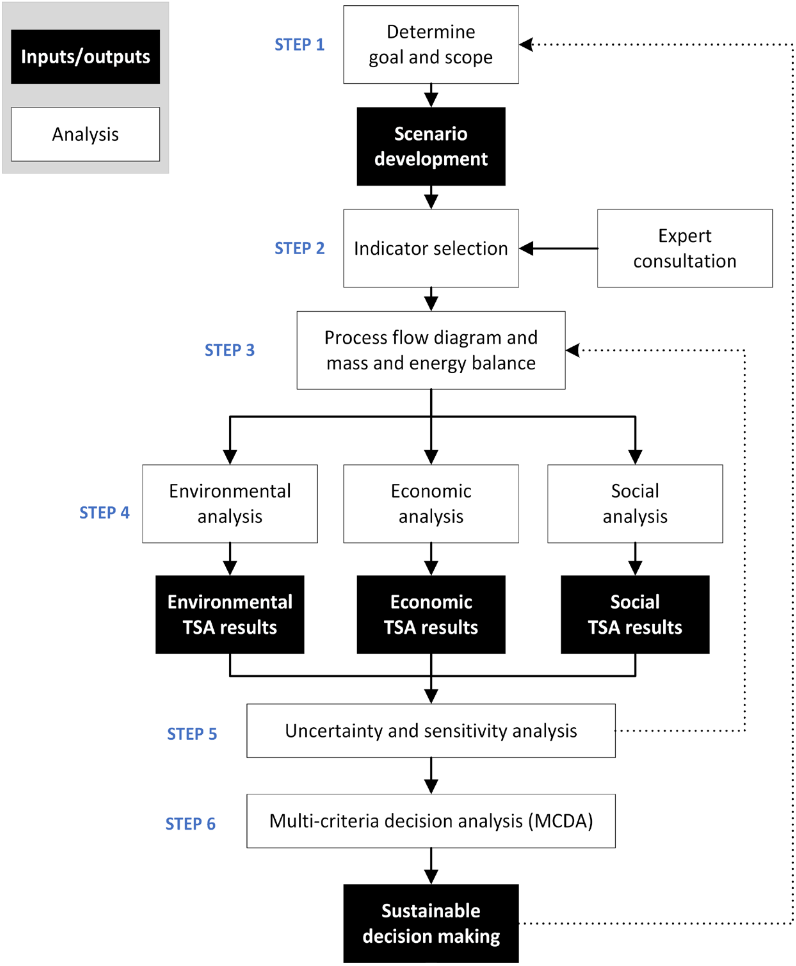

Figure 15. Schematic overview of the integrated techno-sustainability assessment (TSA) framework.

The first five TSA steps rely on previous research methodologies and streamlining methods to select and quantify different sustainability indicators (Thomassen, Van Dael, Van Passel, et al., 2019; Van Schoubroeck et al., 2019). Methods to measure consensus among stakeholders on indicator selection and additional indicator quantification are proposed in the following section. Steps 1 to 5 will be further explained and applied to a biobased chemical case. The case was built to illustrate the TSA and focused on microalgae cultivation systems, in which algae feedstock is grown for the production of food colorants.

3. Results

STEP 1: Goal and scope

The starting point of the case assessed in this chapter is the potential production of feedstock by farmers in Western Europe who have land available for an algae production system. The scale of production is set at one hectare of land, which has been chosen in previous TEAs as well, based on farmers' feedback (Norsker, Barbosa, Vermuë, & Wijffels, 2011; Tredici, Rodolfi, Biondi, Bassi, & Sampietro, 2016). Consumers are increasingly interested in sustainable food value chains, including compliance with environmental regulations and health- and safety aspects (Gebhardt, Sperl, Carle, & Müller-Maatsch, 2020). Consumer-driven demand for natural colorants is changing the food dye market and synthetic colorants, such as azo dyes, are losing their market share (Coultate & Blackburn, 2018). A promising natural alternative is available within the pigments of microalgae (Begum, Yusoff, Banerjee, Khatoon, & Shariff, 2016). Different phyla of microalgae offer a variety of pigments with different characteristics concerning stability, color range, and health applications (Begum et al., 2016). For farmers, growing these microalgae might be a commercially attractive, and sustainable use of their surplus land. However, to maximize sustainability, the heterogeneity of algae strains and cultivation systems must be considered.

Two promising algae types and two different cultivation systems are assessed on their sustainability. The *Porphyridium* algae is cultivated, harvested, and further processed to extract phycoerythrin, a red protein from the light-harvesting phycobiliprotein family (Li et al., 2019). The *Dunaliella salina* algae is cultivated, harvested, and further processed to extract β-carotene, a strongly colored red-orange pigment (Spolaore, Joannis-Cassan, Duran, & Isambert, 2006). The functional unit of the assessment is fixed at one kg of pigments. While β-carotene is already allowed by the European Commission as a food additive (E160a), phycoerythrin is yet to be approved and authorized within the European Union (EU) [EC 1333/2008]. Both natural algae pigments could replace red synthetic dyes such as Allura red (E129). However, Allura red is not included as a synthetic benchmark product because no data is openly available on the production process. The main purpose of this case study is to find the process parameters affecting the sustainability performance of the microalgae scenarios, and to compare multiple algae feedstock and cultivation options.

Both *Porphyridium* and *Dunaliella salina* can be harvested in a horizontal photobioreactor (PBR) or an open raceway pond (OP), each on one hectare of land. The PBR has been shown to reach larger productivities than the OP cultivation, but generally involves higher investment costs (Brennan & Owende, 2010). Two separate production locations are chosen for the analysis. It is assumed that the *Porphyridium* algae will be cultivated in Belgium and the *Dunaliella salina* algae in France. This distinction is necessary as some social indicators can only be populated with location-specific data. Four defined microalgae scenarios are assessed based on their relative sustainability (Table 8).

Table 8. Microalgae scenarios – algae types and cultivation systems.

	Algae type	Cultivation system	Location
Scenario 1 (SC1)	*Porphyridium*	Photobioreactor (PBR)	Belgium
Scenario 2 (SC2)	*Porphyridium*	Open pond (OP)	Belgium
Scenario 3 (SC3)	*Dunaliella salina*	Photobioreactor (PBR)	France
Scenario 4 (SC4)	*Dunaliella salina*	Open pond (OP)	France

STEP 2: Indicator selection

In the second step of the TSA framework, relevant indicators are selected specifically for a microalgae case. Twenty-eight experts in the field of algae processing and products were asked about their agreement with a sustainability indicator ranking for biobased chemicals. The experts were asked to indicate whether they agree or not with the initial indicator ranking, which was retrieved from the Delphi study performed in 2018 (Table 7, chapter 3). The respondents who did not agree with the initial ranking had the opportunity to re-rank the set of indicators. These new experts' rankings were compared with the initial ranking using Kendall's τ rank correlation coefficient (Kendall, 1938). This correlation coefficient is selected to respect the ordinal character of the rankings (De Keyser & Springael, 2009). The value of Kendall's τ ranges from -1 (perfect disagreement) to 1 (perfect agreement). Table 9 provides an overview of the survey results.

Table 9. Survey results – indicator selection by experts. The survey was conducted In October 2019

		Environmental	Economic	Social
#respondents	Total	28	28	28
	"agree"	13	13	16
	"not agree"	13	12	10
	"no idea"	2	3	2
Kendall's τ	Avg τ	0.8729	0.7836	0.8849
	Avg τ "not agree"	0.7457	0.5491	0.7352
	Min τ "not agree"	0.4105	-0.0513	0.4476
	Max τ "not agree"	0.9789	0.8718	0.9810

The τs of the "disagreeing" respondents are shown in Figure 16. Except for one respondent, all rankings have a positive rank correlation coefficient. One expert has a $\tau < 0$ for the economic ranking, which means his/her personal ranking differs significantly from the consensus ranking. All corresponding *z*-values for the environmental and social rankings are larger than 1.645 (that is, the critical *z*). For these, the null hypothesis stating that $\tau = 0$ is rejected at $\alpha = 0.05$. Within the economic rankings, only two *z*-values are not significant at $\alpha = 0.05$. As most of the respondents have a significant positive rank correlation coefficient, it is decided to continue with the initial Delphi ranking for the selection of sustainability indicators. All τs and their corresponding *z*-values are provided in Appendix C1.

The respondents were also asked at which indicator in the ranking they would stop the analysis if limited time was available (Q= "what would be the last indicator of the ranking to take into account?"). The stopping indicator and all the indicators with a higher ranking should be part of the actual sustainability analysis. A frequency analysis was carried out per sustainability dimension of the indicators selected for a sustainability analysis of algae-based chemicals. The stopping criteria were arbitrarily selected where more than half of the respondents reject the indicators on the initial ranking. All of the subsequent indicators were excluded from the analysis. An overview of the frequency analysis and the included and excluded indicators are provided in Appendix C2.

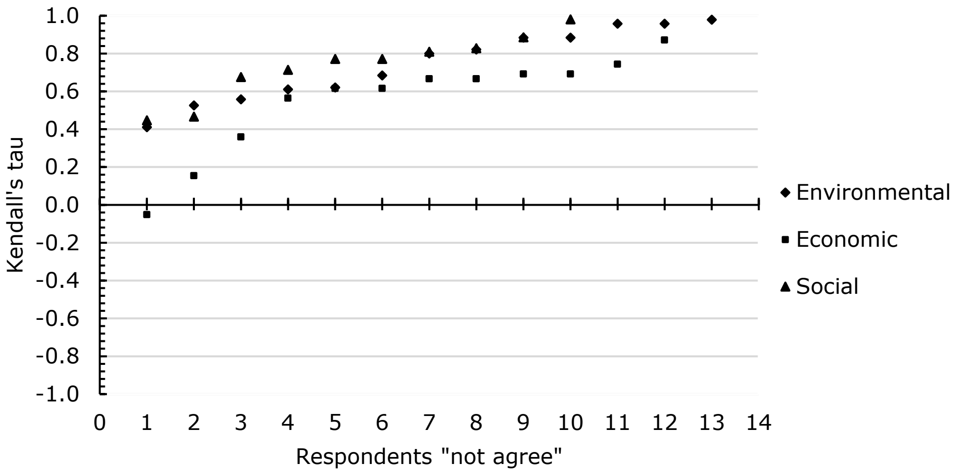

Figure 16. Rank correlation coefficient between initial and new rankings.

STEP 3: Process flows and mass and energy balance

In a third step, technological information about the processes was gathered and a PFD and M&E balance were designed. Figure 17 shows a simplified, schematic overview of the process flows. The case study focuses on the cultivation and harvesting step of the microalgae. The impacts generated by the downstream processes were not considered because little data was available on the extraction of phycoerythrin from *Porphyridium* algae. It is assumed that no pigments were lost during these downstream process steps. In addition, only the pigments were considered as end-products. Given that the case study’s goal is to illustrate the TSA method, additional biorefinery outputs such as exopolysaccharides were excluded from the analysis. These data gaps on downstream processing and end-products need to be handled in the future to have a complete assessment of the value chain.

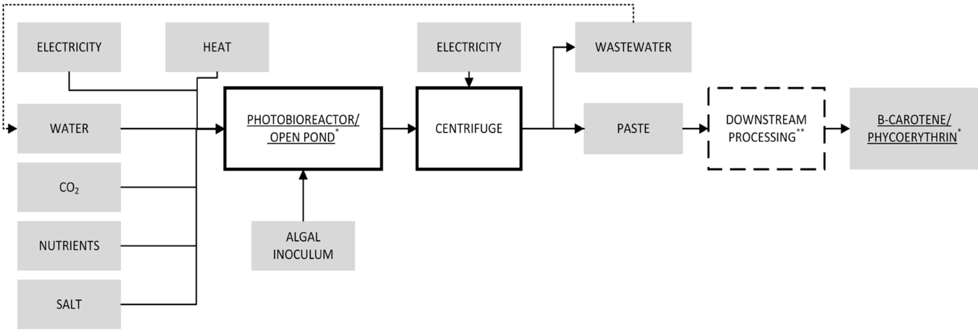

Figure 17. Simplified process flow diagram of the microalgae scenarios. *Underlined processes and products are changing over the scenarios; **Downstream processing steps are unknown.

Figure 18 shows the technical configuration of the cultivation and harvesting processes designed for this case study. Although the downstream process is out of scope, market data should be collected for the final end products for the social and economic indicator calculations. All data were retrieved from suppliers and collected from bibliographic sources. An overview of the data inventory (i.e., all input parameters) is provided in Appendix C3-C5. The medium preparation system, mixing, CO_2 injection system, artificial lighting, and heat pump all consume energy. Additional fugitive water- and CO_2 emissions from the equipment were taken into account. Additional yearly heating was estimated to secure an average algae growth of 0.246 $g.L^{-1}.day^{-1}$ for the *Porphyridium* and 0.197 $g.L^{-1}.day^{-1}$ for the *Dunaliella salina* in the horizontal PBR. If an OP system for cultivation was used, the corresponding productivity diminished to 0.08 $g.L^{-1}.day^{-1}$ for the *Porphyridium* and 0.0135 $g.L^{-1}.day^{-1}$ for the *Dunaliella salina* (Prieto, Pedro Cañavate, & García-González, 2011; Razaghi, Godhe, & Albers, 2014; Rodolfi et al., 2009; Thomassen et al., 2018). The volume-to-surface ratio of the horizontal PBR is 36 $L.m^{-2}$, and 200 $L.m^{-2}$ for the OP. The average temperature was estimated as the country average for Belgium and France.

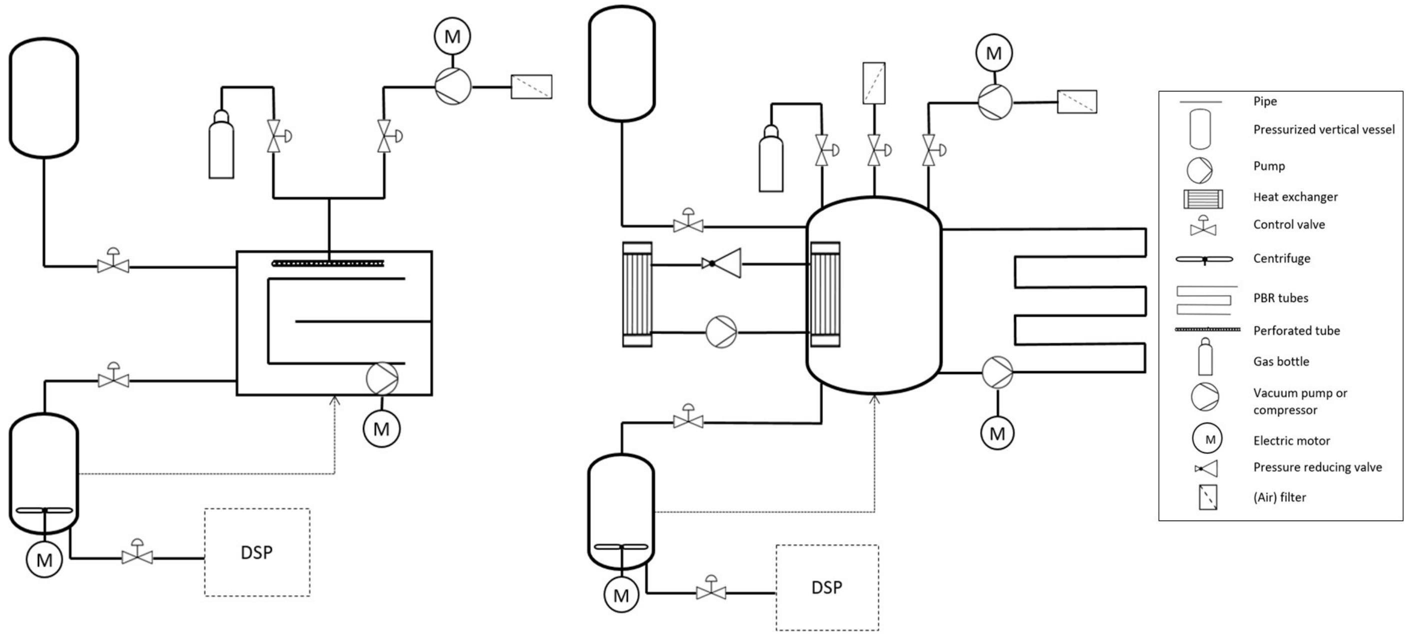

Figure 18. Technical configuration of different cultivation systems: OP (left) and PBR (right). DSP = downstream processing.

The mass and energy results are shown in Table 10. Growing the microalgae in a PBR reaches higher productivity, but volume per land area is larger for the OP cultivation. For the *Porphyridium* algae this leads to a higher biomass output in the OP and for the *Dunaliella salina* more biomass is produced in the PBR. The high biomass output in Scenario 2 requires large amounts of freshwater, nutrients, and CO_2 relative to the other scenarios. Using a heat pump leads to substantial electricity needs for the OP. However, additional electricity needs are much higher for the PBR as the closed system requires a large amount of energy for pumping and artificial lighting. The influence of temperature differences between France and Belgium on the energy needed is only minor. If Scenarios 3 and 4 would be recalculated under Belgian temperatures, the heat consumption would decrease with 0.17 percent and 3.11 percent, respectively.

Table 10. Mass and energy results of microalgae scenarios over the total lifetime (10 years). PBR = photobioreactor, OP = open pond, BE = Belgium, FR = France, and DW = dry weight.

Parameter	**Unit**	**SC1. PBR–BE**	**SC2. OP–BE**	**SC3. PBR–FR**	**SC4. OP–FR**
New salt	$t.y^{-1}$	18	79	157	355
Recycled salt	$t.y^{-1}$	160	683	1,383	3,007
Nutrients	$t.y^{-1}$	35	126	12	27
CO_2	$t.y^{-1}$	73	236	59	39
New water	$m^3.y^{-1}$	1,240	5,321	1,374	3,087
Recycled water	$m^3.y^{-1}$	10,632	45,434	11,813	25,680
Heat	$MWh.y^{-1}$	46	2,149	96	2,996
Electricity	$MWh.y^{-1}$	797	91	800	51
Output biomass (DW)	$t.y^{-1}$	28	52	23	9
Phycoerythrin	$t.y^{-1}$	0.62	1.14	-	-
β-carotene	$t.y^{-1}$	-	-	1.22	0.46

STEP 4: Indicator quantification

In the following paragraphs, the indicators selected in Step 2 are quantified accordingly. To be in line with the heritage of TSA ancestors, upon which the TSA framework builds, these indicators should be integrated with the mass and energy balance whenever possible to make the model dynamic (Thomassen et al., 2018).

However, because of data scarcity at low TRL and lack of quantification methods, this proved infeasible for all indicators. Hence, a number of proxy indicators are not linked to technical data and rely on country-specific data or other scenario-fixed information. Examples of such indicators are ‘patents’ and ‘risk aspects’.

Environmental analysis

For the microalgae case study, the following indicators were quantified: (i) *greenhouse gas (GHG) emissions*, (ii) *ecotoxicity* (including terrestrial, marine, and freshwater), (iii) *land use* (incorporating occupation, transformation, and organic carbon depletion), (iv) *abiotic fossil depletion*, (v) *eutrophication* (including marine and freshwater), (vi) *water consumption*, (vii) *waste generation*, and (viii) *energy efficiency*. *Raw material efficiency* and *end of life options* were not accounted for because of double counting and lack of case differentiation. A detailed explanation of all indicators and their corresponding calculations is provided in the following paragraphs. A general overview of the final environmental results is provided in Table 17, which also summarizes the results for the economic and social dimensions. The fourth column of Table 17 indicates whether the specified indicator should be maximized (+) or minimized (-) to achieve more sustainability.

Most environmental indicators selected by the experts in the present study can be calculated by using the ReCiPe characterization factors (ReCiPe 2016) and the Ecoinvent 3.5 database (allocation at point of substitution – unit). The characterization factors of global warming potential (GWP) were used to quantify the indicator *GHG emissions* in kg CO_2 equivalents. For the *ecotoxicity* indicator, terrestrial, freshwater, and marine ecotoxicity were calculated expressed in kg 1.4 dichlorobenzene (1.4-DB) equivalents to industrial soil, freshwater, and marine water. The ReCiPe method defined *land use* impact as the category that reflects “the process of land transformation, land occupation and land relaxation” (M.A.J. Huijbregts et al., 2017). The ReCiPe method calculates land occupation, transformation, and organic carbon depletion in one land use indicator, expressed in m^2 years crop equivalents. Fossil resource scarcity was quantified to measure the *abiotic fossil depletion*, expressed in kg oil equivalents. *Eutrophication* was measured as freshwater and marine eutrophication from the ReCiPe indicator set, expressed in kg phosphor (P) and kg nitrogen (N) equivalents. Finally, *water consumption* was calculated using the water depletion characterization factors, which correspond to the total amount of water used in m^3.

To avoid double counting, the indicators *raw material efficiency* and *waste generation* were united and quantified by the calculation of the E-factor. The E-factor was developed in the 1980s by Roger A. Sheldon (Roger Arthur Sheldon et al., 2007). It divides kg waste by kg product as shown in Equation (2).

$$\mathrm{E-factor\ (EF)} = \frac{\mathrm{m\ input\ [kg] - m\ output\ [kg]}}{\mathrm{m\ output\ [kg]}} \qquad (2)$$

A higher E-factor means more waste and points to a greater negative environmental impact and extra costs for disposing the waste. Different E-factors were calculated in Table 11, differentiating between inputs with or without water (i.e., mass of water is included or not), and outputs referring to total biomass production or product content (i.e., phycoerythrin or β-carotene). Independent of the calculation method, Scenario 1 always scores best and Scenario 4 worst. Scenarios 2 and 3 change places depending on the calculation with or without water: the OP scenarios score worse when water is encountered as an input. As water consumption is already calculated by the ReCiPe indicator, mass of water could be excluded from the E-factor calculations for this microalgae case study.

Table 11. Yearly average E-factors.

	SC1	**SC2**	**SC3**	**SC4**
E-factor (biomass output, with water)	81	187	146	662
E-factor (biomass output, without water)	3	7	11	46
E-factor (product output, without water)	205	385	223	904
E-factor (product output, with water)	3,888	8,866	2,808	12,660

End of life options are described as 'the possibilities for recycling, composting, biodegrading, burning, … the end product' (Van Schoubroeck et al., 2019). In this case study, the end product is processed as a food colorant and the packaging materials used for the concerning food dye carries environmental concerns. The up and downstream impacts of paper, steel, and plastic packaging are reflected in the other environmental indicators and end of life options is therefore not staged as a separate indicator in the TSA model. This way, double counting can be avoided. For the microalgae case, the end of life impacts per kg pigments were considered the same for all scenarios. As a consequence, they were not included for a comparative analysis.

The last indicator to quantify is the *energy efficiency*. Juodeikiene et al. (2015) quantified energy efficiency by dividing the total energy input by the caloric value (higher heating value) of the end product (Juodeikiene et al., 2015). However, a determination of the caloric value is especially useful when the end product involves an energy-related output like e.g. algae-based biofuels. Within the present case, the end products are biobased chemicals and focus was placed on the energy consumption per kg of product output, instead of caloric values (Equation (3)).

$$\text{Specific energy consumption (SEC)} \left[\frac{\text{MWh}}{\text{kg}}\right] = \frac{\text{Energy}_{\text{input}}[\text{MWh}]}{\text{Product}_{\text{output}}[\text{kg}]} \quad (3)$$

Energy consumption provides a first estimation, but when moving to a higher TRL towards a full scale company, the energy efficiencies should be estimated or an exergy analysis could be applied to expose the inefficient processes (Dewulf et al., 2008). For this microalgae case, the energy consumption of Scenario 4 scores three to nine times higher compared to the other scenarios. This could be explained by the low β-carotene output and the need for additional heat, using a heat exchanger to grow the algae.

Scenario 4 cultivating *Dunaliella salina* in an OP scores the worst on almost all of the described environmental indicators. The only exception is the land use indicator, where Scenario 1 scores worse. On average, Scenario 3 is the most sustainable of the scenarios given the assumptions made, with regard to the reported environmental indicators. Further interpretation of these results is provided within the ‘discussion’ section of this chapter.

Economic analysis
Based on the expert survey and data availability, the following seven indicators were measured for this microalgae case study: (i) *market potential*, (ii) *technical risks*, (iii) *product innovation*, (iv) *process innovation*, (v) *capital productivity*, (vi) *energy cost*, and (vii) *raw materials cost*. *Land productivity* and *product efficiency* were not further accounted for in the case study, even though experts selected them. Land productivity would calculate the sales relative to the amount of land. As the production requires one hectare of land for all scenarios, the land productivity indicator would end up using only sales, which are already accounted for in the market potential and capital productivity indicator. Besides, product efficiency can only be measured for a more mature production volume to compare maximum and actual productivity.

At low TRL, the *market potential* can be calculated based on the market size and price of the end product. Scenarios 1 and 2 include the price for phycoerythrin. Scenarios 3 and 4 the price for β-carotene. World usage of food colors was estimated at 40,000 to 50,000 tonnes in 2013 (Dominguez, 2013). A market report from MarketsandMarkets™ in 2015 predicted that the overall natural food color market would account for nearly 60 percent of the overall global color market. No data was publicly available about the share of different colors within this market. It was assumed that their market share within the natural food color market will be the same. As a consequence, only prices were compared to evaluate the market potential for this case study. Legal factors were disregarded and an assumption was made that both pigments would be allowed in the European food market in the future. Next to its application as a food colorant, phycoerythrin can be sold as a highly valuable biomolecule in niche markets at 254 €.mg^{-1} (Torres-Acosta, Ruiz-Ruiz, Aguilar-Yáñez, Benavides, & Rito-Palomares, 2016). However, the present study aims for a larger product market (i.e., food colorants) and took into account the price of phycobiliproteins which varies from 2.5 €.mg^{-1} to 21.2 €.mg^{-1} (Hu, 2019). The price of β-carotene varies from 215 €.kg^{-1} to 2,150 €.kg^{-1} (Cuellar-Bermudez et al., 2015). Both prices for phycoerythrin and β-carotene vary a lot in literature. It was decided to hold a 'low' price of 36,000 €.kg^{-1} for phycoerythrin because prices at the upper range consider applications in health research such as fluorescent probes (Cuellar-

Bermudez et al., 2015). For the price of β-carotene, an average of 1,183 €.kg^{-1} was considered.

Technical risks are defined as risks associated directly with the supply chain activities, e.g. feedstock supply risk, infrastructure risk, etc. (Van Schoubroeck et al., 2019). Patel et al. (2012) proposed the risk aspects (RA) indicator, which can be used to measure the technical risks (Patel et al., 2012). They defined sub-indicators that are needed to assess risk: (i) Feedstock supply risk, feedstock availability, (ii) regional feedstock availability, (iii) market risk, (iv) infrastructure risk, and (v) application of technical aspects (i.e., inherent functional and pathway aspects). Weights were determined by the CatchBio project based on expert opinion (Patel et al., 2012). Table 12 gives an overview of the scores calculated for the four algae scenarios on the different risk aspects. The higher the scores, the higher the risks. These scores were based on literature and market information. Although the end-product is made from algae, it is water, salt, additional nutrients, and CO_2 that are used as feedstock to cultivate the algae. These feedstocks are largely and regionally available, which means a score of 0 is given to all scenarios. Market risk is small as food dyes are existing commodity chemicals. According to the scoreboard described in Patel et al. (2012), this yields a score of 0.33 for every scenario. The infrastructure risk is the criterion that creates a difference between the scenarios. The target product phycoerythrin as food colorant would need new processing and supply chains while β-carotene is already commercially produced as a food dye. In addition, the cultivation technology changes the infrastructure risk as the technology of raceway open ponds is more mature as the one of horizontal photobioreactors. For the PBR technology, new processing plants would be required. The application-technical risk aspects were considered the same for both pigments.

The RA indicator offers a proxy for technical risks, but it does not take into account every risk aspect. For example, OP technology generally has a higher risk of contamination compared to closed systems and thus, at large scale, the risk of losing large batches of algae feedstock (Cohen & Arad, 1989). Closed photobioreactors have the advantage of better control on culture conditions such as CO_2 supply and temperature control (Gupta, Lee, & Choi, 2015).

Table 12. Risk aspects (RA). *Higher score = higher risk.

	Weights	SC1	SC2	SC3	SC4
Feedstock supply risk	0.25	0	0	0	0
Regional feedstock availability	0.15	0	0	0	0
Market risk	0.25	0.33	0.33	0.33	0.33
Infrastructure (availability) risk	0.20	0.66	0.66	0.33	0
Application-technical aspects	0.15				
Chemicals: functional groups	0.50	0.50	0.50	0.50	0.50
Chemicals: retention of raw material functionality	0.50	0	0	0	0
Final score*		**0.25**	**0.25**	**0.19**	**0.12**

Product- and *process innovation* are two other economic indicators to measure sustainability (Van Schoubroeck et al., 2019). Patent analysis has been used to assess product and process innovation (Abraham & Moitra, 2001; Albino, Ardito, Dangelico, & Messeni Petruzzelli, 2014; Johnstone, Haščič, & Popp, 2010). Patents can be considered as the outputs from the innovation process (Coombs, Narandren, & Richards, 1996). A point of critique is that it rather reflects inventiveness than innovation. Also, some technological advances might not be patentable, and companies and research institutes can have other methods of protecting their technological advantage (Coombs et al., 1996). However, patents have proven to present a close link to economic relevant inventions (Albino et al., 2014). At low TRL, the number of patents approved was considered an interesting proxy for product and process innovation within the present study. The more patents published, the higher the degree of innovation. A patent count was performed on Espacenet, a database provided by the European Patent Office. The results of this analysis are presented in Table 13. It was not the aim to perform a detailed patent analysis, but including additional information such as the average number of scientific citations, geographical origin, and time-scales could improve such analysis in the future (Albino et al., 2014). Considering process innovation in the past 10 years, the scenarios including pond cultivation technologies scored better compared to photobioreactors. For product innovation, most patents were counted for β-carotene but differences with phycoerythrin were small.

Table 13. Patent count [search July 2020]. # = number of patents; #10 = number of patents published in 2010-2020.

Search queries [in title, abstract or claims]					**#**	**Publication range**	**$\#_{10}$**
		AND	AND	AND			
Product	"dye" OR "colorant"	"betacarotene"	"algae"		32	1984-2019	22
				"food"	9	2007-2018	8
		"phycoerythrin"	"algae"		25	1994-2019	16
				"food"	2	2014, 2017	2
Process	"algae"	"cultivation" OR "cultivating"	"pond"		1,634	1973-2020	1,440
			"photobioreactor"		495	1995-2020	431

Capital productivity divides the yearly sales by the average capital cost per year. For the PBR scenarios (i.e., Scenarios 1 and 3), CAPEX of the medium preparation system, bioreactor, heat pump, and artificial lighting were taken into account. For the OP scenarios (i.e., Scenarios 2 and 4) a medium preparation system, heat pump, liner, and paddle wheel were included. The calculations of the capital productivity are shown in Table 14. Higher numbers represent higher productivities. Even though capital costs of the PBR cultivation were significantly higher compared to the OP, the high price of phycoerythrin resulted in higher sales which increased the capital productivity for Scenarios 1 and 2.

Table 14. Yearly average capital productivity. [a]Depending on lifetime per equipment.

	SC1	**SC2**	**SC3**	**SC4**
Average capital cost (€)[a]	376,932	192,854	380,609	168,249
Sales (€)	22,161,598	41,039,996	1,037,190	549,747
Capital productivity	**58.79**	**212.80**	**3.79**	**3.27**

The final indicators that were quantified within the economic dimension were the *cost of raw materials* and the *energy cost*. The total cost of raw materials and energy per year were divided by the total product output. The calculations for the cost of raw materials include the cost of salt, water, fertilizers, and CO_2. Both cost indicators should be minimized to achieve more sustainability. Scenario 4 scores the worst on both cost indicators, while Scenario 3 has relatively low costs of raw materials and energy.

The overall economic performance of the scenarios differs depending on the considered indicator. The scenarios producing phycoerythrin outperform the scenarios producing β-carotene on market potential and capital productivity because of their high market price. However, because phycoerythrin is not yet allowed in the European market as a food colorant, technical risks are higher and product innovation scores lower.

Social analysis

The social indicators selected by the experts and quantified for this case were: (i) *product transparency*, (ii) *human toxicity* (including cancer and non-cancer impacts), and (iii) *income levels*. *Education and training* and *community support and involvement* are not accounted for as these are company-specific indicators and require the process to be operational at high TRL. Furthermore, a*cceptance of biobased materials*, *job creation*, and *workplace accidents and illnesses* did not differentiate between the four assessed scenarios. More information is provided in the following paragraphs. Table 17 includes an overview of all social indicators that are quantified within the social dimension for which the results differ between the scenarios.

Acceptance of biobased materials was selected as the most important social indicator by the microalgae experts in Step 2 of the TSA. Although the perception and associated market uptake of biobased products is recognized to be important, a framework for assessment is often lacking (Falcone & Imbert, 2018). Social acceptance is usually assessed qualitatively using focus groups or questionnaires. In contrast, choice based experiments to investigate consumers' willingness to pay (WTP) have been used in the past to assess consumer acceptance of food in a quantitative way (Alfnes, Guttormsen, Steine, & Kolstad, 2006; J. B. Chang, Moon, & Balasubramanian, 2012; Paci, Danza, Del Nobile, & Conte, 2018). In the case study, two different algae-strains were compared for the same output i.e., food dyes. The acceptance of the algae-based food colorants was considered the same in all scenarios as it was assumed that customers will not deviate between algae strains. Customers will not resist using an end product based on information of that it is being produced from a specific algae strain. Assessing the acceptance would be more relevant if a synthetic benchmark would be included. Previous research from Bearth et al. (2014) and Gebhardt et al. (2020) assessed consumers' expectance and concluded artificial food dyes are disliked more by the public compared to natural alternatives (Bearth, Cousin, & Siegrist, 2014; Gebhardt et al., 2020). A synthetic alternative was not assessed and as a consequence, customer acceptance was considered the same for all scenarios assessed in the present case study.

Product transparency is usually measured in a qualitative or semi-quantitative way. According to the Social-LCA methodological sheets developed by UNEP and SETAC in 2013, transparency should enable the consumer to make an informed choice without intent to mislead or conceal (UNEP SETAC, 2013). They proposed two ways of measuring transparency: (1) a specific and (2) a generic analysis. When analyzing a technology at low TRL, conducting a specific analysis as proposed by UNEP and SETAC is rather difficult. The specific analysis focuses on indicators such as 'consumer complaints regarding transparency', 'publication of a sustainability report', or 'company rating in sustainability indices' where data should be found on a company's website, by interviews with their customers or management, or from the Dow Jones Sustainability index. The generic analysis proposed by UNEP and SETAC offers two indicators which can be used for technology assessment at a lower TRL: 'presence of a law or norm regarding transparency (by country and/or sector)' and 'sector transparency rating: number of organizations by sector which published a sustainability report'. These two generic indicators rely on country and sector data which can already be evaluated at low TRL. Data was collected for Belgium and France within the Global Reporting Initiative (GRI) database in the chemistry- and food sector (2017). Other reporting databases might be selected if deemed relevant for the assessed sector. The country-specific GRI data is compared relative to the number of enterprises present. As the indicator considers the effective implementation of sustainability reporting, this proxy for transparency can be chosen as an input for the TSA (Table 15). A higher proxy number leads to a higher level of transparency. It was assumed that the entire value chain is located in Belgium for Scenarios 1 and 2 and in France for Scenarios 3 and 4. When more data become available, more specific assumptions can be made about the location of the different processes along the value chain. To provide a benchmark, the transparency proxy was calculated for all countries within the EU for which data is available on the OECD website (Appendix C6). Belgium scores better on the transparency proxy compared to France. However, this difference is rather small compared to other EU countries.

Table 15. Transparency proxy. [a]OECD, 2017; [b]GRI, 2017.

	Belgium	**France**
Manufacture of chemicals and chemical products [a]	614	3,042
Manufacture of food products [a]	6,720	51,288
Total # of enterprises	7,334	51,387
# sustainability reports [b]	6	13
% sustainability reports per enterprise	**0.082**	**0.024**

When technology matures and a full scale company is assessed, another method to measure organizational transparency is proposed by Zakaria et al. (2018). They developed an indicator for transparency in sustainability reporting, which measures the relative entropy between the probability distributions of words in the sustainability dictionary and those in a corporate report (Zakaria, Liginlal, & Aoun, 2018).

At low TRL, direct *job creation* is calculated by counting the jobs needed within the cultivation and harvesting step. An integration with technical parameters is possible by making the number of employees dependent on the scale of the plant. As only one hectare of production area was assessed for the case, the direct job creation was the same for all scenarios (i.e., three employees). Supervision and clerical labor can be estimated as 10 to 20 percent of the operating labor (Peters, Timmerhaus, & West, 2003). To include indirect job impacts, input-output multipliers can be determined which represent an additional or direct change to the economy resulting from each change in a selected industry (Madugu, 2015). This was done for an algal biofuel manufacturing site by Madugu in 2015.

However, input-output multipliers are very case dependent and thus cannot be transferred for use in the present case study.

Human toxicity was calculated by using the ReCiPe characterization factors and the Ecoinvent 3.5 database. The carcinogenic as well as non-carcinogenic human toxicity potential (HTP) were both taken into account. Results are displayed in Table 17 at the end of this section. Scenario 4 scores the worst on both HTP indicators while Scenarios 2 and 3 score best.

Income levels and the fairness of these incomes can be assessed by calculating the fair wage potential (FWP) (Rafiaani, Kuppens, et al., 2020). Neugebauer et al. (2017) developed the FWP taking into account working time, equal remuneration, and living wage (Equation (4)). The Gini-coefficient can be used as an approximation for the income inequalities factor (IEF). Table 16 presents the calculations for the different microalgae scenarios. It was again assumed that the entire value chain is present in one country, i.e., Belgium or France. Under the assumptions made, the scenarios present in Belgium score better with a higher fair wage potential compared to the French algae production systems.

$$\mathrm{FWP_n} = \frac{\mathrm{RW_n}}{\mathrm{RWT_n}} * \mathrm{CF_{FW,n}}$$

$$\mathrm{CF_{FW,n}} = \frac{1}{\mathrm{MLW_n}} * \mathrm{CWT_n} * (1 - \mathrm{IEF_n^2}) \qquad (4)$$

(with n = process, RW = real (average) wage, RWT = real working time, CF = fair wage characterization factor, MLW = minimum living wage, CWT = contracted working time, and IEF = inequality factor)

Table 16. Fair wage potential: Belgium versus France. [a]Real (average) wage – OECD 2018; [b]Real working time (RWT) – Eurostat 2018; [c]Min. living wage (MLW) – Eurostat 2018; [d]Contracted working time (CWT) – ILO 2009; [e]Inequality factor (IEF) – Gini 2015.

	RW[a] €/month	*RWT*[b] hours/week	*MLW*[c] €/month	*CWT*[d] hours/week	*IEF*[e] %	*FWP*
Belgium	3,677.97	41.00	1,330	38.00	0.277	**1.340**
France	3,143.36	40.40	1,510	35.00	0.327	**0.817**

Finally, a quantification method needs to be found to assess the *workplace accidents and illnesses*. Kidam and Hurme (2013) analyzed 364 equipment's related accidents cases within the chemical industry. Process accidents within an equipment category were calculated relative to the other equipment categories (Kidam & Hurme, 2013). The biggest difference in equipment within the microalgae case study is the use of an OP versus a PBR which can be categorized as a 'storage tank' and 'reactor' holding the same accident rate. Both 'storage tanks' and 'reactors' are each responsible for 14 percent of the accidents (Kidam & Hurme, 2013). However, the number of accidents per equipment type is not only dependent on the risks per equipment, but also a function of the required labor (Rafiaani, Thomassen, et al., 2020). For the microalgae case assessed, required labor was in all cases considered the same. As a consequence, workplace accidents will not deviate between the scenarios.

In general, Scenario 4 scores the worst on all social indicators. Scenario 2 seems to benefit from Belgium as the location for cultivation, and lower human toxicity risks.

STEP 5: Uncertainty and sensitivity analysis

A fifth step in the TSA framework performs a sensitivity and uncertainty analysis to identify the relative influence of the input parameters on the individual sustainability indicators measured for the microalgae processes. A sensitivity analysis identifies the influential parameters when a large amount of input data and calculations are involved. Ten thousand trials are performed varying all input data by -10 percent to +10 percent following a triangular distribution. The full sensitivity analysis can be consulted in Appendix C7. Some proxy indicators are omitted from the analysis because they were independent of technological data and rely on a limited amount of social or economic input data. This was the case for the following indicators: market potential, technical risks, product- and process innovation, transparency, and income levels.

Table 17. Environmental, economic, and social indicators – results for the microalgae scenarios. SC = scenario, PBR = photobioreactor, OP = open pond, BE = Belgium, FR = France, GHG = greenhouse gas emissions, FETP/METP/TETP = freshwater/terrestrial/marine ecotoxicity potential, LUP = land use potential, AFD = abiotic fossil depletion potential, FEP/MEP = freshwater/marine eutrophication potential, WCP = water consumption potential, SEC = specific energy consumption, HTP c/nc = human toxicity potential cancer/non-cancer, and FWP = fair wage potential.

Indicator	**Measurement**	**Unit**	**+/-***	**SC1. PBR–BE**	**SC2. OP–BE**	**SC3. PBR–FR**	**SC4. OP–FR**
Environmental							
GHG emissions	GWP ReCiPe	kg CO_2 eq.	-	626	831	188	1,759
Terrestrial ecotoxicity	TETP ReCiPe	kg 1.4-DB eq.	-	1,945	1,711	1,113	2,783
Marine ecotoxicity	METP ReCiPe	kg 1.4-DB eq.	-	23	10	12	34
Freshwater ecotoxicity	FETP ReCiPe	kg 1.4-DB eq.	-	17	15	9	23
Land transformation & occupation	LUP ReCiPe	m^2a crop eq.	-	36	9	6	14
Abiotic fossil depletion	AFD ReCiPe	kg oil eq.	-	156	223	33	561
Freshwater eutrophication	FEP ReCiPe	kg P eq.	-	0.21	0.13	0.07	0.22
Marine eutrophication	MEP ReCiPe	kg N eq.	-	0.03	0.02	0.02	0.04
Water consumption	WCP ReCiPe	m^3	-	8	7	4	12
Waste generation	E-factor	Index	-	205	385	187	904
Energy efficiency	SEC	$MWh.kg^{-1}$	-	1.37	1.96	0.73	6.55
Economic							
Market potential	Price	$€.kg^{-1}$	+	36,000	36,000	1,183	1,183
Technical risks	Risk aspects indicator	Index	-	0.25	0.25	0.19	0.12
Product innovation	Patent count (avg)	#patents	+	16	16	22	22
Process innovation	Patent count (avg)	#patents	+	431	1,440	431	1,440
Capital productivity	Sales/cost of capital	Index	+	59	213	4	3
Raw materials cost (yr avg)	Cost calculation	$€.kg^{-1}$	-	63	101	29	153
Energy cost (yr avg)	Cost calculation	$€.kg^{-1}$	-	181	51	76	150
Social							
Transparency	Sustainability reporting	%	+	0.082	0.082	0.024	0.024
Human toxicity cancer	HTP_C ReCiPe	kg 1.4-DB eq.	-	27	14	15	28
Human toxicity non-cancer	HTP_{NC} ReCiPe	kg 1.4-DB eq.	-	373	294	257	807
Income levels	FWP	Index	+	1.340	1.340	0.817	0.817

*Positive or negative impacts are indicated by respectively '+' or '–' in the fourth column. This is important for final aggregation performed in chapter 5.

There are some rules of thumb for interpreting the values of the resulting rank correlations. If the absolute values of the correlations are ≥ 0.4, a moderate to very strong correlation between the input data and output indicator can be observed (Schober, Boer, & Schwarte, 2018). The results of the sensitivity analysis show that most sustainability indicators were strongly influenced by the pigment content, the algae growth rate, and the recycled salt ratio. Large amounts of salt are being used by the algae cultivation system, and an optimized recycling system could improve the sustainability of the processes. Data on algae growth models and pigment content were still unsure in current literature and are further related to factors such as light, temperature, stress factors, and pressure. Optimizing these conditions could increase pigment content and algae growth, which would benefit many of the included sustainability aspects. In addition, other input parameters such as water recycling, electricity purchase price, and PBR investment costs also had a big influence on some individual indicators such as water consumption and raw material costs, land use potential and energy cost, and capital productivity, respectively.

Pigment price was considered highly uncertain within this analysis, as was mentioned in the economic analysis of Step 4. Product price drives market potential and the sensitivity analysis shows that the price is a crucial parameter when assessing capital productivity. If both prices for phycoerythrin and β-carotene would converge to similar pigment prices in the future, Scenario 2 would still score best; however, Scenario 1, which was ranked second best when current price data was considered, could have the lowest capital productivity (Figure 19).

A what-if analysis was performed to assess the influence of the location-specific energy-mix on the environmental impact indicators, which uses Belgian location factors for Scenarios 3 and 4. In Scenario 3 this leads to an increase in land use (+13 m^2a crop eq.) and GWP (+134 kg CO_2 eq.) under Belgian conditions. No remarkable indicator changes were present in Scenario 4 resulting from differences between French and Belgian location factors.

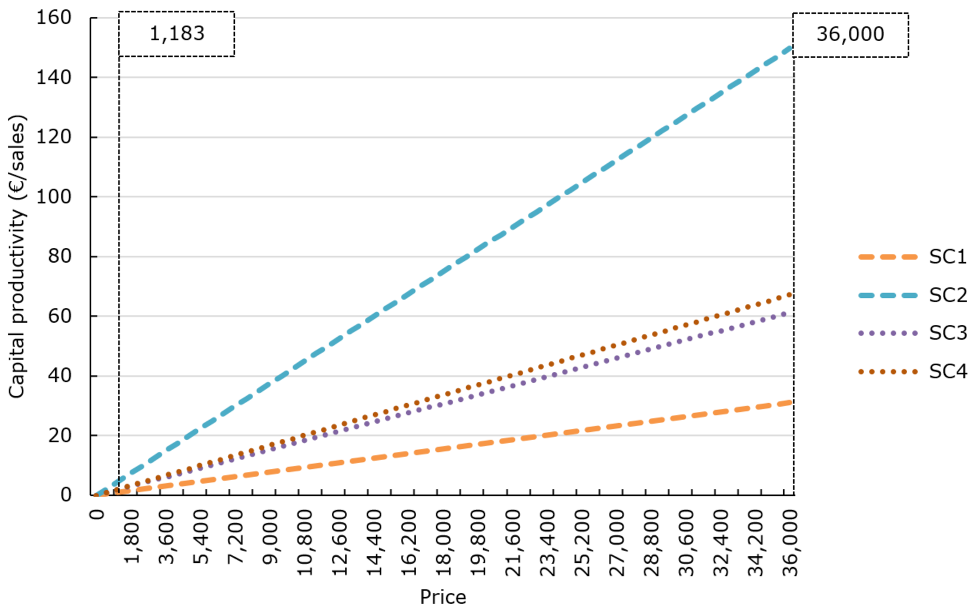

Figure 19. What-if analysis – the effect of pigment price on capital productivity.

4. Discussion

4.1 Scenario comparison

The sustainability indicators calculated within the TSA framework enable the evaluator to compare the different scenarios under the assumptions made. To allow for a general comparison between the different microalgae scenarios, the scores were converted into rank numbers and a counting analysis shows how many times a scenario was ranked on a specific position for all 22 sustainability indicators (Table 18). The rank order was reversed for indicators with an opposite direction. When equal scores between the scenarios occurred, the average ranking position is rounded to the higher ranking position. Scenario 3, cultivating the *Dunaliella salina* algae in a PBR, is ranked best on 13 out of 22 indicators. Scenario 4, cultivating the *Dunaliella salina* in the open pond, scores the worst and is ranked third or fourth on 19 out of 22 indicators.

Table 18. Ranking results – a counting analysis.

Rank position	22 sustainability indicators SC1	SC2	SC3	SC4
1	3	8	13	3
2	6	7	4	0
3	11	7	5	5
4	2	0	0	14

Rank position	4 social indicators				7 economic indicators				11 environmental indicators			
	SC1	SC2	SC3	SC4	SC1	SC2	SC3	SC4	SC1	SC2	SC3	SC4
1	2	3	1	0	1	4	2	3	0	1	10	0
2	0	1	1	0	2	0	2	0	4	6	1	0
3	2	0	2	2	3	3	3	2	6	4	0	1
4	0	0	0	2	1	0	0	2	1	0	0	2

This general counting analysis assumes equal weighting for all 22 indicators, which creates imbalances between the three sustainability domains. An analysis per domain is added in Table 18 showing the separate rankings of the scenarios. The high integrated ranking position of Scenario 3 is driven by the lower environmental impacts for which the concerned scenario is ranked first on 10 out of 11 indicators. The sensitivity analysis showed that both pigment content and growth parameters have a large influence on the output indicators. For Scenario 3, pigment production is the highest relative to the other scenarios. Growing the *Dunaliella salina* algae in a PBR leads to a pigment production which is 2.6 times higher than an OP cultivation, which explains the high environmental scores of Scenario 3 compared to Scenario 4. The same results apply for the *Porphyridium* algae where the OP cultivation is more productive. As a consequence, the environmental indicators per functional unit score better for the *Porphyridium* cultivated in an open pond compared to the PBR scenario. To achieve an environmentally sustainable microalgae process, it seems that the growth rate plays a crucial role. Growth conditions should be monitored and optimized within the cultivation of algae. Scenario 2 scores relatively high on the social and economic indicators compared to the other scenarios. This can be related to the high pigment price of phycoerythrin, favorable social conditions thanks to Belgium as the location of cultivation, and lower human toxicity risks. However, a counting analysis might lead to a wrong interpretation of the indicator results as the magnitude of the differences in scores and the trade-offs between the domains are not represented by the ranking.

4.2 Application challenges

While assessing the microalgae case using the TSA approach, data availability and (social) indicator quantification posed difficulties, especially at low TRL. Data availability concerns are mostly present during Step 3 (process flows and mass and energy balance) and Step 4 (the economic, environmental, and social analyses) of the TSA, in which an extensive data collection was required. Step 3 requires technological data including mass and energy information. Step 4 starts with the collection of social, economic, and environmental data based on the indicators that were selected in Step 2. When a full scale company does not yet exist, country or sector data (that is, secondary data) can be the only available data source. Some indicators might be excluded based on the TRL and the impossibility of finding data. An example is measuring 'education and training', for which mature company data is essential. When moving higher on the TRL scale, information becomes more certain, and data sources become more comprehensive. A sensitivity analysis estimates the crucial input parameters, which provides insights for further data needs and technology development when moving to a higher TRL. In addition, it is possible to take into account the stochasticity of data in the final decision-making step (i.e., Step 6).

In practice, sustainability assessments often neglect social impact categories due to a lack of quantification methods (Van Schoubroeck et al., 2018). In Step 4 of the TSA, it is recommended to calculate proxies for the selected social impacts such as transparency and income levels. The same applies for the environmental and economic dimensions, where some indicators might be difficult to measure as well. For example, process- and product innovation are quantified using patent analysis as a proxy, and the E-factor developed by Sheldon (2007) is included in the environmental analysis. By using proxies, such as risk aspects (RA) developed by Patel et al. (2012) and fair wage potential (FWP) by Neugebauer et al. (2017), the sustainability assessment goes beyond profit calculations and common widespread indicators. It is essential to include a comprehensive indicator selection that precedes the actual analysis to include all relevant sustainability impacts, preferably by using expert participation (Bockstaller & Girardin, 2003). However, when no valid proxy is available, and quantification seems impossible, a qualitative description could offer additional information on missing values. For example, the risk of contamination within an OP compared to a PBR is not accounted for within the RA indicator, as this is specific for algae cultivation systems. Such impacts should be added separately to avoid bypassing non-quantifiable indicators. When making decisions based on the quantitative models, qualitative data should be consulted to draw valid and complete conclusions for a comprehensive sustainability evaluation.

5. Conclusion

Technologies should be assessed from low TRL and onwards to make R&D and investment decisions, and proceed on the TRL scale in a sustainable way. Therefore, a techno-sustainability assessment (TSA) method for a sustainability analysis of (new) products and technologies has been developed within this chapter. A combination of the first five TSA steps results in three separate assessments per sustainability domain, all dynamically linked to technological and country-specific data. The TSA framework goes beyond the standard inclusion of well-known impact categories, such as GWP and NPV, by involving case-dependent indicator selection. Environmental, economic, and social indicators were selected and quantified to compare different microalgae scenarios for the production of biobased chemicals (i.e., food colorants). The general biobased chemical indicator ranking, developed in chapter 3, was considered directly applicable to the microalgae case study by the experts. Based on a counting analysis, Scenario 3 cultivating the *Dunaliella salina* in a photobioreactor in France scored best on most sustainability indicators, and Scenario 4, cultivating *Dunaliella salina* in an open pond scored the worst. These results should be interpreted as relative outcomes compared to the other assessed scenarios.

The TSA framework encourages a practical approach to support product- and technology developers, and decision makers. The framework provides the opportunity to assess sustainability, including economic, environmental, and social aspects by identifying potential hurdles and opportunities. A dynamic quantification of the selected indicators in Step 4 enables using sensitivity analysis, and the ability to perform multi-criteria decision analysis in a final step (i.e., Step 6). The sixth TSA step will be explained in chapter 5, which integrates and interprets the selected indicators expressed in different units to enable integrated decision-making. A stochastic approach should be applied as this allows for data uncertainty at low TRL. A combination of MCDA and TSA results in an integrated techno-sustainability assessment (TSA) method with the aim of providing a balanced, holistic framework for sustainability analysis and corresponding decision-making.

CHAPTER 5

Integrating sustainability indicators: a decision-making analysis

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ABSTRACT

A better understanding of the potential sustainability of emerging technologies and products is essential to guide additional research and further technology development. To this end, a techno-sustainability assessment (TSA) framework was developed in chapter 4 and measures the environmental, economic, and social impacts over the life cycle of a biobased chemicals. However, the quantification of multiple impact categories in different metrics makes a comparison between alternative scenarios complex. In this fifth chapter, a hierarchical, stochastic outranking approach for sustainable decision-making is developed with the aim of integrating multiple sustainability indicators. A multi-criteria decision analysis (MCDA) is applied, which allows for performance uncertainty and the development of a ranking of scenarios. Different weighting schemes and preference structures are considered and compared to check for the robustness of the results. The decision analysis is applied to the microalgae case study from chapter 4, in which four alternative scenarios based on two different strains of red microalgae and two different cultivation systems were assessed. The aim of chapter 5 is to develop an integrated TSA where decision-making is included in order to compare the potential sustainability performance of different scenarios and to make better-informed choices between alternatives by evaluating environmental, economic, and social sustainability impacts.

1. Introduction

A full sustainability analysis incorporates technological aspects as well as economic, social, and environmental impact categories in a comprehensive way. TEA as well as (social) LCA have been used already for sustainability evaluation of technologies (Hoogmartens, Van Passel, Van Acker, & Dubois, 2014). In chapter 4 of this dissertation, a techno-sustainability assessment (TSA) framework was developed which integrates these methods. However, the interpretation of the results of these assessments is complex because social, economic, and environmental indicators are represented in different units. For example, environmental LCA indicators such as global warming potential (GWP) can be quantified in CO_2 equivalents, ecotoxicity potential (ETP) in kg 1.4-DCB_{eq}, and water consumption in m^3. The complexity increases when these environmental impacts are compared with economic or social indicators which are expressed in units such as 'euro' or 'number of jobs', and the use of an appropriate decision analysis method is necessary. These decision-support methods are influenced by the preferences of specific stakeholders, such as sustainability analysis practitioners. The methodological choices within sustainability evaluation tools should be consistent with the values of the affected stakeholders (Alexandros Gasparatos, 2010). Specific decision-making methods are needed that integrate multiple indicators and the presence of perceptions and values within the assessment of sustainability (Martin, 2015).

Multi-criteria decision analysis (MCDA) provides a solution for comprehensive decision-making. Wang et al. (2009) described MCDA as a decision support approach that is suitable for addressing complex problems featuring high uncertainty, conflicting objectives, different forms of data and information, and multi-interests and perspectives (Wang et al., 2009). The combination of LCA and MCDA has been used in the past, for example, by implementing the AHP and PROMETHEE to rank alternative scenarios (Rita, Marques, Garcia, Freire, & Dias, 2015). Examples can be found in the bioproducts, energy, transportation, and chemical industry (Adisa Azapagic, Stamford, Youds, & Barteczko-Hibbert, 2016; Klein & Whalley, 2015; Maxim, 2014; Narayanan, Zhang, & Mannan, 2007; Reeb, Venditti, Gonzalez, & Kelley, 2016). A combination of MCDA with all sustainability dimensions (environmental, economic, and social impacts) has also been reported to achieve 'full' integration. Examples are the studies of Santoyo-Castelazo and Azapagic (2014), in which multi-attribute value theory was used to determine a global value function, and Zhang and Haapala (2015), in which the principles of PROMETHEE were used to combine the three sustainability dimensions (Santoyo-Castelazo & Azapagic, 2014; Zhang & Haapala, 2015). However, these decision-making approaches are often deterministic or limited to fixed methodological choices regarding preference structures and weighting schemes. Deterministic decision analysis does not allow for data uncertainties; this issue is particularly relevant for the valuation of technologies at low TRL. In addition, all MCDAs have to deal with the subjectivity of weighting and selection of preference structures. Decision makers often make prior fixed choices instead of comparing multiple options to check for the robustness of their results. Opon and Henry (2020) described this as methodological uncertainty, where different methods result in divergent and sometimes conflicting conclusions and decisions (Opon & Henry, 2020).

Step 6 of the techno-sustainability assessment (TSA) framework proposes that the sustainability indicator results are integrated using MCDA. This combination of TSA and MCDA is hereafter referred to as the **integrated** techno-sustainability assessment (TSA). Because the assessment of technologies and processes at a low TRL contains many uncertainties, a stochastic outranking approach was chosen to build an appropriate MCDA method for the case study herein. A stochastic multi-attribute analysis (SMAA) was used as a base model, completed with different preference structures and weighting scheme extensions. The study of Prado and Heijungs (2018) was consulted as a guideline to build these SMAA models. SMAA follows a stochastic PROMETHEE approach, performing pairwise comparisons to assess the significance of mutual differences between scenarios (Prado-lopez et al., 2014). Afterwards, the pairwise distances – being the differences between scenarios on a specific indicator – are evaluated against thresholds, which reflect the preference structure. The use of outranking in decision-making makes it possible to focus on those indicators in which the alternative scenarios show critical differences (Prado-lopez et al., 2014). In addition, PROMETHEE is considered to be a pragmatic approach, facilitating the combination of independent indicators expressed in different units (Prado & Heijungs, 2018).

The aim of chapter 5 is to develop a decision-making method that integrates environmental, social, and economic sustainability indicators with different units, taking into account stochastic and flexible methodological choices. In the next section, a stochastic, hierarchical outranking approach for sustainable decision-making is proposed. With this method, a comparison between different scenarios can be structured and more sustainable choices on e.g. technologies and feedstocks can be made, when technologies are still under development. Later in this chapter, the developed MCDA method is applied to the case study initiated in chapter 4, in which microalgae feedstock were used to produce biobased chemicals. Different preference structures and weighting schemes are compared that could take into account prior knowledge of microalgae experts on a prioritization of sustainability indicators.

2. Method

Previous studies have used uncertainty analysis within integrated sustainability assessment to reflect variations in indicator results (Byun & Han, 2020). Uncertainty and sensitivity analyses were already included within the TSA framework in Step 5 (see chapter 4). Inherent uncertainty about the product system reflects the data uncertainty in early development stages (Blanco et al., 2020). Uncertainty analysis could also provide input for further indicator integration. The decision-making model developed in this chapter starts by performing Monte Carlo simulations on TSA indicator results to take into account performance uncertainty (Step 5 of TSA). Next, a multi-level approach is followed consisting of two levels to aid decision-making (Step 6 of TSA). At Level 1, SMAA is performed within the individual sustainability dimensions. At Level 2, an overarching sustainability result is calculated. This multi-level approach allows decision makers to zoom in on the underlying dimensions at the same time as having an integrated result (Bann et al., 2017).

On the first level, three separate SMAAs are performed to calculate individual sustainability scores (that is, an environmental, economic, and social SMAA) with corresponding rankings of the scenarios. Pairwise differences between the scenarios are calculated, preference structures and weights are defined, and the relative performance of a scenario is measured within each sustainability domain. The resulting scores and rankings from the SMAA show how a particular scenario is performing compared to the other scenarios within a sustainability dimension.

On the second level, the results of the first-level SMAAs are used as input values for final integration. Pairwise distances are calculated again with appropriate thresholds and weighting schemes. The result of the second-level SMAA is an integrated sustainability score and ranking for each alternative scenario. A more detailed schematic overview of the full hierarchical MCDA method is shown in

Figure 20. The main features of this MCDA method are explained in the following subsections.

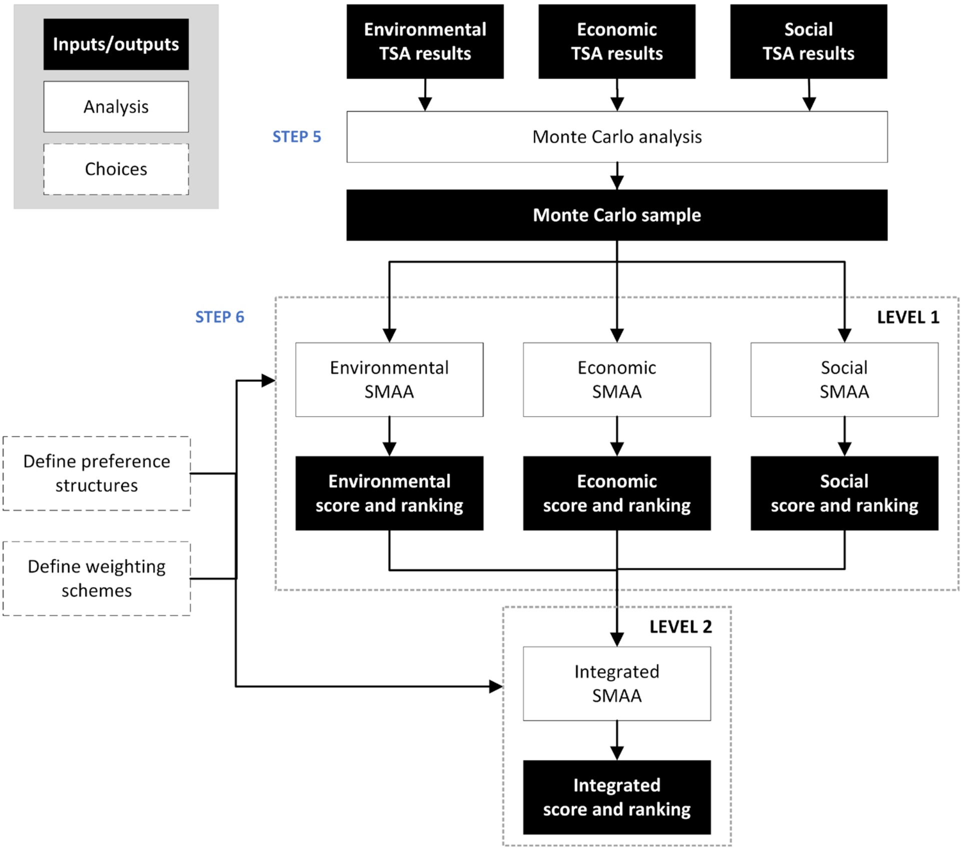

Figure 20. A hierarchical, stochastic outranking approach for decision-making. SMAA = stochastic multi-attribute analysis, and TSA = techno-sustainability assessment.

2.1 Stochastic input parameters

A large variety of input data are collected and used in the TSA framework to calculate the sustainability indicators as was presented in chapter 4. Examples of these data include growth rates of biobased feedstocks, energy requirements of specified technologies, or price data of raw materials and equipment. Stochasticity within this data can be included by repeated random sampling of a set of input parameter values. A selection of input parameters is based on two criteria: (1) data uncertainty and (2) contribution to the sensitivity of the sustainability indicator. When performing a sustainability assessment of emerging technologies, the data used often stem from lab analyses, computer models, or the available literature. A number of parameters might be estimated with a high level of uncertainty or large data ranges might be found in literature. The uncertainty of the output indicators can be assigned to these stochastic input parameters. Sensitivity analysis can check which input parameters are driving the variation of the indicator results (Wender, Prado, Fantke, Ravikumar, & Seager, 2018). The input parameters with the highest uncertainty and largest contribution to the variation of the indicators are selected for a Monte Carlo simulation. The Monte Carlo simulation creates a data sample in which sustainability indicators are calculated multiple times for the different alternatives. The selected input data are varied according to a defined distribution and data range, depending on the case. The minimum amount of iterations for the Monte Carlo simulation can be determined by monitoring the accuracy for 1 percent precision at 95 percent confidence for the means and standard deviations of the simulation.

2.2 Preference structures

After a Monte Carlo sample is computed, pairwise distances *d* are calculated within every Monte Carlo iteration *r* between the indicator results *IR* of indicator *h* for the scenarios *i* and *j* (Equation (5)).

$$d_{hijr} = IR_{hir} - IR_{hjr} \quad (h = 1, \dots, m\,; i, j = 1, \dots, n\,; r = 1, \dots, R) \tag{5}$$

Thresholds need to be selected which reflect the preference structure used to assign a score based on the length of the pairwise distance. Internal normalization is performed by evaluating the pairwise distances against pseudo-criteria: a preference threshold (P) and an indifference threshold (Q) (Prado-lopez et al., 2014). The use of thresholds could reduce the degree of compensation between sustainability indicators and dimensions, protecting the decision-model against extremes that might compensate for other indicator performances (Cinelli, Coles, & Kirwan, 2014; Prado & Heijungs, 2018). The use of thresholds restricts the enforcement of a weak sustainability view, including full compensation, but partial compensation will still be present (Cinelli et al., 2014). Xu (2001) summarized six possible thresholds commonly used in outranking MCDAs, ranging from simplelevel criteria to linear or gaussian preference functions (Xu, 2001). The chosen thresholds should match the data and be case-specific. Based on these thresholds, an outranking score *S* is assigned, reflecting the magnitude of the pairwise distance *d*. Table 19 gives an overview of three types of preference structures further used in the decision-making model. When working with ranking data, one can decide to choose thresholds such as true or level criteria. When working with ratio data, a more advanced preference structure uses linear preference *P* and indifference *Q* thresholds, which can be based on the average standard deviations SD_{hi} of the selected sustainability indicators. Equations (6) and (7) show how *P* and *Q* can be calculated for the latter preference structure.

Table 19. A selection of preference structures (Xu, 2001). *S* = outranking score, *d* = distance, *p* = preference, and *q* = indifference.

Type 1 True criterion	Type 4 Level criterion	Type 5 Linear preference and indifference criterion
$S = \begin{cases} 1 & if\ d > 0 \\ 0 & if\ d \leq 0 \end{cases}$	$S = \begin{cases} 1 & if\ d > p \\ 0.5 & if\ q < d \leq p \\ 0 & if\ d \leq q \end{cases}$	$S = \begin{cases} 1 & if\ d > p \\ \frac{(d-q)}{(p-q)} & if\ q < d \leq p \\ 0 & if\ d \leq q \end{cases}$

$$P_h = \frac{1}{n}\sum_{i=1}^{n} SD_{hi} \quad (h = 1, \dots, m) \tag{6}$$

$$Q_h = \frac{1}{2}P_h \quad (h = 1, \dots, m) \tag{7}$$

In addition, it is important to derive whether an indicator needs to be maximized or minimized in order to increase sustainability. For example, within a sustainability analysis, human toxicity is preferred to be as low as possible, while an indicator related to job creation or profit is preferably as high as possible. The preference structures can be adapted accordingly by making the thresholds negative when the indicators need to be minimized.

Within every iteration *r*, the next step is to calculate the net flows *F* based on the outranking scores *S* (Equation (8)).

$$F_{hir} = \sum_{\substack{j=1 \\ j \neq i}}^{n} (S_{hijr} - S_{hjir}) \quad (h = 1, \dots, m\,; j = 1, \dots, n\,; r = 1, \dots, R) \tag{8}$$

2.3 Weighting

Weighting includes the process of aggregating indicator results by using numerical factors based on value choices (ISO 14044 2006) (ISO, 2006). The allocation of weights is a complex and subjective process. Different weighting schemes are considered within the developed SMAA models and compared to check for the robustness of the results. Based on previous literature, four different weighting schemes can be applied: stochastic random weights (SRW), equal weights (EW), rank-order centroid weights (ROCW), and rank exponent weights (REW) (Prado & Heijungs, 2018; Roszkowska, 2013).

The use of EW and SRW can imply that the preference between indicators is unknown to the stakeholders. The use of EW makes the assumption that each indicator is as important as the other. The use of SRW explores stochastic weight spaces rather than point values to include a wide variety of possible values (Prado-lopez et al., 2014). For the ROCW and REW methods, case-specific stakeholder preference information can be applied. An example of such an information source is the Delphi ranking of sustainability indicators for biobased chemicals developed in chapter 3. Existing indicator prioritizations can be converted into numerical weights and used in MCDA models (Equations (9) and (10)). ROCW reflect the centroid of the simplex defined by the ranking of indicators (Roszkowska, 2013). REW take different parameters into account to consider different steepness in the weights (Roszkowska, 2013). The parameter ρ describes the exponents used in the REW scheme. In the SMAA models, the exponents can be randomized to be compatible with the Monte Carlo iterations in the SMAA flow results. When the exponent is zero, equal weights are derived. When the exponent equals 1, linear rank sum weights are encountered. If $0 < \rho < 1$, weight distribution tends to be relatively flat. If $\rho > 1$, the distribution of weights is steep, and relatively more weight is given to the indicators ranked first. The selection of this parameter ρ could be based on the degree of consensus on the indicators between experts, or by asking for stakeholder opinions on these weight distributions. Figure 21 provides an example of how weights can change depending on different exponents.

$$REW_h = \frac{(m-rank_h+1)^{\rho}}{\sum_{k=1}^{m}(m-rank_k+1)^{\rho}} \qquad (h = 1,2,\dots,m) \tag{9}$$

$$ROCW_h = \frac{1}{m}\sum_{k=h}^{m}\frac{1}{Rank_k} \qquad (h = 1,2,\dots,m) \tag{10}$$

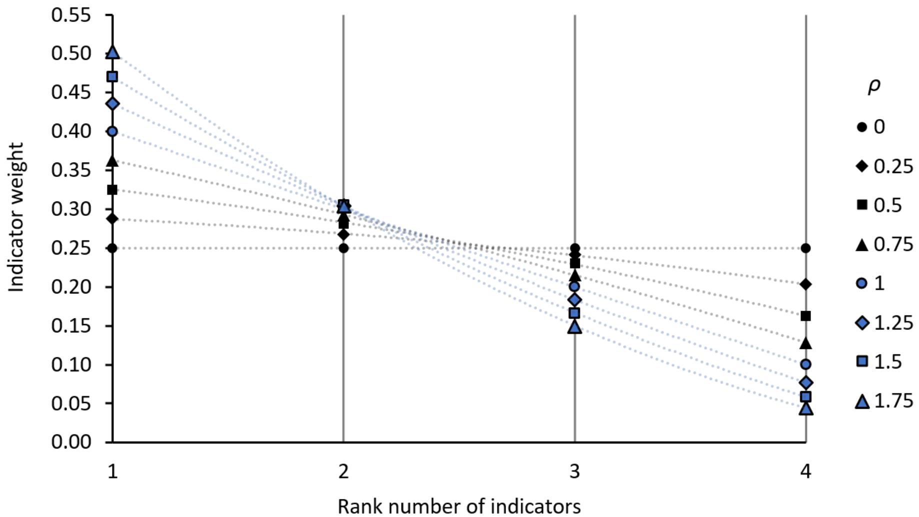

Figure 21. Example of REW used in SMAA models with four indicators. ρ = exponent, blue = steep distribution, and black = flat distribution.

The chosen weight distribution *w* is multiplied by the net flows *F* to calculate the final score *FS* per iteration *r* (Equation (11)). A corresponding ranking or average score can then be derived to make a final comparison between the assessed scenarios.

$$FS_{ir} = \sum_{h=1}^{m} w_{ir} \times F_{hir} \quad (h = 1,\dots,m\,; r = 1,\dots,R) \tag{11}$$

2.4 Final integration

The MCDA results per sustainability dimension can still provide conflicting rankings. A final integration is proposed to make decisions based on one integrated score or ranking. The output, given by Equation (11), from the individual social, environmental, and economic SMAA models at Level 1, is used to formulate a decision matrix with multiple scenarios and different sustainability dimensions for the integrated SMAA at Level 2. In other words, the same SMAA steps are followed, but the indicator results *IR* are now represented by the score (or ranking) results from the individual sustainability dimensions. The use of SMAA to integrate the results in one ranking can provide a way for practitioners to select preferred and less favorable scenarios based on a full sustainability analysis. When a variety of scenarios are compared, MCDA can narrow down the choices, and exclude the most unsustainable scenarios. However, the integration of data also leads to information loss and is highly dependent on stakeholders' views and goals. Decision makers could increase transparency by disclosing all methodological information and the separate rankings within the three sustainability dimensions. Decisions cannot be made without first observing the underlying reasons for a specified sustainability performance.

3. Results

3.1 Case description

The decision-making analysis developed in this chapter is applied to a microalgae case study, the details of which have been described in chapter 4. This case was built to illustrate the integrated TSA methodology. Four possible scenarios (SC1-SC4) were identified based on different microalgae and cultivation systems. The microalgae are used as feedstock for the production of red food colorants. The *Porphyridium* algae is cultivated, harvested, and further processed to extract phycoerythrin. The *Dunaliella salina* algae is cultivated, harvested, and further processed to extract β-carotene. Both algae types can be grown in a horizontal photobioreactor (PBR) or open raceway pond (OP). For the present case study, focus remains on the cultivation and harvesting step. The downstream process was not considered due to the lack of data. To assess the relative sustainability performance of these scenarios, relevant environmental, economic, and social data were collected and sustainability indicators were quantified accordingly. Table 20 shows data sources which were used for the sustainability analysis in chapter 4.

Table 20. Data sources used in TSA. *Global Reporting Initiative; **Organisation for Economic Co-operation and Development; ***International Labour Organization.

	Data sources
Environmental data	Ecoinvent 3.5 database and scientific literature
Economic data	Company quotations, country reports, and scientific literature
Social data	GRI*, OECD**, ILO***, EUROSTAT reports and databases, and scientific literature

In the second step of the TSA framework, relevant sustainability indicators were selected by combining the initial Delphi rankings (described in chapter 3) and an additional microalgae-specific survey (described in chapter 4). Some indicators are excluded because they are not quantifiable at low TRL or they score the same for all scenarios, which is redundant in a comparative analysis. As was explained in the previous chapter, the 'market potential' indicator depends solely on price data. To avoid double counting, this indicator was excluded from the MCDA. Other indicators, such as capital productivity, already involve using prices by calculating sales. Furthermore, some indicators were already aggregated, such as ecotoxicity potential (ETP), eutrophication potential (EP), and human toxicity potential (HTP). Using the ReCiPe indicator quantifications in chapter 4, freshwater-, marine-, and terrestrial ecotoxicity, freshwater- and marine eutrophication, and cancer and non-cancer human toxicity potential were measured. In order to include ETP, EP and HTP as separate environmental and social indicators in the SMAA, aggregation was done beforehand by first integrating the separate ReCiPe indicators. For the final decision analysis, seventeen sustainability indicators were selected. Figure 22 shows a summary of the eight environmental, six economic, and three social indicators used in the outranking models.

3.2 Decision-making analysis

Consequently, a Monte Carlo simulation was performed by varying the input parameters used for the quantification of the sustainability indicators. The selected stochastic parameters are presented in Table 21 with their corresponding distributions and ranges. Uniform, discrete or Beta PERT distributions were assumed. (Discrete) uniform distributions are applied to input data where values are equally likely to occur, and beta PERT distributions are used when a three-point estimation technique is advisable and minimum, maximum, and most likely values are known (Bann et al., 2017). The minimum and maximum values were retrieved from literature and suppliers. The distribution and ranges from the most sensitive parameters should be determined as accurately as possible. When the former data is lacking, the approach of Brun et al. (2002) was adopted where a choice could be made from three classes of relative uncertainty: "accurately known parameters (class 1: relative uncertainty 5 percent), moderately inaccurate known parameters (class 2: relative uncertainty 20 percent) and very poorly known parameters (class 3: relative uncertainty 50 percent)" (Brun, Kühni, Siegrist, Gujer, & Reichert, 2002). It took 43,300 Monte Carlo iterations to reach a sample where the true means and standard deviations of the indicators did not deviate by more than 1 percent from the simulated statistics (Appendix D1). These 43,300 trial values were used in the SMAA models to calculate the pairwise distances, thresholds, outranking scores, net flows, and final scores and rankings. The stochastic outranking model was developed using Python 3.7.4. The pseudocode is attached in Appendix D2 and can be used for other case studies as well.

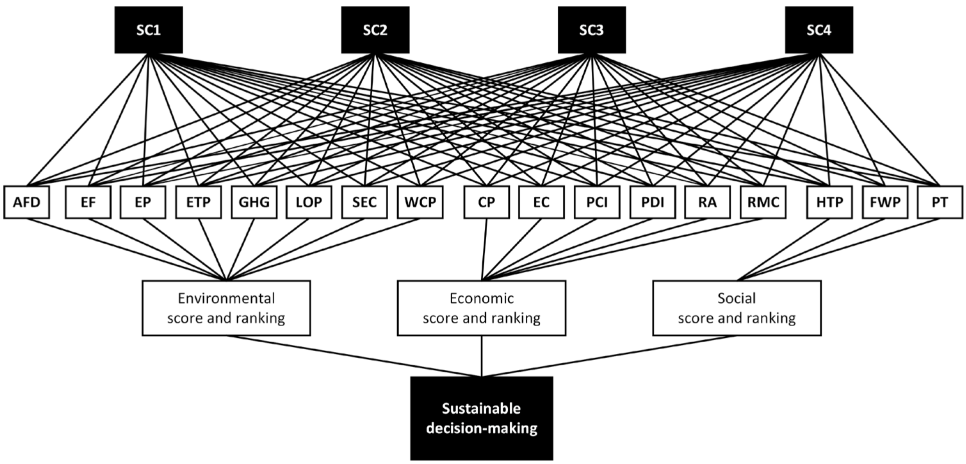

Figure 22*.* Sustainable decision-making: an integration of environmental, economic, and social indicators to assess different microalgae systems. SC = scenario, AFD = abiotic fossil depletion, CP = capital productivity, EC = energy cost, EF = E=factor, FEP/MEP = freshwater/marine eutrophication potential, FETP/METP/TETP= freshwater/terrestrial/marine ecotoxicity potential, FWP = fair wage potential, GHG = greenhouse gas emissions, HTP c/nc = human toxicity potential cancer/non-cancer, LUP = land use potential, PCI = process innovation, PDI = product innovation, PT = product transparency, RA = risk aspects, RMC = raw materials cost, SEC = specific energy consumption, and WCP = water consumption potential.

Table 21. Stochastic input parameters – Monte Carlo variables and distributions. PBR = photobioreactor, and OP = open pond.

Parameter[*]	**Unit**	**Deterministic TSA value**	**Distribution**	**Range**	**Source(s) for ranges**
Recycled water[a]	%	90%	Uniform	[72%; 99%]	20%[e]
Recycled salt[a]	%	90%	Uniform	[72%; 99%]	20%[e]
Growth rate					
• Scenario 1	$g.L^{-1}.day^{-1}$	0.25	Beta PERT	[0.12; 0.37]	50%[e]
• Scenario 2	$g.L^{-1}.day^{-1}$	0.08	Beta PERT	[0.04; 0.12]	50%[e]
• Scenario 3	$g.L^{-1}.day^{-1}$	0.20	Beta PERT	[0.10; 0.30]	50%[e]
• Scenario 4	$g.L^{-1}.day^{-1}$	0.01	Beta PERT	[0.007; 0.02]	50%[e]
Phycoerythrin content	%	0.02	Beta PERT	[0.01; 0.036]	[f] and supplier info
β-carotene content	%	0.05	Beta PERT	[0.03; 0.078]	[g]
PBR cost cte	$€.m^2$	15,237	Beta PERT	[12,190; 18,284]	20%[e]
Phycoerythrin price[b]	$€.kg^{-1}$	36,000	Uniform	[36,000; 18,000]	[h] and -50%[e]
β-carotene price	$€.kg^{-1}$	1183	Uniform	[215; 2,150]	[i]
Electricity LUP eq. Belgium	$impact.kWh^{-1}$	0.02	Beta PERT	[0.011; 0.033]	50%[e]
Sustainability reports France[c]	#	13.00	Discrete uniform	[13; 20]	50%[e]
Sustainability reports Belgium[c]	#	6.00	Discrete uniform	[6; 9]	50%[e]
Real working time Belgium	$h.week^{-1}$	41.00	Beta PERT	[32.8; 49.2]	20%[e]
Real working time France	$h.week^{-1}$	40.40	Beta PERT	[32.32; 48.48]	20%[e]
Real average wage Belgium	$\$.year^{-1}$	52,080	Uniform	[41,664; 62,496]	20%[e]
Real average wage France	$\$.year^{-1}$	44,510	Uniform	[35,608; 53,412]	20%[e]
Patent count PBR[d]	#	431	Discrete uniform	[431; 517]	20%[e]
Patent count OP[d]	#	1,440	Discrete uniform	[1,440; 1,728]	20%[e]
Patent count phycoerythrin[d]	#	16	Discrete uniform	[16; 19]	20%[e]
Patent count β-carotene[d]	#	22	Discrete uniform	[22; 26]	20%[e]
Electricity price Belgium	$€.MWh^{-1}$	138.80	Beta PERT	[129.7; 139.8]	Eurostat data, min and max last 5 years

[*]No correlation is assumed between the parameters.

[a]It is assumed that recycling can never reach an efficiency of 100 percent; [b]It is assumed that the price of phycoerythrin as a food colorant will converge closer to the β-carotene price as soon as phycoerythrin will be sold on the food market; [c]The GRI database only includes reports that GRI is aware of, which could lead to an underestimation; [d]Some technological advances are not patentable or have other methods of protecting their technologies, which could lead to an underestimation (Coombs et al., 1996); [e](Brun et al., 2002); [f](Guihéneuf & Stengel, 2015); [g](García-González et al., 2003; Prieto et al., 2011); [h](Hu, 2019); [i](Cuellar-Bermudez et al., 2015).

Once it has decided which indicators need to be maximized or minimized, thresholds and weights were defined to fit the case. Concerning the preference structure, Type 5 “linear preference and indifference thresholds” were applied when integrating towards the individual sustainability dimensions on Level 1. The resulting outranking score *S* has a corresponding non-linear preference structure and full compensation is avoided between the indicators. Concerning the weighting schemes, the ETP, EP, and HTP indicators were calculated first using equal weighting (EW). Their final scores per scenario were included as input data for the environmental and social SMAA. At Level 1, four different weighting options were compared. ROCW and REW are based on prior ranking information about the preferences of stakeholders. As prior information is available based on the expert surveys performed in chapter 3 and 4, three different weighting options based on expert rankings were compared: (1) ROCW, (2) flat REW with $0 < \rho < 1$, and (3) steep REW with $1 < \rho < 2$. Ranking information on the prioritization of indicators is provided in Table 22. An additional fourth weighting option is added applying (4) SRW, to enable comparison with an option where no prior stakeholder information would be available.

Table 22. A priori indicator ranking (based on results chapter 4).

Environmental	Economic	Social
1. GHG emissions (GHG)	1. Raw materials cost (RMC)	1. Transparency (PT)
2. Waste generation (EF)	2. Process innovation (PCI)	2. Human toxicity (HTP)
3. Ecotoxicity (ETP)	3. Product innovation (PDI)	3. Income Levels (FWP)
4. Energy efficiency (SEC)	4. Technical risks (RA)	
5. Land use (LUP)	5. Capital productivity (CP)	
6. Abiotic fossil depletion (AFD)	6. Energy cost (EC)	
7. Eutrophication (EP)		
8. Water consumption (WCP)		

The Level 1 SMAA models resulted in scores and rankings per iteration. The average scores per weighting scheme are provided in Appendix D3. Table 23 presents the ranking results for the separate environmental, economic, and social SMAAs using four different weighting options. These summarizing ranking results show the percentage of time a certain scenario is ranked at a specific ranking position, with rank 1 being the best alternative with the lowest environmental impact and highest economic and social scores. Scenario 3, growing *Dunaliella salina* in a PBR in France, scored best out of all scenarios in the environmental and economic dimensions, but worse in terms of its social sustainability. Scenario 4, cultivating the *Dunaliella salina* in an OP in France, had the worst environmental and social performance. The *Porphyridium* scenario cultivating algae in an OP in Belgium (Scenario 2) had better economic and social results than the Belgian PBR scenario (Scenario 1). Socially, both *Porphyridium* scenarios have an advantage due to location factors in Belgium compared to France, where the *Dunaliella* is cultivated. The separate social indicators 'transparency' and 'income levels' were both measured by proxies and future research should elaborate on these quantifications to check their validity. Human toxicity, on the other hand, is already used widely in (social) LCAs and has a remarkably negative score for Scenario 4. The assessment of the environmental sustainability is relatively similar for both Belgian scenarios cultivating *Porphyridium*. The environmental results are visualized in Appendix D4, comparing different weighting schemes. The underlying reasons for the SMAA scores and rankings can be derived from the individual indicator and sensitivity results presented in chapter 4.

As an input for the second level SMAA, the reversed ranking results from the individual models were used (i.e., the environmental, economic, and social SMAAs). The choice of using rankings stems from the idea that the results of three different SMAA models become mathematically comparable and that the robustness of the final SMAA aggregation increases, in addition to the improved interpretability of the results. As ranking data is now used instead of absolute values, different preference structures are appropriate. Both the true- and the level criterion (Type 1 and Type 4) are applied and compared within the final integration level of the MCDA model (Table 19). The 43,300 results per scenario, per sustainability dimension under the flat REW scheme are used as input for the final integration. One could choose to allocate specific weights to the sustainability dimensions depending on the goal of the assessment. For the microalgae case study, random and equal weights (ROW and EW) were used, considering the complexity of assigning weights to the individual sustainability domains. A total of 43,300 different iterations were executed for three different preference structures and two weighting schemes. Table 24 presents the percentage of times a scenario is ranked in a defined position. The average scores per weighting scheme and preference structure are provided in Appendix D5.

Table 23. SMAA ranking results per weighting scheme at Level 1 (in %) – showing the percentage of times a scenario is ranked at a specific ranking position. Rank 1 being the best alternative with the highest sustainability score. SC = scenario, SRW = stochastic random weights, ROCW = rank-order centroid weights, and REW = rank exponent weights.

		ROCW				REW flat				REW steep				SRW			
		SC1	**SC2**	**SC3**	**SC4**	**SC1**	**SC2**	**SC3**	**SC4**	**SC1**	**SC2**	**SC3**	**SC4**	**SC1**	**SC2**	**SC3**	**SC4**
		Environmental															
Rank position	1	3.64	2.27	94.08	0	2.88	4.45	92.66	0	3.68	3.33	92.99	0	2.64	6.45	90.91	0
	2	53.06	41.82	5.10	0.02	41.65	52.26	5.98	0.12	50.93	43.31	5.75	0.02	34.63	57.39	7.49	0.48
	3	43.21	54.53	0.82	1.45	54.94	41.63	1.36	2.07	45.30	52.01	1.26	1.43	58.93	34.35	1.56	5.15
	4	0.09	1.38	0	98.53	0.52	1.66	0.00	97.82	0.09	1.36	0	98.55	3.79	1.81	0.04	94.36
		Economic															
Rank position	1	0.35	2.05	97.36	0.24	0	9.78	82.31	7.91	0	2.13	94.55	3.31	0.09	38.11	41.89	19.92
	2	8.31	63.81	2.27	25.60	0	39.16	14.59	46.25	0.13	23.97	4.90	70.99	1.78	29.67	35.83	32.73
	3	19.94	19.62	0.30	60.14	0.42	50.71	3.03	45.85	7.25	66.67	0.38	25.70	11.31	30.52	21.43	36.74
	4	71.39	14.52	0.07	14.02	99.58	0.35	0.07	0	92.61	7.22	0.17	0	86.83	1.71	0.85	10.62
		Social															
Rank position	1	7.12	89.52	0	0.00	7.12	89.52	0	0	7.12	89.52	0	0	6.90	88.24	1.72	0.00
	2	92.88	10.48	0	0.00	92.73	10.48	0.15	0	92.88	10.48	0	0	80.70	10.70	11.48	0.04
	3	0	0	99.11	0.65	0.15	0	98.96	0.65	0	0	99.11	0.65	12.14	1.04	85.93	0.89
	4	0	0	0.89	99.35	0	0	0.89	99.35	0	0	0.89	99.35	0.27	0.02	0.88	99.07

Table 24. Integrated SMAA ranking results at Level 2 (in %) – showing the percentage of times a scenario is ranked at a specific ranking position. Rank 1 being the best alternative with the highest sustainability score. SC = scenario, SRW = stochastic random weights, EW = equal weights, p = preference, and q = indifference.

		SC1	SC2	SC3	SC4	SC1	SC2	SC3	SC4	SC1	SC2	SC3	SC4
		EW, TYPE 1				**EW, TYPE 2 (*p*=1, *q*=0)**				**EW, TYPE 2 (*p*=2, *q*=1)**			
Rank position	1	0.93	14.62	87.48	0.03	1.14	40.35	61.77	0.01	0.88	14.53	87.61	0.03
	2	6.99	79.35	10.84	0.89	11.14	50.51	36.38	0.33	6.94	79.45	10.75	0.92
	3	90.85	5.38	1.32	4.18	87.00	8.48	1.39	4.78	90.82	5.37	1.28	4.23
	4	1.24	0.65	0.36	94.90	0.72	0.67	0.46	94.88	1.36	0.66	0.36	94.81
		SRW, TYPE 1				**SRW, TYPE 2 (*p*=1, *q*=0)**				**SRW, TYPE 2 (*p*=2, *q*=1)**			
Rank position	1	2.52	37.04	59.95	0.49	3.56	40.10	55.89	0.44	2.06	33.38	63.95	0.62
	2	14.51	48.44	33.30	3.75	20.00	40.17	35.03	4.79	9.93	56.01	31.42	2.63
	3	66.75	13.55	6.28	13.41	61.21	17.68	8.46	12.66	71.25	9.70	4.24	14.80
	4	16.22	0.97	0.46	82.35	15.23	2.05	0.61	82.11	16.76	0.91	0.39	81.95

Scenario 3, defined as the *Dunaliella salina* algae cultivated in the horizontal PBR in France, is considered the most sustainable scenario relative to the alternative scenarios, with a 55.89 percent to 87.61 percent probability of being ranked first. Scenario 4, where the *Dunaliella salina* algae is cultivated in an OP in France, has the highest chance of being ranked as the least sustainable alternative, with a 81.95 percent to 94.9 percent chance of being ranked last. These overall results are compliant with the counting analysis performed in chapter 4. However, the results of the SMAA models consider the input uncertainties and different weighting and preference distributions which increase the validity of the model and the robustness of the results. For a detailed interpretation of the SMAA results, the sensitivity analysis performed in chapter 4 should again be consulted. The included sustainability indicators are highly influenced by the pigment content, the algae growth rate, and the recycled salt ratio. The algae growth and pigment content influence the productivity and final pigment output of the system. The mass and energy results in chapter 4 already showed that Scenario 3 produced the highest amount of pigments (Table 10, chapter 4). The data on these growth and pigment ratios from the literature have a large variability in parameter values. The SMAA models' stochasticity partially accounts for these uncertainties at low TRL, given the assumptions made on parameter values and distributions. Scenario 2, cultivating the *Porphyridium* in an open raceway pond in Belgium, is the second most sustainable scenario. Using the stochastic random weighting scheme might push Scenario 2 towards the first ranking position, compared to the use of equal weights. More phycoerythrin is produced in the OP compared to the PBR, which is due to the high volume per land for the OP and the estimated growth when comparing both cultivation options. These results show that the interaction between an algae cultivation type and algae variety plays an essential role in its corresponding sustainability. Overall, it can be concluded that Scenarios 2 and 3 are in all cases superior to Scenarios 1 and 4 on their integrated relative sustainability.

4. Discussion

The stochastic MCDA approach assesses in a hierarchical way the relative sustainability of different scenarios with the aim of advising and guiding decision makers. In chapter 4 of this dissertation, different sustainability indicators were quantified and a sensitivity analysis showed which input parameters had a significant influence on these separate sustainability impacts. However, this list of indicators can get too large to make rational comparisons and decisions between alternative scenarios. A counting analysis gave some first impressions on the final interpretation in chapter 4, but the magnitude of the differences on the indicators between the scenarios was not taken into account. In addition, performance uncertainty of (emerging) technologies was not considered within the individual indicator results, neither in the counting analysis. For that reason, chapter 5 provides a solution which integrates the independent indicators by applying a stochastic MCDA and providing a variety of methodological options concerning thresholds for preference structures and weighting schemes.

4.1 Integrated assessment

One of the core challenges within sustainability assessment is to properly integrate. The novel integrated TSA framework, developed in chapters 4 and 5, allows for three types of 'integration': merging different categories of impacts (horizontal integration), linking separate assessments undertaken at different stages in the value chain (vertical integration), and integrating assessments into decision-making (Hacking & Guthrie, 2008; N. Lee, 2002).

In Step 4 of the framework, one can horizontally integrate by including economic, social, and environmental sustainability impact categories. Wherever possible, these sustainability impacts are linked with the technological and country-specific parameters.

Vertical integration happens along the value chain (that is, the life cycle). When life cycle inventory data for the environmental impacts (such as GWP and ETP) are used, upstream impacts are taken into account. For the microalgae case, the focus remained on integrating the cultivation and harvesting processes, supplemented with end-product information. It can be necessary to leave out certain processes at first, but to add information when moving to a higher TRL. These decision should be made in the first TSA step where goal and scope are defined. The feedback loop that returns from Step 6 to Step 1, provides the opportunity to repeat and adjust based on new information, when moving along the TRL scale.

A final type of integration is the conversion of the separate sustainability indicators into decision-making results. Therefore, the TSA framework offers a sixth, MCDA step that integrates sustainability indicators and dimensions. An outranking approach allows the decision maker to discard those categories in which the alternative scenarios are deemed equivalent and focus attention on critical differences. By using pairwise judgements as an evaluation approach, semi-quantitative and qualitative ordinal data could be incorporated into the SMAA (Prado-lopez et al., 2014). This is especially interesting for social impact categories that are difficult to quantify.

4.2 Robustness check

The entire decision-making analysis developed in this chapter was applied to the microalgae case for which algae pigments are produced for food colorants. The robustness of the integrated TSA results can be evaluated by comparing multiple thresholds and weights in the MCDA method. Overall, the average microalgae scenario rankings provided similar results when different methodological choices were applied. However, rank reversal occurs in some specific cases. Within the economic dimension, for example, the preference of Scenario 4 over Scenario 2 changes when different weighting schemes are involved. When a steeper weight distribution is applied, relatively more weight was given to the economic indicators ranked first, which score better on Scenario 4 than on Scenario 2. However, because the magnitude of the differences between Scenarios 2 and 4 on the lower-ranked indicators (that is, capital productivity and energy cost) was relatively high, they switched ranking position when weights were distributed more equally, such as when using SRW. This is also shown by the average SMAA scores in Appendix D3. It is up to the decision maker to choose the most appropriate weighting scheme depending on prior information on the values of stakeholders and availability of this stakeholder information.

For the microalgae case assessed in this dissertation, the ranking of scenarios appeared to be robust. However, for other cases considering different biobased feedstocks, technologies, and end-products, the SMAA results might be conflicting and highly dependent on weights and chosen thresholds. This should warn the decision maker that the relative sustainability of an alternative scenario is unsure and dependent on methodological choices. In such cases, more information on weights and preference structures should be gathered to refine the model. The inclusion of data uncertainty and large data ranges for the Monte Carlo analysis can also lead to ambiguity in the final SMAA results, meaning that no clear 'winner' or 'loser' can be identified. Inconclusive results should stimulate decision makers to gather more data, perform additional lab- or pilot tests, and consult experts again on the scenario development, indicator selection and quantification, and data inventory and uncertainty.

4.3 Limitations

Creating an integrated sustainability result to compare alternative scenarios has an important limitation concerning transparency. Communicating a final sustainability ranking of scenarios lacks clarity on the underlying sustainability dimensions, indicators, and input parameters. For a comprehensive interpretation, decision makers should refer to the individual sustainability indicators and the corresponding sensitivity analysis resulting from previous TSA steps. A second limitation concerns the non-exhaustive list of preference structures and weighting schemes provided in this chapter. More methodological options exist and other thresholds and weights might fit the case-specific decision models. For that reason, they are illustrated as a "choice" in Figure 20 to represent the variety of options that a decision maker can encounter. Third, the microalgae case study used to illustrate the decision-making analysis included no data on the downstream process. It is important to note that all the steps of the value chain should be included to provide a full picture of its sustainability. After harvesting, different chemical extraction steps can be included to extract the pigments. The use of extraction technologies depends on many algae- and technology-specific characteristics, such as the density of the algae broth leaving the centrifuge. The conclusions regarding the sustainability performance for the microalgae scenarios in this chapter are only applicable to the cultivation and harvesting technologies within the value chain. Finally, a full value chain analysis would include multiple biorefinery outputs. Consequently, sustainability impacts should be allocated using physical or economic proportions, as is common practice within LCSA (Valdivia et al., 2013).

It is stressed that the SMAA follows a 'bottom-up' approach where the most and least sustainable scenarios can be selected based on technological, economic, environmental, and social data. Future research should integrate a top-down feedback loop where this data can be optimized and target output values could be determined which would optimize the sustainability of the alternative scenarios. A common approach to execute this is multi-objective optimization (MOO). Past research already developed a MOO for an optimization towards both economic and environmental objectives (Thomassen, Van Dael, You, & Van Passel, 2019). This could be extended with social objectives to be compatible with the integrated TSA framework.

5. Conclusion

This chapter discusses the final step (i.e., Step 6) of the integrated techno-sustainability assessment (TSA) framework for technology evaluation, which was first proposed in chapter 4. A hierarchical, stochastic outranking approach for sustainable decision-making is developed combining TSA and MCDA. The MCDA method combines four major strengths: (i) the use of stochastic input data based on real data ranges and distributions, the inclusion of multiple (ii) preference structures and (iii) weighting schemes according to (a variety of) stakeholder values, and (iv) a multi-level perspective providing results within the separate sustainability dimensions as well as an integrated outranking result for sustainable decision-making. A variety of methodological choices takes into account case-specific characteristics such as stakeholder preferences and different data types and ranges of indicators. The robustness of the models can be checked by comparing different methodological options. When the weighting schemes are combined with the outranking net flows, scores and ranking results can be estimated and trade-offs are made. It is essential to remain transparent about the methodological choices incorporated in the model when communicating decisions based on MCDA. The MCDA pseudocode provided in Appendix D2 is compatible with the Monte Carlo sample. If additional input is added or existing input values are adjusted as a result of new available data and technology development, the sustainability indicators and MCDA decision output change accordingly. This makes the entire integrated TSA framework iterative and dynamic.

The process of determining weights and choosing thresholds for benchmarking remains subjective. Different sustainability impacts might be more or less relevant depending on the scope of the assessment and decision makers' preferences. The indicator ranking for biobased chemicals developed in chapter 3 is confirmed by experts to be valid for the microalgae case. Future research should gather more stakeholder preference data for different products and technologies in order to further validate the indicator ranking for an accepted selection of weights. In addition, expert data could be gathered on the second level of the decision-making framework by questioning stakeholders on their view towards sustainability and the relative importance of the individual sustainability domains.

Chapter 5 concludes the development of the integrated TSA framework by providing an integrated method for sustainable decision-making applied to a biobased chemical case study using microalgae as feedstock. The results provide the decision maker with extensive knowledge on the relative sustainability of these technologies and the ability to make better-informed choices. The proposed MCDA method can be used to direct further technology-development as TRLs progress. For the case study assessed in this study, the results show that stimulating algae growth leads to productivity gains, positively affecting the overall sustainability. Moreover, company management choices such as the degree of recycling and the level of transparency can influence the relative sustainability performance. In general, TSA provides a framework for companies and scientists to assess different technologies and the value chains they are part of. The integrated TSA could steer investment decisions towards the most sustainable option, given the methodological assumptions made. Policy makers can use the integrated TSA to support sustainability within R&D and guide technologies along the TRL scale.

CHAPTER 6

Conclusion

1. Introduction

Many chemicals are hazardous to the environment and human health (Goldenman et al., 2017). To reduce these negative impacts, green chemistry was introduced which can be translated into the production of biobased chemicals. New or improved industrial processes are being built to convert biomass into a variety of chemical products. However, the use of biobased feestocks does not necessarily imply that these chemicals are safer for the environment, human health, or have any other sustainability gains compared to their alternatives. For that reason, sustainability impacts should be measured and monitored, preferably already during the research and development phase of new biobased technologies. This dissertation covers the development of an integrated techno-sustainability assessment framework to better understand emerging (biobased) technologies and products' potential sustainability. In the introductory chapter (i.e., chapter 1), four major research questions (RQs) were defined. The following paragraphs provide concluding answers and remarks to these questions.

2. Integrated techno-sustainability assessment

2.1 Indicator selection

The first two research questions concern an adequate selection of indicators for a sustainability assessment of biobased chemicals. **RQ 1**, "Which indicators are available in current scientific literature for the sustainability assessment of biobased chemicals?", can be answered by conducting an extensive literature review. Chapter 2 reports the full review analysis. **RQ 2**, "Which indicators are needed and preferred for the sustainability assessment of biobased chemicals?", can be investigated by a combination of experts' opinion and multi-criteria decision analysis (MCDA) for the construction of a consensus ranking on indicators. Chapter 3 provides an overview of the methods used for the expert survey and the details on the full analysis. The summarizing results of chapters 2 and 3 will be further elaborated in the following paragraphs.

A state-of-the-art literature search was performed which found 38 articles published up to and including 2017 on ISI Web of Science. The decision for inclusion of articles was based on two criteria: (1) the focus on ‘sets’ of indicators instead of stand-alone indicators, and (2) enclosing sets which assess only on product- and/or activity level. Next, the included studies were analyzed according to (i) the inclusion of different sustainability dimensions (i.e., environmental, economic, and social), (ii) the focus (i.e., general sustainability, general biomass, chemicals, and biobased chemicals), (iii) the overlap between indicators (derived from description and formula), and (iv) interlinkages between the sustainability domains. Based on the results of the performed review, an indicator list is presented that captures all indicators currently used in scientific literature for sustainability assessments of biobased chemicals (Appendix A2).

The review study shows that, for the existing body of literature, existing sets of indicators lack a holistic view on sustainability. The sets are mostly incomplete, meaning they lack a balanced inclusion between the environmental, social, and economic dimension. There is a clear hierarchy present within these sustainability domains with a preference for environmental indicators and ignorance towards social aspects. In addition, the existing sets lack focus because the biobased chemical case studies have to rely on the use of indicators of more generic assessment frameworks with no adaptation to case-specific characteristics. In conclusion, no generally accepted set of indicators had been developed for sustainability assessment of biobased chemicals. Sustainability indicator sets did exist, yet not on a mature and complete level. The need existed to elaborate and enhance a standardized and comprehensive list of indicators, specifically for biobased chemicals.

As a result, a first framework for indicator selection was proposed which is illustrated again in Figure 23. According to this framework, the developed list of indicators from the review should be used as an input to consult stakeholders from the public as well as the academic and private sector on regional, national, or international level, depending on the scope. Chapter 3 gathered feedback from different experts in Europe to develop a comprehensive set of indicators specifically for biobased chemicals. In chapter 3, the goal was to collect and interpret information about sustainability indicators on the one hand, and rank the indicators based on their relevance on the other hand. Therefore, a Delphi study was combined with a MCDA to fully address the research question.

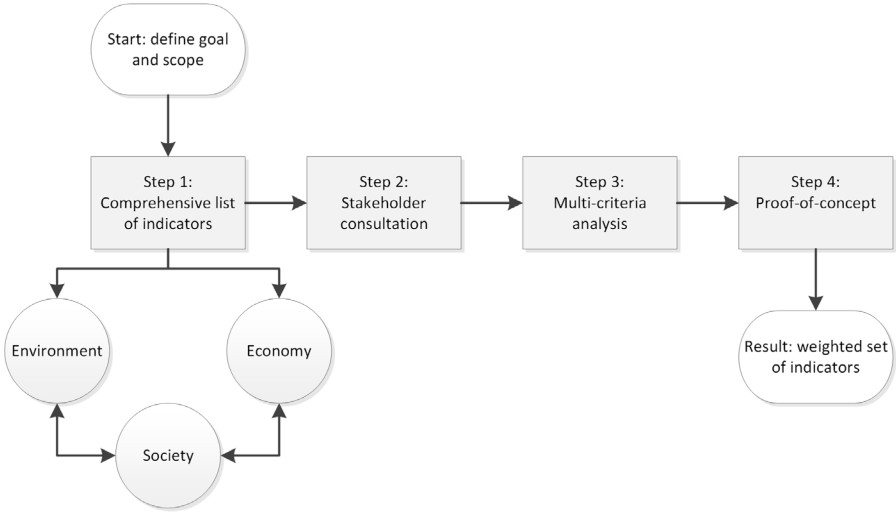

Figure 23. Constructing an indicator set to assess sustainability: a framework.

A Delphi survey aims to reach consensus among experts on a research question by conducting an iterative group facilitation methodology (Hasson et al., 2000). Participants were selected based on their expertise in sustainability and biobased chemistry and were divided into three core groups: the private, public, and academic sector. For the Delphi performed in this dissertation, two iterative survey rounds were developed: a first open round to select indicators and a closed second round to rank indicators. The second round used best-worst scaling (BWS) and asked the experts to indicate the 'best' and 'worst' item from a set of indicators per sustainability domain (J. A. Lee et al., 2008). The survey data was used to compose a ranking per respondent, which provided the input needed to perform AURORA, an outranking MCDA method (De Keyser & Springael, 2009). All the detailed methodological information on the combination of Delphi, BWS, and AURORA can be found in chapter 3. A combination of these methods could be replicated and applied to other product categories as well. BWS proves to be an efficient way of obtaining data from experts and provokes discrimination for 'easy' indicator selection. AURORA is capable of using the BWS output and constructs a consensus ranking which complies with the goal of a Delphi study to reach consent among experts.

The Delphi study resulted in the construction of one final consensus ranking which represents how experts elaborated on the concept of sustainability within biobased chemistry, and offers prioritization of indicators to practitioners of sustainability analysis within Europe (Table 25). Consensus between the rankings of the respondents was measured by the median Kendall's τ and proved to be positive within all three sustainability domains. The strongest consensus was measured within the environmental sustainability ranking and the weakest, however still strong consent, was found for the social sustainability ranking. The experts indicated *GHG emissions*, *market potential*, and *acceptance of biobased materials* as the most crucial indicators for respectively environmental, economic, and social sustainability. In a following next step, the selected indicators needed to be quantified and integrated in one holistic assessment. This follow-up research was performed in chapters 4 and 5.

Table 25. Final consensus rankings of sustainability indicators for the assessment of biobased chemicals.

	Environmental		**Economic**		**Social**
1	GHG emissions	1	Market potential	1	Acceptance of biobased materials
2	Raw material efficiency	2	Raw materials cost	2	Product transparency
3	End of life options	3	Product innovation	3	Job creation
4	Ecotoxicity	4	Process innovation	4	Human toxicity
5	Waste generation	5	Technical risks	5	Income levels
6	Energy efficiency	6	Capital productivity	6	Workplace accidents and illnesses
7	Natural land transformation	7	Energy cost	7	Education and training
8	Abiotic fossil depletion	8	Land productivity	8	Community support and involvement
9	Eutrophication	9	Product efficiency	9	Fatal work injuries
10	Agricultural land occupation	10	Labor productivity	10	Security measures
11	Water consumption	11	Subsidies	11	Social security
12	Organic carbon depletion	12	Waste disposal cost	12	Child labor
13	Management practices (crops)	13	Transportation cost	13	Working hours
14	Soil erosion			14	Discrimination
15	Acidification			15	Cultural heritage
16	Particular matter formation				
17	Abiotic mineral depletion				
18	Stratospheric ozone depletion				
19	Photo-oxidant formation				
20	Ionising radiation				

2.2 Techno-sustainability assessment

Chapters 2 and 3 focus on "what" should be assessed. From chapter 4 onwards, the research continued by answering the question "how" one should assess sustainability. Chapter 4 of this dissertation handles **RQ 3**: "How are sustainability indicators quantified for the assessment of emerging biobased technologies?". An integrated techno-sustainability assessment (TSA) framework is proposed which uses indicator information from the previous chapters, and deals with quantification and final decision-making. In order to illustrate the integrated TSA framework, a case study was used for which the sustainability of the cultivation and harvesting processes of microalgae was assessed, for the final production of biobased food colorants. The first step within TSA is to determine goal and scope and consequently define different scenarios. For the algae case, four different scenarios were constructed for which different cultivation systems (i.e., an open and closed system) are combined with different algae types (i.e., *Porphyridium* and *Dunaliella salina*). In the second step, environmental, social, and economic indicators are selected for a specific case study based on literature review and expert opinion. The review study performed in chapter 2 and the Delphi study from chapter 3 were consulted for a comprehensive indicator selection. The third step gathers technological information and constructs a process flow diagram (PFD) and a mass and energy (M&E) balance. Data for the microalgae case were gathered using literature and supplier information to model the product value chain. In a fourth step, the actual environmental, economic, and social analysis is performed and the selected indicators are measured per scenario and compared relative to the other scenarios. The quantification of the different selected indicators are fully explained in chapter 4 and relies on a combination of methods such as techno-economic assessment (TEA) and (social) life cycle analysis (LCA). In the fifth step, results are interpreted by an uncertainty and sensitivity analysis which identifies the crucial connections between the indicators and the stochastic input data. The identification of important parameters within the analyzed system can help decision makers with further technology development. In the final step, i.e., Step 6, a stochastic outranking approach was developed to integrate all sustainability indicators and help decision makers in selecting the most and least sustainable scenarios. This last step is further explained in chapter 5 and will be summarized in the next section of this conclusion.

2.3 A decision-making method

RQ 4, "How can sustainability indicators be integrated in order to make decisions?", is dealt with in chapter 5. The quantification of multiple impact categories expressed in different units makes a comparison between alternative scenarios complex. Complexity grows when more scenarios are compared and the amount of indicators increases. If a decision maker wants to know which scenario scores best or worst compared to the others, MCDA offers a solution for the integration of these indicators over the scenarios. A hierarchical, stochastic outranking approach for sustainable decision-making was therefore developed in this dissertation. The decision-making method allows for performance uncertainty and different weighting and preference schemes, which can be chosen and justified according to the assessed case and values of the stakeholders. Based on the results of chapter 4, a Monte Carlo simulation was performed by varying a selection of input parameters. An illustration was again provided using the microalgae case, in which uniform, discrete, and Beta PERT distributions described the data probability of different input parameters. A number of 43,300 iterations were further assessed using stochastic outranking modelled in Python 3.7.4. The pseudocode, as presented in Appendix D2, can be used for any other case in the future, when decisions based on different indicators need to be made. The model includes three different preference structures and four general weighting schemes where corresponding parameters (such as preference and indifference values, and rank data) can be chosen as is convenient for the case, stakeholders, and decision makers.

For the microalgae case assessed, the scenario in which the *Dunaliella salina* algae is cultivated in a horizontal photobioreactor (PBR) in France, was considered the most sustainable scenario, with a 55.89 percent to 87.61 percent probability to be ranked first on the integrated ranking. The scenario where *Porphyridium* is cultivated in an open pond (OP), was the second most sustainable option, relative to the other assessed microalgae scenarios. The *Dunaliella salina* scenario where the algae are cultivated in an OP in France, had the highest chance of being ranked as the least sustainable alternative, with a 81.95 percent to 94.9 percent chance of being ranked last. The overall results showed that the interaction between an algae cultivation type (i.e., PBR or OP) and algae variety (i.e., *Dunaliella salina* or

Porphyridium) plays an important role for its corresponding sustainability. The included sustainability indicators used for the assessment are highly influenced by the pigment content and the algae growth rate, which affect productivity and final pigment output of the system.

2.4 General conclusion

Figure 24 provides an overview of all the methods used in the integrated TSA framework. The different colors represent the different sections and research questions (RQs) of this PhD thesis: *grey* for RQ 1 and 2, *blue* for RQ 3 and *green* for RQ 4. These methods were applied specifically to biobased chemicals and microalgae as a case, however, they can be generalized towards any other application.

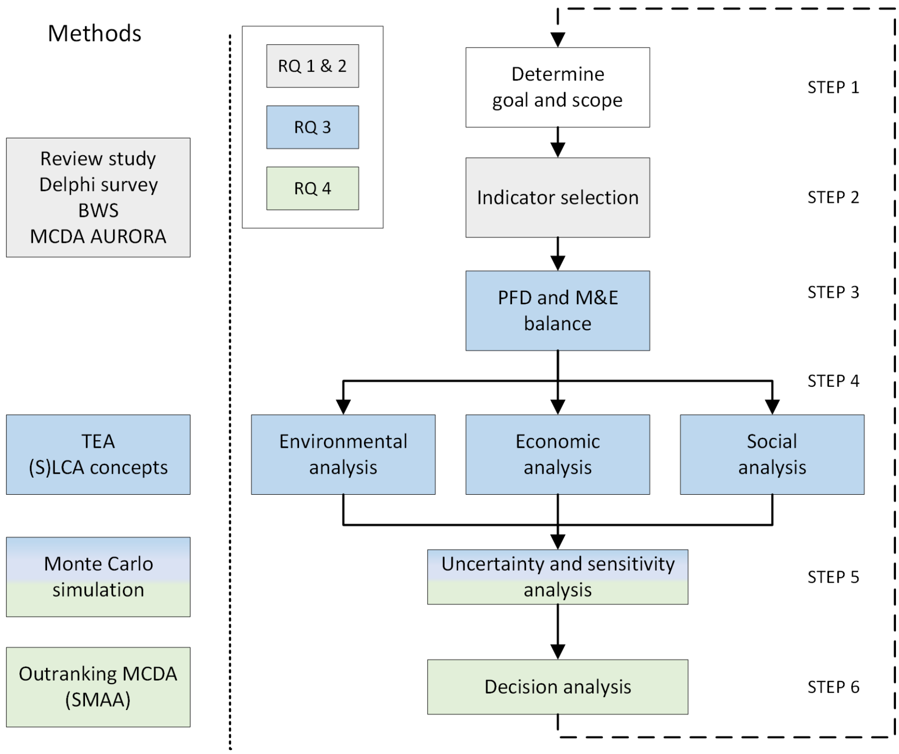

Figure 24. Methods used within the integrated techno-sustainability assessment framework. RQ = research question, BWS = best-worst scaling, MCDA = multi-criteria decision analysis, TEA = techno-economic assessment, (S)LCA = (social) life cycle assessment, SMAA = stochastic multi-attribute analysis, PFD = process flow diagram, and M&E = mass and energy.

The novel integrated techno-sustainability assessment framework is the first to focus on a combination of methods for (i) a comprehensive indicator selection, (ii) a dynamic integration of sustainability dimensions in one assessment, and (iii) a multi-criteria decision making tool allowing for data uncertainty and flexible method options. Academics, policy makers, and companies can use the integrated TSA to gain insights in the sustainability performance of their technologies, products, and value chains, and make better-informed decisions. More information on the valorization potential is provided in the following section.

3. Valorization potential

A distinction can be made between the practitioners of sustainability assessment and the users of its results. **Practitioners** such as (social) LCA or TEA consultants, research institutes, or other private companies could use the framework developed in this dissertation to perform a full sustainability assessment including environmental, social, and economic impacts in an integrated way, for technologies and products already at a low TRL. Academic researchers in statistics, economics, or other behavioral sciences could utilize and further improve the (combination of) methods applied in this dissertation and elaborate on the indicator selection and need for quantification of social indicators, such as for product acceptance or transparency. Expertise centers for sustainability assessments could be established in the future where experts are gathered and the integrated TSA could offer a harmonized framework for practitioners.

Furthermore, the results and insights that the integrated TSA offers can be valuable to different stakeholders (Figure 25). **Policy makers** have to make sustainable funding decisions to support R&D and upscaling of technologies. Integrated TSA can guide these decisions towards sustainable alternatives by providing a method for comparative analysis that is integrated over all sustainability domains. Based on the TSA results, policy makers can redirect roadmaps and strategies and safeguard sustainability impacts by monitoring innovative technologies and products along the value chain. Stakeholders from **academia and industry** can be divided into two separate categories: **technology developers** working in R&D, and **decision makers**, usually at management level. First, technology developers gain insights into the

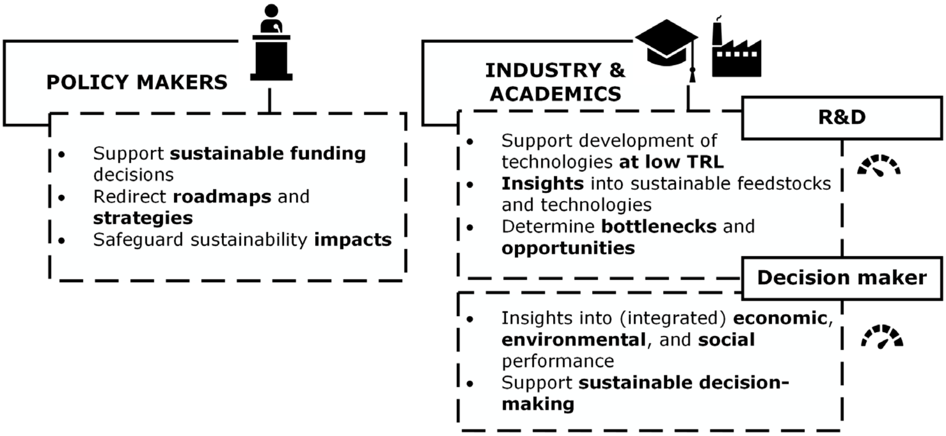

Figure 25. Users of the results from the integrated TSA.

sustainability of their technologies, products, and value chains. TSA uncovers the bottlenecks and opportunities of technologies and processes that could potentially be interesting for companies. Second, integrated TSA can steer decision makers in companies and academia towards more sustainable investments. Insights are provided within the three separate sustainability dimensions and integrated by providing a single score and ranking of alternative scenarios. By performing integrated TSA at early development stages, unsustainable expenditures can be prevented, and time can be saved collecting data when assessing the technology again at higher TRL.

4. Limitations

Important limitations of this dissertation concern the microalgae case study used within chapters 4 and 5 to illustrate the integrated TSA framework. First, a fossil based colorant was not included as a benchmark scenario. It would have been valuable to include the value chain of Allura Red (E129), which is a red synthetic colorant. This way, the biobased algae feedstocks could be compared with conventional oil-based products. Another interesting comparison could be made with carmine (E120) as a natural food colorant which is gained from aphid and is present in beverages, bakery products, meat, and dairy products, etc. (Müller-maatsch, Jasny, Henn, Gras, & Carle, 2018). Comparing carmine with microalgae-based colorants would provide an animal-plant comparison which can have potential differences on several impact categories, such as social acceptance, transparency, or land use changes. The synthetic alternatives as well as the animal-based alternative were not included due to data limitations. An attempt was made to try and contact experts on Allura Red and Carmine, however no useful responses were received. As a consequence, algae feedstocks were compared relative to each other, including different cultivation systems and locations.

Furthermore, it is stressed that the microalgae case is hypothetical. The use of *Porphyridium* as a food colorant in Europe is not yet approved, and as such, no full-scale process data is available on the value chain. In addition, many data is based on scientific literature and specific information on the downstream processing is lacking. The use of primary data is preferred over the use of secondary data. However, when emerging technologies are evaluated, primary data is not fully available and often confidential. For that reason, the outcomes of the integrated TSA must be seen as potential results concerning the relative sustainability of the different scenarios and not as a final truth. The integrated TSA is therefore framed as an iterative process where, at different steps of the framework, feedback loops provide information to the above steps to change, improve, and fine-tune the results.

Finally, for a full picture on the practicability of the TSA framework, more case studies, outside the field of microalgae, should be conducted. It was chosen in this dissertation to focus on one elaborated case study on microalgae. However, further research should check if the integrated TSA method works, and is applicable to different products and feedstocks. This is further explained in the next section.

5. Future research needs

The Delphi ranking constructed in chapter 3 is in general applicable to biobased chemicals and their value chains. Within the field of biobased chemistry, there exists many different feedstocks, which all deviate from each other in terms of biological characteristics and applications. It would be interesting to check the applicability of the Delphi ranking on a multitude of cases, such as biochar, bioplastics from starch, etc. In chapter 4, the pertinence of the indicator ranking on microalgae as feedstock was checked with experts, and found to be suitable without additional reranking. The applicability was explored by conducting a survey among algae experts and measuring consensus by using a correlation coefficient (i.e., Kendall's τ). This method should be elaborated and further used to explore other biobased feedstocks, and check the robustness of the developed set of indicators for general use in the entire field of biobased chemicals. Next to a validation of the selected indicators, the entire TSA framework should be monitored and verified by its end-users. The developed integrated TSA should correspond to the needs and expectations of different users. A follow-up stakeholder consultation could further address the validity of the framework.

In addition, the Delphi indicators should be cross-referenced with established criteria, such as the United Nations development goals and the green chemistry principles (Anastas, Paul T; Warner, 1998; United Nations, 2015). These well-known sets provide goals and principles towards sustainable development and green chemistry, and offer valuable insights on sustainability criteria that should be met, and how chemicals should be assessed. The set of indicators developed by the Delphi study within this dissertation is currently based on other existing indicator sets available in literature and expert opinion. Future research could check if the indicator set also fits the overarching criteria and goals, which could again improve the validity and reliability of the defined indicators.

The indicator ranking gives a clear overview on which indicators are relevant and preferred for the social assessment of biobased chemicals. However, when trying to quantify the indicators in chapter 4, many lack clear methodologies on how to evaluate them. A major challenge is the inclusion of an indictor regarding social acceptance, which is the number one important indicator in the social ranking. Based on choice modeling, the attributes which influence consumer's choice could be revealed. An additional scoring system based on the results of these attributes could potentially provide quantification, in a case-specific context. It would be interesting for further research to explore the field of social acceptance of biobased products, and develop evaluation systems which fit the TSA method.

The MCDA approach developed in chapter 5 offers a bottom-up approach where the most and least sustainable scenarios can be selected based on technological, economic, environmental, and social data. A next step could be to provide results 'the other way around' by integrating a top-down feedback loop. Here, input data can be optimized and target values could be determined, which would enhance the final sustainability of the scenarios. Thomassen et al. (2019) used multi-objective optimization (MOO) to optimize towards both economic and environmental objectives (Thomassen, Van Dael, You, et al., 2019). As is stated in the discussion part of chapter 5, this MOO could be extended with social objectives to be compatible with the integrated TSA framework.

Finally, the integrated TSA results should be properly communicated to all actors in the value chain. For the end-consumer, this is automatically linked with the social acceptance as is described above. Consumers, suppliers, and governments should be informed about the sustainability of the products they buy and use. In the Green Paper on integrated product policy the commission states *"Consumers must have easy access to understandable, relevant, credible information either through labelling on the product or from another readily accessible source"*. Certification schemes and labels could use integrated TSA to perform impact assessments, and translate the developed methods towards communication tools for sustainable buying behavior. A stakeholder consultation could determine how the results of the integrated TSA should be visualized and communicated internally, and to the general public.

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APPENDICES

Appendix A. Supplementary information chapter 2

1. Bibliography for review study.

Author(s)	Year	Title
Eissen & Metzger	2002	Environmental performance metrics for daily use in synthetic chemistry
Guinée, et al.	2002	Handbook on life cycle assessment. Operational guide to the ISO standards. I: LCA in perspective. IIa: Guide. IIb: Operational annex. III: Scientific background.
Bare, et al.	2003	TRACI - The Tool for the Reduction and Assessment of Chemical and Other Environmental Impacts
Jolliet et al.	2003	IMPACT 2002+: A New Life Cycle Impact Assessment Methodology
Goedkoop, et al.	2008	ReCiPe 2008
Sugiyama, Fischer & Hungerbühler	2008	Decision framework for chemical process design including different stages of environmental, health and safety assessment
Tufvesson & Börjesson	2008	Wax production from renewable feedstock using biocatalysts instead of fossil feedstock and conventional methods
Groot & Borén	2010	Life cycle assessment of the manufacture of lactide and PLA biopolymers from sugarcane in Thailand
Tabone, et al.	2010	Sustainability metrics: life cycle assessment and green design in polymers
Uhlman & Saling	2010	Measuring and communicating sustainability through eco-efficiency analysis
JRC European Commission	2011	ILCD Handbook: Recommendations for Life Cycle Impact Assessment in the European context
Sheldon	2011	Utilisation of biomass for sustainable fuels and chemicals: Molecules, methods and metrics
Patel, et al.	2012	Sustainability assessment of novel chemical processes at early stage: application to biobased processes
Sacramento-Rivero	2012	A methodology for evaluating the sustainability of biorefineries: framework and indicators

Nuss & Gardner	2013	Attributional life cycle assessment (ALCA) of polyitaconic acid production from northeast US softwood biomass
Patel, et al.	2013	Early-stage comparative sustainability assessment of new bio-based processes
Posada, et al.	2013	Potential of bioethanol as a chemical building block for biorefineries: Preliminary sustainability assessment of 12 bioethanol-based products
Akanuma, Selke & Auras	2014	A preliminary LCA case study: comparison of different pathways to produce purified terephthalic acid suitable for synthesis of 100% bio-based PET
Muñoz, et al.	2014	Life cycle assessment of bio-based ethanol produced from different agricultural feedstocks
Hong, Zhou & Hong	2015	Environmental and economic impact of furfuralcohol production using corncob as a raw material
Juodeikiene, Vidmantiene & Basinskiene	2015	Green metrics for sustainability of biobased lactic acid from starchy biomass vs chemical synthesis
Khoo & Isoni	2015	Bio-chemicals from lignocellulose feedstock: sustainability, LCA and the green conundrum
Moncada, Posada & Ramirez	2015	Early sustainability assessment for potential configurations of integrated biorefineries. Screening of bio-based derivatives from platform chemicals.
Nguyen, et al.	2015	A new approach for the design and assessment of bio-based chemical processes toward sustainability
Patel, et al.	2015	Analysis of sustainability metrics and application to the catalytic production of higher alcohols from ethanol
Sheldon & Sanders	2015	Towards concise metrics for the production of chemicals from renewable biomass
Belboom & Léonard	2016	Does biobased polymer achieve better environmental impacts than fossil polymer? Comparison of fossil HDPE and biobased HDPE produced from sugar beet and wheat
Cespi, et al.	2016	Butadiene from biomass, a life cycle perspective to address sustainability in the chemical industry
Daful, et al.	2016	Environmental impact assessment of lignocellulosic lactic acid production: integrated with existing sugar mills
Gargalo et al.	2016	Assessing the environmental sustainability of early stage design for bioprocesses under uncertainties: an analysis of glycerol bioconversion
Krzyżaniak, et al.	2016	Life cycle assessment of new willow cultivars grown as feedstock for integrated biorefineries

Benalcázar et al.	2017	Production of bulk chemicals from lignocellulosic biomass via thermochemical conversion and syngas fermentation: a comparative techno-economic and environmental assessment of different site-specific supply chain configurations
Chen et al.	2017	Production of caproic acid from mixed organic waste: an environmental life cycle perspective
Daful & Görgens	2017	Techno-economic analysis and environmental impact assessment of lignocellulosic lactic acid production
Gunukula & Anex	2017	Evaluating and guiding the development of sustainable biorenewable chemicals with feasible space analysis
Gunukula, Runge, & Anex	2017	Assessment of biocatalytic production parameters to determine economic and environmental viability
Isola et al.	2017	Life cycle assessment of photodegradable polymeric material derived from renewable bioresources
Moncada, Posada & Ramirez	2017	Comparative early stage assessment of multiproduct biorefinery systems: an application to the isobutanol platform

2. Overview of indicators included in sustainability assessments for biobased chemicals.

2.1 Environmental indicators.

		Indicator name	Description
CLIMATE CHANGE		GWP/ carbon footprint/ GHG	measures sources of greenhouse gas emissions (including CO_2, NH_4, and N_2O) and their contribution to climate change (Nguyen et al., 2015). GWP represents the global warming potential, which is a combination of radiative forcing and atmospheric lifetime, for a time horizon 100 years (IPCC) (M.A.J. Huijbregts et al., 2017; Scheutz et al., 2009)
CLEAN AND EFFICIENT ENERGY USE		Cumulative energy demand (CED)	represents the primary, direct and indirect energy use in the process during the entire life cycle (Nguyen et al., 2015). The CED indicator is often calculated specifically for a certain aspect in the process (e.g. CED of raw materials)
		Non-renewable energy use	calculates the primary non-renewable energy use. An example is the fossil energy consumption (FEC), calculated based on CED of raw material and utilities (Nguyen et al., 2015)
		Energy efficiency	calculates the caloric value of the end product and all the useful side products, divided by the sum of all fossil and renewable energy inputs (Roger A. Sheldon & Sanders, 2015)
		Energy loss index (ELI)	estimates energy-related efforts in the process using reaction information only, aggregating five indicators: water in reactor outlet, product concentration, boiling point, MLI and reaction enthalpy (Sugiyama et al., 2008)
		Non-renewable energy share	measures how much fossil energy is displaced by the new process/product (Sacramento-Rivero, 2012)
RESOURCE MANAGMENT	Land	Land use: ED	calculates the impacts concerning ecosystem damage (ED) as a result of land use, including the loss of biodiversity and life-support functions (Sacramento-Rivero, 2012)
		Land use: occupation and transformation	serves as an umbrella covering all land use indicators
		Agricultural land occupation	calculates the amount of agricultural area occupied (in m^2) (M.A.J. Huijbregts et al., 2017)
		Natural land transformation	calculates the amount of transformed area per year. 'Natural land' represents the type of land that arises without human distortion (M.A.J. Huijbregts et al., 2017)
		Urban land occupation	calculates the amount of urban area occupied (in m^2) (M.A.J. Huijbregts et al., 2017)

		Soil organic matter (SOM)	calculates the impact on fertile land use as it influences properties like buffer capacity, soil structure and fertility (JRC European commission, 2011)
		Indirect land use change	calculates greenhouse gas emissions caused by land use change (Eissen & Metzger, 2002)
	Materials	Renewable sources	represents the % of material from biological sources in the final product, by mass (Tabone et al., 2010)
		Use local sources	accounts for the categorical distance of the furthest feedstock location: international, national and regional (Tabone et al., 2010)
		Raw-material consumption	indicates if the consumption rates of renewable raw materials is lower than their regeneration rates. RMC is only applicable on renewable sources (Sacramento-Rivero, 2012)
		Mass index S^{-1}	calculates the mass of raw materials used for synthesis including solvents, catalysts, auxiliaries, and workup per mass unit of the purified product (Eissen & Metzger, 2002)
		Material efficiency	gives the total weight of useful products, divided by the total weight of useful products and waste (Roger A. Sheldon & Sanders, 2015)
		Material efficiency: density	measures the efficient use of a material through its density. Less dense materials are able to serve many purposes with less mass (Tabone et al., 2010)
		Design products for recycle	can be measured by the % recovery of a material in the U.S. municipal recycle stream (Tabone et al., 2010)
	Abiotic depletion	Abiotic depletion potential (ADF)	calculates each extraction of minerals and fossils based on concentration reserves and rate of de-accumulation (Guinee, 2002)
		Mineral depl.	indicates the extraction of mineral resources in kg (M.A.J. Huijbregts et al., 2017)
		Fossil fuel depl.	indicates the extraction of fossil resources in kg (M.A.J. Huijbregts et al., 2017)
		Fossil fuel index	considers the increase in energy input requirements per unit of consumption of fuel and the consumption of fuel per unit of product (Bare, 2002)
	Water	Freshwater-use reduction (WR)	indicates the water-use reduction achieved by a product or a biorefinery (Sacramento-Rivero, 2012)
		Water depletion/ water use	gives an estimation of the potential amount of water embodied inside a bio-based chemical (Cespi et al., 2016; M.A.J. Huijbregts et al., 2017)
	Air	Acidification	represents the decrease of pH by calculating at the base saturation (M.A.J. Huijbregts et al., 2017)
		Ionising radiation	calculates the level of exposure related to releases of radioactive material to the environment (M.A.J. Huijbregts et al., 2017)
		Particulate matter formation	gives an indication of the air quality and the presence of PM10 in the air (M.A.J. Huijbregts et al., 2017)

ECOSYSTEM CARE		Photo-oxidant formation	estimates the formation of reactive substances, also indicated as "summer smog" (Guinee, 2002; M.A.J. Huijbregts et al., 2017)
		Stratospheric ozone depletion	calculates the stratospheric ozone concentration (M.A.J. Huijbregts et al., 2017)
	Eutrophication	Eutrophication	includes all effects due to excessive levels of macronutrients in the environment caused by emissions of nutrients to air, water and soil (Krzyżaniak, Stolarski, Szczukowski, & Tworkowski, 2016)
		Freshwater eutrophication	refers to the eutrophication of fresh water with phosphor and nitrogen (M.A.J. Huijbregts et al., 2017)
		Marine eutrophication	refers to the eutrophication of marine water with phosphor and nitrogen (M.A.J. Huijbregts et al., 2017)
		Terrestrial eutrophication	refers to the enrichment of terrestrial ecosystems with phosphor and nitrogen (Guinee, 2002)
	Ecotoxicity	Ecotoxicity	refers to the impact on ecosystems caused by emissions of toxic substances
		Freshwater ecotoxicity	refers to the impact on freshwater systems caused by emissions of toxic substances to air, water and soil (Guinee, 2002)
		Marine ecotoxicity	refers to the impact on marine ecosystems caused by emissions of toxic substances to air, water and soil (Guinee, 2002)
		Terrestrial ecotoxicity	refers to the impact on terrestrial ecosystems caused by emissions of toxic substances (Krzyżaniak et al., 2016)
	Waste	Atom economy (AE)	accounts for a rough estimate of the amount of waste that will be generated by different processes (Roger A. Sheldon, 2011)
		Design biodegradable products	is measured by categorical classifications: non-biodegradable, biodegradable in an industrial facility and biodegradable in typical backyard conditions (Tabone et al., 2010)
		E-factor	accounts for the actual amount of waste produced in the process, defined as everything but the desired product (Roger A. Sheldon, 2011)
		Environmental quotient (EQ)	takes into account not only the amount of waste (E-factor), but also the nature of the waste (Roger A. Sheldon, 2011)
		Mass loss indices (MLI)	refers to the mass ratio of all substances except for the product, measuring how much unwanted substances are produced in the reaction (Sugiyama et al., 2008)
INDICES		Reduction of baseline emissions (RBE)	aggregates abiotic depletion, GWP, ozone depletion, photochemical oxidation, human- and eco-toxicities, acidification, and eutrophication (Sacramento-Rivero, 2012)
		EI of raw materials	relates to the environmental impacts (EI) of raw materials per unit of product represented by GHG and CED (de Assis et al., 2018a)

		Biodiversity and ecosystem services (BES)	aggregates climate regulation potential, biodiversity damage potential, biotic production potential, freshwater regulation potential, erosion regulation potential and water purification potential (Muñoz et al., 2014)
		Process costs and environmental impact (PCEI)	aggregates the presence of water in reactor outlet, product concentration, boiling point, MLI, reaction enthalpy, number of co-products and pre-treatment of feedstock (Patel et al., 2012)
		Damage to resource availability	is based on the marginal increase in costs due to the extraction of a resource (MCI). The MCI represents the increase of the cost of a commodity, due to an extraction or yield of the resource (M.A.J. Huijbregts et al., 2017)

2.2 Economic indicators.

		Indicator name	**Description**
LOW COSTS	Feedstock	Costs of raw materials	calculates the cost of feedstock
		Raw materials cost ratio (RCR)	calculates the cost ratio of raw materials of two processes, producing the same comparable goods (Sacramento-Rivero, 2012)
		Transportation cost	calculates the cost of fuel consumption, capital recovery of transportation equipment and (un)loading (Nguyen et al., 2015)
	Production	Production cost/ conversion cost	calculates the costs of raw materials, utilities, depreciation and others (including labor, maintenance, supplies and taxes) (Nguyen et al., 2015)
		Depreciation expense	calculates the cost of depreciation
		Capital costs	calculates the costs that change according to the scale of production and includes main equipment, feedstock pre-treatment, reactor vessels, product purification, etc. (Nguyen et al., 2015)
		Taxes	calculates the taxes
		Energy cost	calculates the cost of energy
		Maintenance activities	calculates the cost of maintenance activities

		Total production cost	calculates the sum of transportation costs and conversion costs (Nguyen et al., 2015)
	EoL	Waste disposal	calculates the costs related to waste disposal
	People	Cost of labor	calculates the cost of labor
		Illnesses and accidents	calculates the cost related to illnesses and accidents
VALUE CREATION	Feedstock profitability	Normalized biotechnological-valorization potential (BVP)	measures the viability of biomass sources as feedstock for biorefineries based on 12 criteria, including economic, technological, geographical, and biological-chemical aspects. Each aspect is given a score between 0 and 3 (Sacramento-Rivero, 2012)
		Economic constraint	provides information about the raw material cost (feedstock) relative to the market value of the products (Patel et al., 2012)
		Fraction of revenue for feedstock (FRF)	represents the quotient of costs of the feedstock and the economic value of the product (Sacramento-Rivero, 2012)
	General profitability	Cost efficiency	can be measured by using a median price per unit product. If the products are more competitively priced, they will more effectively integrate into markets (Tabone et al., 2010)
		Economic index	calculates the ratio between the product price and the cost of synthesis (i.e., utilities and raw materials) (Cespi et al., 2016)
		Modified gross margin (GM)	a financial ratio that relates the gross profit (GP) to the net sales (NS) (Sacramento-Rivero, 2012)
	Investment value	Net present value (NPV)	measures the difference between the present value of cash in- and outflows
		Internal rate of return (IRR)	provides the discounted cash flow analysis that gives a zero NPV (Gezae Daful & Görgens, 2017)
		Minimum selling price (MSP)	calculates the selling price that would bring the NPV to zero at a defined number of years (de Assis et al., 2018b)
RISKS		Risk aspects (RA)	is based on external economic and technical aspects, taking into account factors not covered explicitly by prices (feedstock supply risk, regional feedstock availability, infrastructure risk and application-technical aspects) (Patel et al., 2013)

2.3 Social indicators.

	Indicator name	Description
HEALTH	DALY (Disability-adjusted loss of life years)	calculates the sum of years of life lost and years of life disabled (M.A.J. Huijbregts et al., 2017)
	Human toxicity	accounts for the effects of toxic substances on the human environment, usually not focused on the working environment (Guinee, 2002)
	Human health: criteria air pollutants	accounts for human health effects due to exposure to ambient particulates (Bare, 2002)
	Human health: cancer	is the potential for toxicological impacts related to cancer effects (Bare, 2002)
	Human health: non-cancer	is the potential for toxicological impacts related to non-cancer effects (Bare, 2002)
SAFETY	Chemical inherent safety (ICI)	aggregates: heat of main reaction (IRM), heat of potential side reaction (IRS), flammability (IFL), explosiveness (IEX), toxicity (ITOX), corrosiveness (ICOR), and incompatibility of chemicals (IINT) (Nguyen et al., 2015)
	Process inherent safety (IPI)	aggregates: inventory of chemicals (II), process temperature (IT) and pressure (IP), type of equipment (IEQ), and structure of process (IST) (Nguyen et al., 2015)
	Workplace accidents and illnesses	deals with workplace accidents and illnesses. An example is the Recordable incident rate (RIR), calculating the number of recordable incidents for each 100 full-time employees per year (2,000 hours worked per employee per year) (Sacramento-Rivero, 2012)
	Rate of fatal work injuries (RFWI)	calculates the number of recordable incidents for each 100,000 full-time employees per year (2,000 hours worked per employee per year) (Sacramento-Rivero, 2012)
SOCIAL CARE	Social investment	accounts for the contribution through employment and philanthropic and community development projects (Sacramento-Rivero, 2012)

INDICES	Environment, health, and safety index (EHSI)	aggregates: environment (persistency, air hazard, water hazard and solid waste), health (irritation and chronic toxicity) and safety (mobility, fire/explosion, reaction/decomposition and acute toxicity) (Patel et al., 2012)
	Environment, health, and safety management system compliance (EMSC)	represents the degree of compliance with an adopted EHSMS. An external audit assesses the compliance and assigns a %EMS. If the company reaches a minimum %EMS, a certification is issued (Sacramento-Rivero, 2012)
	Health and safety compliance (HSC)	represents the degree of compliance with the normative OHS (Occupational Health and Safety) (Sacramento-Rivero, 2012)

Appendix B. Supplementary information chapter 3

1. Pseudocode Branch-and-Bound algorithm.

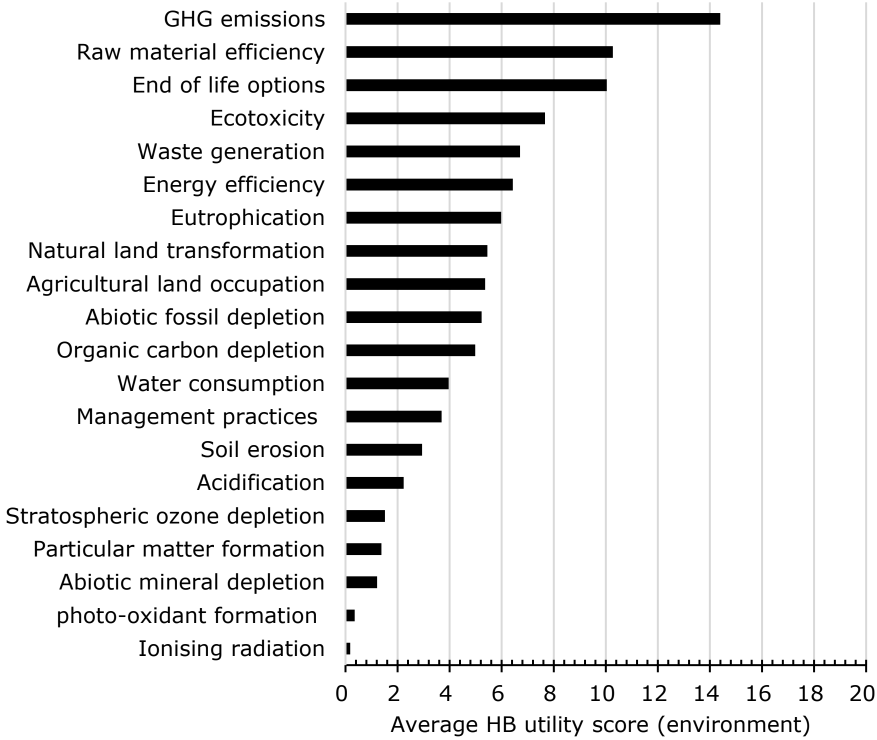
```
Start
    Initialize
    Start
        Set to investigate := Set of all solutions
        Best bound for median τ found until now := -1
          Bound for median τ :=1
        Set of optimal solutions := ø
    End
    Repeat
        Set to investigate := Branch with highest bound for median τ and most alternatives ranked
        i := number of alternatives ranked in chosen branch
        If i < n then
            i := i+1
            Expand the branch by adding i subbranches
            Foreach subbranch do
                Calculate corresponding bound
                If bound for median τ < best bound for median τ found until now then
                    Remove this branch
                End if
            End foreach
        Else if bound for median τ > best bound for median τ found until now then
            Best bound for median τ found until now := bound for median τ
            Set of optimal solutions := {branch}
        Else if bound for median τ = best bound for median τ found until now then
            Set of optimal solutions := Set of optimal solutions U {branch}
        End if
    Until Set to investigate = ø
End
```

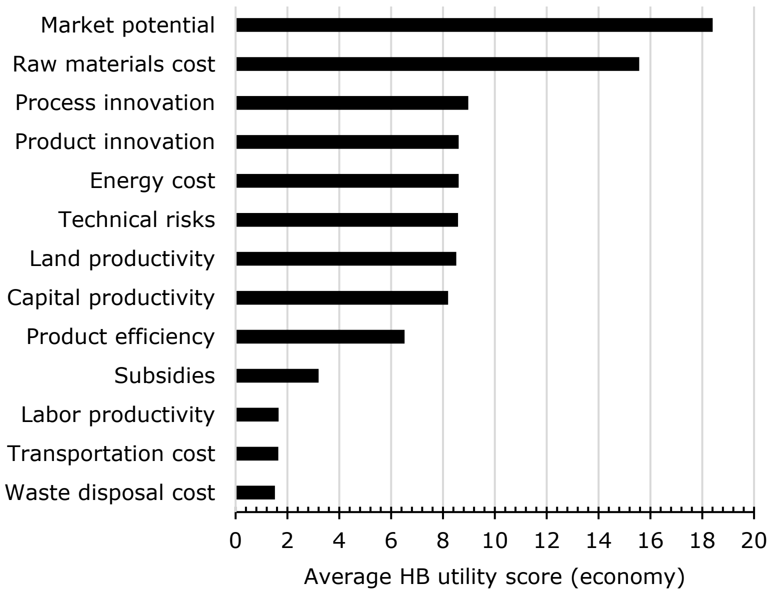
2. Sustainability indicators for biobased chemicals (input Delphi round 2).

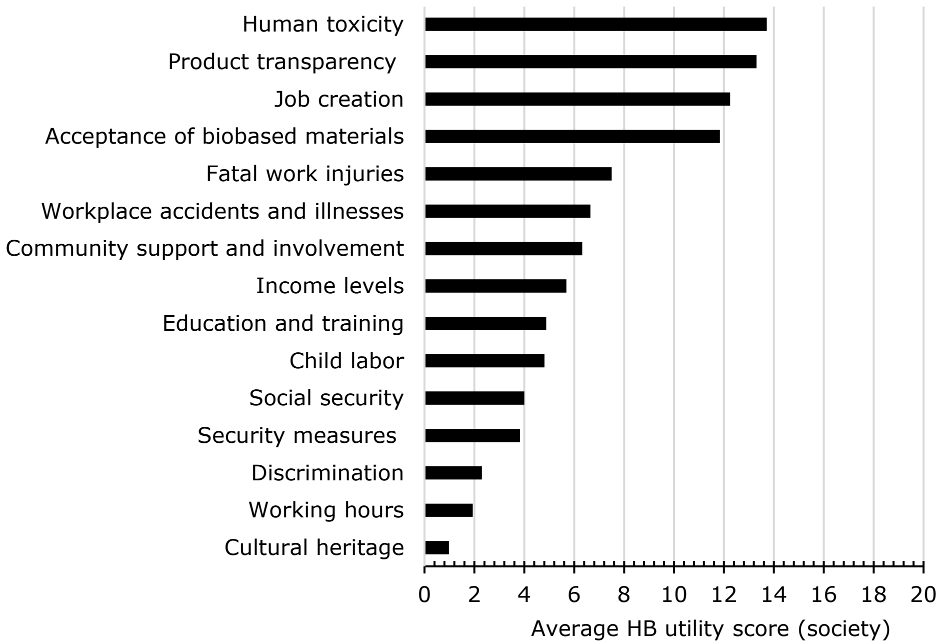
	INDICATOR	DESCRIPTION
ENVIRONMENTAL	Abiotic fossil depletion	Fossil resources required to produce a biobased chemical
	Abiotic mineral depletion	Mineral resources required to produce a biobased chemical
	Acidification	Emissions causing acidifying effects to the environment
	Agricultural land occupation	Amount of agricultural area occupied
	Ecotoxicity	Emissions of toxic substances to air, water and soil
	End of life options	Possibilities for recycling, composting, biodegrading, burning, … the end product
	Energy efficiency	Amount of energy from renewable and non-renewable resources needed per biobased chemical
	Eutrophication	Emissions (including phosphor and nitrogen) that cause eutrophication of marine water, fresh water and terrestrial environment
	GHG emissions	Greenhouse gas emissions and their contribution to climate change (including biogenic carbon and direct and indirect land use change)
	Ionising radiation	Level of exposure related to releases of radioactive material to the environment
	Management practices in crop production	The type of practices used for crop production
	Natural land transformation	Amount of transformed 'natural land' area (=no human distortion)
	Organic carbon depletion	Amount of organic carbon in the soil lost
	Particular matter formation	Presence of PM10 in the air
	Photo-oxidant formation	Formation of summer smog
	Raw material efficiency	Amount of raw materials needed per biobased chemical
	Soil erosion	Displacement of the upper layer of the soil
	Stratospheric ozone depletion	Emissions causing depletion of the ozone layer
	Waste generation	Amount and type of waste generated (e.g. by calculating 'atom economy')
ECONOMIC	Capital productivity	Capital needed for the production per biobased chemical
	Energy cost	Cost of energy per biobased chemical
	Labor productivity	Direct and indirect labor needed for the production per biobased chemical
	Land productivity	Direct land needed for the production per biobased chemical
	Market potential	Market price and size per biobased chemical

	Process innovation	Effects on price and output of improvement of facilities, skills and technologies, etc.
	Product efficiency	Actual productivity divided by maximum productivity
	Product innovation	Effects on price and output of new products, new features, improvement of performance, etc.
	Raw materials cost	Cost of feedstock per biobased chemical
	Subsidies	Amount of subsidies per biobased chemical
	Technical risks	Risks associated directly with the supply chain activities, e.g. feedstock supply risk, infrastructure risk, etc.
	Transportation cost	Cost of transportation per biobased chemical
	Waste disposal cost	Cost of waste disposal per biobased chemical
SOCIAL	Acceptance of biobased chemicals	Perception of consumers towards the biobased chemical
	Child labor	Presence of child labor
	Community support and involvement	Support and involvement from the local community
	Cultural heritage	Respect towards local cultural heritage (including language, religion, etc.)
	Discrimination	A "fair chance" for everybody, e.g. equal payment male/female
	Education and training	Education and training initiatives and opportunities
	Fatal work injuries	Number of fatal work injuries
	Human toxicity	Effects of toxic substances on the human environment
	Income levels	Level of income of the workers
	Job creation	Number of jobs created
	Product transparency	Creation of an informed choice for the consumer without intent to mislead or conceal
	Security measures	Security measures taken at the workplace
	Social security	Compensation for retirement, disability, illness, injury, etc.
	Working hours	Number of hours worked
	Workplace accidents and illnesses	Number of workplace accidents and illnesses

3. Rankings per sustainability dimension (based on HB utility scores).







Human toxicity
Product transparency
Job creation
Acceptance of biobased materials
Fatal work injuries
Workplace accidents and illnesses
Community support and involvement
Income levels
Education and training
Child labor
Social security
Security measures
Discrimination
Working hours
Cultural heritage
0
2
4
6
8
10
12
14
16
18
20
Average HB utility score (society)

Appendix C. Supplementary information chapter 4

1. Kendall's τ and corresponding z-values

	Environmental		Economic		Social	
#respondent	τ	z	τ	z	τ	z
1	0.884	5.451	0.692	3.294	0.981	5.097
2	0.958	5.905	0.667	3.172	0.886	4.602
3	0.958	5.905	0.615	2.928	0.829	4.305
4	0.821	5.061	0.615	2.928	0.448	2.326
5	0.411	2.531	0.154	0.732	0.810	4.206
6	0.684	4.218	0.667	3.172	0.714	3.712
7	0.526	3.244	0.744	3.539	0.676	3.514
8	0.611	3.764	-0.051	-0.244	0.771	4.008
9	0.558	3.439	0.564	2.684	0.467	2.425
10	0.884	5.451	0.872	4.149	0.771	4.008
11	0.979	6.035	0.692	4.759	1.000	5.196
12	0.800	4.932	0.359	4.759	1.000	5.196
13	0.621	3.828	1.000	4.759	1.000	5.196
14	1.000	6.164	1.000	4.759	1.000	5.196
15	1.000	6.164	1.000	4.759	1.000	5.196
16	1.000	6.164	1.000	4.759	1.000	5.196
17	1.000	6.164	1.000	4.759	1.000	5.196
18	1.000	6.164	1.000	4.759	1.000	5.196
19	1.000	6.164	1.000	4.759	1.000	5.196
20	1.000	6.164	1.000	4.759	1.000	5.196
21	1.000	6.164	1.000	4.759	1.000	5.196
22	1.000	6.164	1.000	4.759	1.000	5.196
23	1.000	6.164	1.000	4.759	1.000	5.196
24	1.000	6.164	1.000	4.759	1.000	5.196
25	1.000	6.164	1.000	4.759	1.000	5.196
26	1.000	6.164			1.000	5.196

2. A frequency analysis of indicators included/excluded for a sustainability analysis of algae-based chemicals based on expert opinion.

Note: the indicators above the dashed line should be included in the assessment.

Environmental (n=26)			**Economic** (n=25)			**Social** (n=26)		
Indicator	Excl.	Incl.	Indicator	Excl.	Incl.	Indicator	Excl.	Incl.
GHG emissions	1	25	Market potential	0	25	Acceptance of biobased materials	0	26
Raw material efficiency	1	25	Raw materials cost	1	24	Product transparency	0	26
End of life options	2	24	Product innovation	3	22	Job creation	1	25
Ecotoxicity	3	23	Process innovation	4	21	Human toxicity	1	25
Waste generation	1	25	Technical risks	5	20	Income levels	5	21
Energy efficiency	1	25	Capital productivity	6	19	Workplace accidents and illnesses	9	17
Natural land transformation	5	21	Energy cost	6	19	Education and training	7	19
Abiotic fossil depletion	4	22	Land productivity	9	16	Community support and	13	13
Eutrophication	3	23	Product efficiency	10	15	Fatal work injuries	19	7
Agricultural land occupation	4	22	Labor productivity	15	10	Security measures	20	6
Water consumption	3	23	Subsidies	18	7	Social security	21	5
Organic carbon depletion	13	13	Waste disposal cost	16	9	Child labor	18	8
Management practices for	17	9	Transportation cost	20	5	Working hours	23	3
Soil erosion	18	8				Discrimination	22	4
Acidification	22	4				Cultural heritage	22	4
Particular matter formation	23	3						
Abiotic mineral depletion	22	4						
Stratospheric ozone	25	1						
Photo-oxidant formation	26	0						
Ionising radiation	26	0						

3. Technological input data TSA.

Note: input numbers can deviate from sources because of unit conversions and additional calculations.

Abbreviations: PBR = photobioreactor, OP = open pond, FR = France, BE = Belgium, CSU = CO_2 supply unit, and MPS = medium preparation system.

Cultivation

Algae specific

	Porphyridium	**Unit**	**PBR**	**OP**	**Source(s)**
Mass	HNO_3 consumption	g.g biomass^{-1}	0.090	0.090	Supplier information (2019)
	$MgSO_4$ consumption	g.g biomass^{-1}	0.862	1.989	Supplier information (2019)
	Fe DTPA consumption	g.g biomass^{-1}	0.003	0.006	Supplier information (2019)
	H_3PO_4 consumption	g.g biomass^{-1}	0.012	0.012	Supplier information (2019)
	KOH consumption	g.g biomass^{-1}	0.248	0.248	Supplier information (2019)
	CO_2 fixation efficiency	% CO_2	75	41.23	(Acién, Fernández, Magán, & Molina, 2012; Doucha, Straka, & Lívanský, 2005; Ramanan, Kannan, Deshkar, Yadav, & Chakrabarti, 2010)
	CO_2 fixation	g.g biomass^{-1}	1.8	1.8	(Šingliar, Mikulec, Kušnír, & Polakovičová, 2013)
	Salt use	g.L^{-1}	15	15	Supplier information (2019)
	Phycoerythrin	%	2.18	2.18	(Guihéneuf & Stengel, 2015; Kavitha, Kathiresan, Bhattacharya, & Sarada, 2016; Rebolloso Fuentes, Acién Fernández, Sánchez Pérez, & Guil Guerrero, 2000; Torres-Acosta et al., 2016)
Process	Cultivation time	days	10	13	(Cohen & Arad, 1989; Guihéneuf & Stengel, 2015)
	Growth rate	g.L^{-1}.day^{-1}	0.246	0.082	Averages (Razaghi et al., 2014; Rodolfi et al., 2009)
	Growth PBR/OP		3	3	(Das, Bhowmick, & Mutharaj, 2019)
	Cultivation temperature	°C	20	20	(Rebolloso Fuentes et al., 2000; Román, Alvárez-Pez, Fernández, & Grima, 2002)
	Water recycling	%	90	90	Assumption
	Salt recycling	%	90	90	Assumption

	Dunaliella salina	Unit	PBR	OP	Source(s)
Mass	$MgSO_4$ consumption	g.g biomass^{-1}	0.140	0.775	(Tafreshi & Shariati, 2006)
	KNO_3 consumption	g.g biomass^{-1}	0.286	1.628	(Tafreshi & Shariati, 2006)
	$NaHCO_3$ consumption	g.g biomass^{-1}	0.095	0.541	(García-González et al., 2003)
	KH_2PO_4 consumption	g.g biomass^{-1}	0.008	0.044	(Tafreshi & Shariati, 2006)
	$FeCl_3.6H_2O$ consumption	g.g biomass^{-1}	0.002	0.009	(Tafreshi & Shariati, 2006)
	CO_2 fixation efficiency	% CO_2	75	41.23	(Acién et al., 2012; Doucha et al., 2005; Ramanan et al., 2010)
	CO_2 fixation	g.g biomass^{-1}	1.8	1.8	(Šingliar et al., 2013)
	Salt use	g.L^{-1}	117	117	(Tafreshi & Shariati, 2006)
	β-carotene	%	5.40	5.40	(García-González et al., 2003; Prieto et al., 2011)
Process	Cultivation time	days	10	23	(Thomassen et al., 2018)
	Growth rate	g.L^{-1}.day^{-1}	0.197	0.0135	(Prieto et al., 2011; Thomassen et al., 2018)
	Cultivation temperature	°C	25	25	(García-González et al., 2003)
	Water recycling	%	90	90	Assumption
	Salt recycling	%	90	90	Assumption

Equipment	**Parameter**	**Unit**	**PBR**	**OP**	**Source(s)**
Process and equipment	Electricity use Air blower	kW	1.1		Supplier information (2019)
	Electricity use Pumping	kW	0.8		Supplier information (2019)
	Electricity use mixing (blower + paddle wheel)	kW.m^{-3}		0.00372	(Jorquera, Kiperstok, Sales, Embiruçu, & Ghirardi, 2010)
	Electricity use CO_2 supply unit (CSU)	kWh.t CO_2^{-1}	0	22.2	(Kadam, 2001)
	Electricity use medium preparation system (MPS)	kW.m^{-3}.h	0.275	0.275	(Acién et al., 2012)
	Electricity use artificial light	kW	0.056		Supplier information (2019)
	> Artificial light use	h.day^{-1}	3		Supplier information (2019)
	> Lamps/volume PBR		0.024		Supplier information (2019)
	Heat loss	%.day^{-1}	30	100	Assumption

	Additional heating due to sollar irradiation	°C	5		(Thomassen et al., 2018)
	COP heat exchanger	-	3.25	3.25	AquaCal
	MPS hours	h	6	6	(Acién et al., 2012)
	Mixing hours	h	24	24	Assumption
	Number of reactors	#	20		Supplier information (2019)
	Inoculum system/reactor volume	$L.L^{-1}$	0.01	0.01	Supplier information (2019)
	Volume ground area	$L.m^{-2}$	36		Supplier information (2019)
	Height pond	m		0.2	(de Vree, 2016)
Emissions	N_2O emissions	kg N_2O.kg N^{-1}	0.0039	0.000024	(Fagerstone, Quinn, Bradley, De Long, & Marchese, 2011)
	NH_3 emissions	kg NH_3.kg N^{-1}	0.05	0.05	(Yuan, Kendall, & Zhang, 2015)
	O_2 emissions	g.g $biomass^{-1}$	1.07	1.07	(Buehner et al., 2009)
	Fugitive emissions open ended line	$kg.h^{-1}$	0.002	0.002	(Hassim, Pérez, & Hurme, 2010)
	Fugitive emissions tank	$kg.h^{-1}$	0.082	0.082	(Hassim et al., 2010)
	Fugitive emissions pumping (liquid)	$kg.h^{-1}$	0.0199	0.0199	(Hassim et al., 2010)
Harvesting	**Parameter**	**Unit**			**Source(s)**
Process and equipment	Biomass Loss	%	3		(Thomassen et al., 2018)
	Maximum concentration	%DW	12		(Grima, Acie, Medina, & Chisti, 2003)
	Electricity use centrifuge	$kWh.m^{-3}$	1.4		(Milledge & Heaven, 2011)
	Operating hours	h	24		Assumption
Emissions	Fugitive emissions centrifuge light liquid	$kg.h^{-1}$	0.0199		(Hassim et al., 2010)
Others	**Parameter**	**Unit**			**Source(s)**
	Average temperature Belgium	°C	11.50		KMI (2020)
	Average temperature France	°C	12.77		Tradingeconomics (2020)
	Operation rate	%	90		Assumption

4. Economic input data TSA.

	Parameter	Unit		Source(s)
General	Evaluation period	yr	10.00	Assumption
	Nominal discount rate	%	15.00	(Mercken, 2004)
	Equity - Debt ratio	%	20-80	Assumption
	Interest rate	%	4.50	Assumption
	Inflation rate	%	2.00	Eurostat (2019)
	Tax rate BE|FR	%	29|33.30	OECD (2019)
	CEPCI oct 2019	Index	599.30	("Economic indicators," 2020)
	Site preparation	$\%I_0$	10	(Caputo, Palumbo, Pelagagge, & Scacchia, 2005)
CAPEX	Cost PBR	$€.m^{-3}$	15,571 capacity $[m^3]^{-0.103}$	(Acién et al., 2012) and supplier information (2019)
	Lifetime PBR	yr	10.00	(Acién et al., 2012)
	Cost liner	$€.ha^{-1}$	90,438	(R. E. Davis et al., 2014; Lundquist, Woertz, Quinn, & Benemann, 2010; Norsker et al., 2011)
	Lifetime liner	yr	20	(R. Davis, Fishman, Frank, & Wigmosta, 2012)
	Cost paddle wheel	$€.ha^{-1}$	11,776	(Lundquist et al., 2010; Norsker et al., 2011; Rogers et al., 2014)
	Lifetime paddle wheel	yr	20	(Rogers et al., 2014)
	Cost inoculum	$€.ha^{-1}$	144,999	(Tredici et al., 2016) and supplier information (2019)
	Lifetime inoculum	yr	20	(R. E. Davis et al., 2014)
	Cost MPS	$€.m^{-3}.h$	7,144 capacity $[m^3.h^{-1}]^{-0.484}$	(Acién et al., 2012; Tredici et al., 2016)
	Lifetime MPS	yr	10	(Tredici et al., 2016)
	Cost artificial lighting	$€.unit^{-1}$	9	Gamma
	Lifetime artificial lighting	Yr	10	Gamma
	Cost heat exchanger	$€.m^{-3}$	702 capacity $[m^3]^{-0.013}$	Supplier information (2019)
	Lifetime heat exchanger	yr	15	(Thomassen et al., 2018)
	Cost centrifuge	$€.L^{-1}.h$	6,130 capacity $[L.h^{-1}]^{-0.425}$	Supplier information (2019)
	Lifetime centrifuge	yr	10	(Tredici et al., 2016)

OPEX	Price salt	€.t^{-1}	71	USGS -National Minerals Information Center (2017)
	Purchase price CO_2	€.t^{-1}	80	(Gorre, Ruoss, Karjunen, Schaffert, & Tynjälä, 2020)
	Purchase price HNO_3	€.t^{-1}	707	Alibaba (2019)
	Purchase price $MgSO_4$	€.t^{-1}	297	Alibaba (2019)
	Purchase price FeDTPA	€.t^{-1}	13,559	Mbferts (2019)
	Purchase price H_3PO_4	€.t^{-1}	9,323	Alibaba (2019)
	Purchase price KOH	€.t^{-1}	1,843	Alibaba (2019)
	Purchase price KNO_3	€.t^{-1}	1,594	Mbferts (2019)
	Purchase price $NaHCO_3$	€.t^{-1}	870	Intra Laboratories (2019)
	Purchase price KH_2PO_4	€.t^{-1}	1,993	Mbferts (2019)
	Purchase price $FeCl_3.6H_2O$	€.t^{-1}	488	Alibaba (2019)
	Labor cost	€.h^{-1}	39.70	Eurostat (2019)
	Working hours/day BE|FR	h.day^{-1}	7.6|7	ILO (2019)
	Working days	days	260	ILO (2019)
	Wage rate personnel BE|FR	€.h^{-1}	40.5|36.6	Eurostat (2019)
	Personnel on site	Persons	3	(Norsker et al., 2011)
	Ha for 1 additional person	ha.PBR^{-1}	10	(Thomassen et al., 2018)
	Ha for 1 additional person	ha.OP^{-1}	30	(Thomassen et al., 2018)
	Electricity cost BE|FR	€.MWh^{-1}	138.8|113.6	Eurostat (2019)
	Natural gas cost	€.MWh^{-1}	23.3	Eurostat (2019)
	Insurance cost	%I_0	1	(Peters et al., 2003)
	Repair cost	%I_0	1	Assumption
	Water purchase cost	€.m^{-3}	3.76	VMM (2020)
	Water disposal cost	€.m^{-3}	2	VMM (2020)
Revenues	Selling price phycoerythrin	€.kg^{-1}	36,000	(Hu, 2019)
	Selling price β-carotene	€.kg^{-1}	1,183	(Cuellar-Bermudez et al., 2015)
	Total market size food colorants	t.yr^{-1}	450,000	(Dominguez, 2013)

5. Environmental input data TSA.

Note: characterization factors are retrieved from the Ecoinvent 3.5 database. The additional material information needed is found in the tables below.

PBR (/unit)	**Unit**		**Source**
Scale: length	m	5,800	Supplier information
Scale: volume	m^3	18	Supplier information
Scale: sizing factor		0.897	Economic regression
Input: borosilicate glass	kg	5,800	Supplier information
Input: steel	kg	2,000	Supplier information
Input: PET	kg	49	Supplier information
Input: EPDM	kg	98	Supplier information
Input: PP	kg	70	Supplier information
Input: PE	kg	100	Supplier information
Input: RVS (steel)	kg	70	Supplier information

Paddle wheel (/unit)	**Unit**		**Source**
Scale: surface	ha	0.81	(Rogers et al., 2014)
Scale: sizing factor		1	Economic regression
Input: paddle width	m	12.2	(Rogers et al., 2014)
Input: paddle thickness	m	0.01	(Thomassen et al., 2018)
Input: paddle radials		8	(Lundquist et al., 2010)
Input: paddle material		HDPE	(Collet et al.,
Input: engine material		steel	(Collet et al., 2014)
Input: engine steel	kg	83	Rotary power (2019)
Input: paddle depth	m	0.15	(Tafreshi & Shariati, 2006)
Input: HDPE	kg	141.31	Calculated

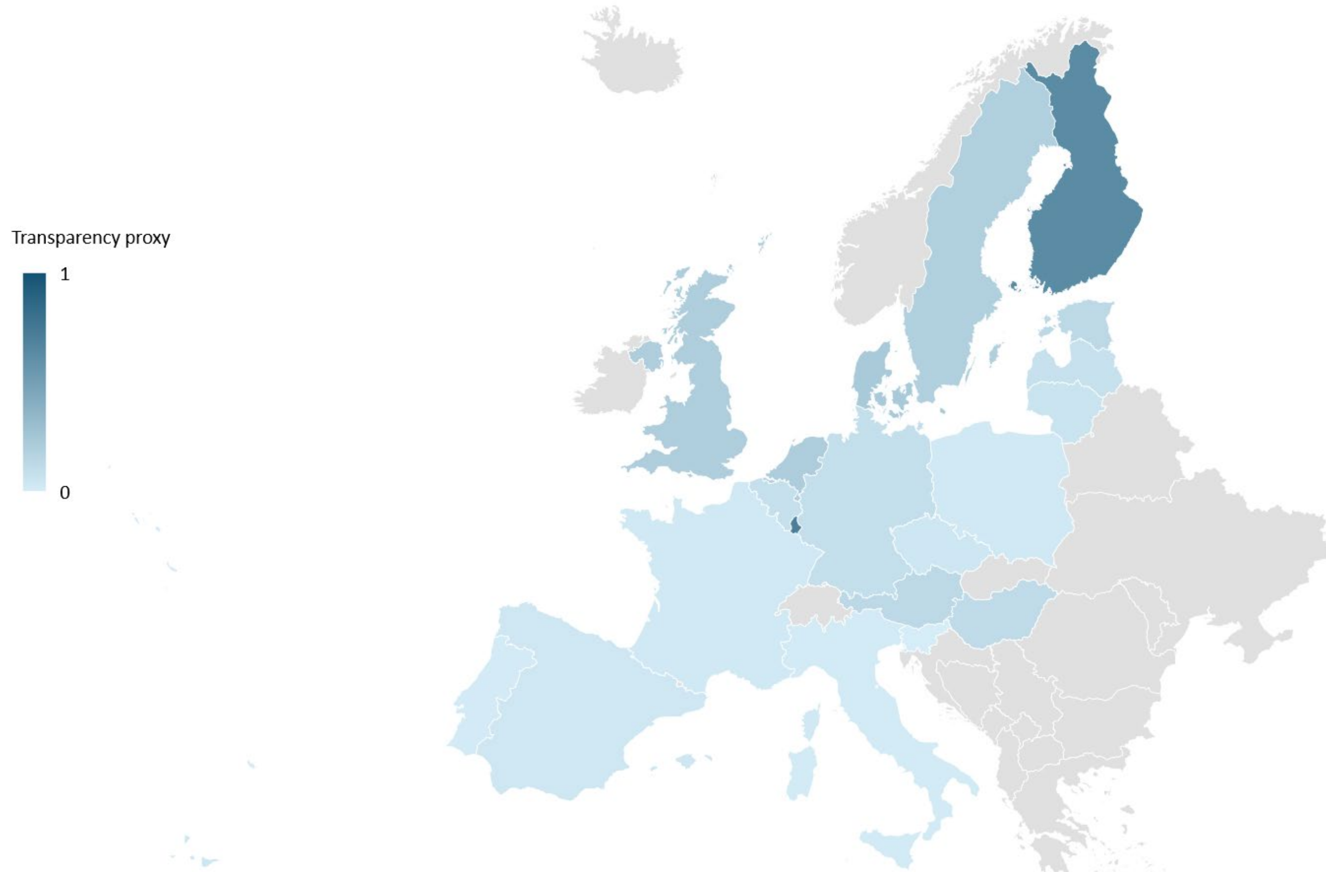
Liner (/unit)			
Scale: surface	ha	0.81	(Rogers et al., 2014)
Scale: sizing factor		1	Economic regression
Mass: material		HDPE	(R. E. Davis et al., 2014)
Mass: liner thickness	mil	40	(R. E. Davis et al., 2014)
Mass: liner width	m	12.2	(Rogers et al., 2014)
Mass: additional height	m	0.05	(Thomassen et al., 2018)
Mass: liner depth	m	0.2	(Tafreshi & Shariati, 2006)
Mass: HDPE	kg	81,444	Calculated

Centrifuge (/unit)			
Scale: input flow	$L.h^{-1}$	4,000	Supplier information
Scale: sizing factor		0.575	Economic regression
Input: steel	kg	2,905	Supplier information

6. Additional social input data TSA – a proxy for transparency.

Note: the transparency proxy was calculated for all countries within the EU for which data was available on the OECD website (2017). No data was found for Bulgaria, Croatia, Greece, Ireland, Romania, Slovakia, Malta, and Cyprus. The lowest transparency was present in Slovenia, and the highest in Luxembourg and Finland. These numbers were specifically calculated for transparency in the food and chemical sector. The higher the proxy number, the better.

Country	**# companies in manufacturing of chemical products**	**# companies in manufacturing of food products**	**# sustainability reports in food and chemicals**	**Transparency proxy**
Slovenia	218	2,263	0	0
Portugal	843	9,327	1	0.0098
Italy	4,250	52,542	9	0.0158
Poland	2,487	14,436	4	0.0236
France	3,042	51,288	13	0.0239
Spain	3,542	23,151	10	0.0375
Czech republic	1,793	8,087	4	0.0405
Lithuania	143	1,541	1	0.0594
Latvia	228	1,055	1	0.0779
Belgium	614	6,720	6	0.0818
Germany	3,019	21,498	23	0.0938
Hungary	672	4,558	6	0.1147
Austria	370	3,535	5	0.1280
Estonia	126	640	1	0.1305
Sweden	833	3,868	9	0.1914
United Kingdom	2,897	8,036	22	0.2012
Netherlands	912	5,924	14	0.2048
Denmark	277	1,466	4	0.2295
Finland	290	1,610	12	0.6316
Luxembourg	16	125	1	0.7092


Transparency proxy
1
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7. Sensitivity analysis.

Note: the sensitivity analysis was performed using Oracle Crystal Ball software, 10,000 trials, varying all input data by -10% to +10%, following a triangular distribution. The following tables show Spearman's rho (i.e., a rank correlation coefficient) values which are ≥ 0.2.

Environmental

Parameter	Unit	GHG	TETP	METP	FETP	LUP	AFD	FEP	MEP	WCP	EF	SEC
SCENARIO 1												
Recycled water	%									-0.8		
Recycled salt	%		-0.23	-0.21	-0.2				-0.24		-0.69	
Growth rate	$g.L^{-1}.day^{-1}$	-0.46	-0.39	-0.47	-0.46	-0.5	-0.49	-0.47	-0.45	-0.32	-0.2	-0.55
CO_2 fixation	$g.g\ biomass^{-1}$		0.24								-0.29	
Pigment content	%	-0.66	-0.72	-0.63	-0.63	-0.55	-0.6	-0.65	-0.62	-0.36	-0.55	-0.57
CO_2 eq.	$impact.kg^{-1}$		0.24									
Artificial light ratio	%	0.2		0.21	0.2	0.26	0.22	0.2	0.21			0.31
Artificial light	$h.day^{-1}$				0.22	0.26	0.24		0.21			0.3
Artificial light power	kW	0.22			0.21	0.26	0.23	0.21	0.21			0.3
Electricity eq.	$impact.kWh^{-1}$	0.36		0.33	0.34	0.43	0.39	0.34	0.34			
SCENARIO 2												
Recycled water	%									-0.45		
Pigment content	%	-0.97	-0.97	-0.97	-0.97	-0.97	-0.95	-0.97	-0.97	-0.84	-0.96	-0.93
SCENARIO 3												
Cultivation time	#days										-0.2	
Recycled salt	%			-0.2				-0.25	-0.21		-0.48	
Growth rate	$g.L^{-1}.day^{-1}$	-0.64	-0.64	-0.67	-0.67	-0.67	-0.66	-0.64	-0.66	-0.7	-0.56	-0.72
Pigment content	%	-0.71	-0.7	-0.65	-0.67	-0.67	0.69	-0.67	-0.66	-0.64	-0.62	-0.64
SCENARIO 4												
Recycled water	%									-0.41		
Recycled salt	%		-0.48	-0.48	-0.5	-0.46		-0.5	-0.54		-0.58	
Growth rate	$g.L^{-1}.day^{-1}$	-0.43	-0.34	-0.41	-0.38	-0.39	-0.44	-0.37	-0.36	-0.41	-0.34	-0.46
Pigment content	%	-0.8	-0.75	-0.74	-0.72	-0.74	-0.77	-0.73	-0.71	-0.74	-0.67	-0.76
Dunaliella optimal temp.	°C	0.26					0.31					0.34

Economic

Parameter	Unit	RMC	EC	CP
SCENARIO 1				
Recycled water	%	-0.59		
Cultivation time	#days	-0.21		
Growth rate	$g.L^{-1}.day^{-1}$	-0.23	-0.49	0.49
Pigment content	%	-0.59	-0.5	0.48
Electricity price	$€.MWh^{-1}$		0.48	
Pigment price	$€.kg^{-1}$			0.48
Artificial light ratio	%		0.28	
Artificial light	$h.day^{-1}$		0.29	
Artificial light power	kW		0.28	
PBR cost cte	$€.m^{-3}$			-0.41
PBR cost power	$€.m^{-3}$			-0.25
KOH consumption	$g.g[biomass]^{-1}$	0.21		
SCENARIO 2				
Pigment content	%	-0.96	-0.93	0.91
Centrifuge cost power	$€.L^{-1}.h$			-0.21
SCENARIO 3				
Cultivation time	#days	-0.25		
Recycled salt	%	-0.24		
Growth rate	$g.L^{-1}.day^{-1}$	-0.65	-0.72	0.71
Pigment content	%	-0.63	-0.62	0.62
SCENARIO 4				
Recycled salt	%	-0.3		
Growth rate	$g.L^{-1}.day^{-1}$	-0.44	-0.45	0.48
Pigment content	%	-0.79	-0.76	0.79
Dunaliella optimal temp.	°C		0.32	

Social

Parameter	Unit	HTP_c	HTP_{nc}
SCENARIO 1			
Recycled salt	%		-0.31
Growth rate	$g.L^{-1}.day^{-1}$	-0.55	-0.44
Pigment content	%	-0.67	-0.66
Electricity eq.	$impact.kWh^{-1}$	0.23	0.29
Steel eq.	$impact.kg^{-2}$	0.22	
SCENARIO 2			
Pigment content	%	-0.97	-0.97
SCENARIO 3			
Recycled salt	%		-0.28
Growth rate	$g.L^{-1}.day^{-1}$	-0.7	-0.65
Pigment content	%	-0.66	-0.65
SCENARIO 4			
Recycled salt	%	-0.44	-0.49
Growth rate	$g.L^{-1}.day^{-1}$	-0.41	-0.39
Pigment content	%	-0.75	-0.73

List of abbreviations: GHG = greenhouse gas emissions, TETP/METP/FETP = terrestrial/marine/freshwater ecotoxicity potential, LUP = land use potential; AFD = abiotic fossil depletion, FEP/MEP = freshwater/marine eutrophication potential, WCP = water consumption potential, EF = E-factor, SEC = specific energy consumption, RMC = raw materials cost, EC = energy cost, CP = capital productivity, MP = market potential, and HTP c/nc = human toxicity potential cancer/non-cancer

Appendix D. Supplementary information chapter 5

1. Indicator values for 43,300 trials – A Monte Carlo simulation.

Note: all the below values were converted to a non-beneficial (minimizing) shape in order to be compliant for the SMAA models.

SC1	**AFD**	**CP**	**EC**	**EF**	**FEP**	**FETP**	**FWP**	**GHG**	**HTP_C**	**HTP_{NC}**	**LUP**	**MEP**	**METP**	**PCI**	**PDI**	**PT**	**RA**	**RMC**	**SEC**	**TETP**	**WCP**
Base	156	-31	181	205	0.21	17	-1.34	626	27	373	36	0.03	23	-431	-16	-0.08	0.25	63	1.37	1,945	8
Mean	167	-24	194	230	0.22	19	-1.35	672	30	407	39	0.03	25	-474	-17	-0.1	0.25	71	1.48	2,096	10
Min	77	-69	81	108	0.11	9	-1.97	322	14	194	13	0.01	12	-517	-19	-0.12	0.25	34	0.63	1,045	3
Max	491	-5	623	657	0.65	56	-0.91	1,905	90	1,182	146	0.09	75	-431	-16	-0.08	0.25	188	4.71	5,681	32

SC2	**AFD**	**CP**	**EC**	**EF**	**FEP**	**FETP**	**FWP**	**GHG**	**HTP_C**	**HTP_{NC}**	**LUP**	**MEP**	**METP**	**PCI**	**PDI**	**PT**	**RA**	**RMC**	**SEC**	**TETP**	**WCP**
Base	223	-150	51	385	0.13	15	-1.34	831	14	294	9	0.02	10	-1,440	-16	-0.08	0.25	101	1.96	1,711	7
Mean	240	-113	55	407	0.14	16	-1.35	883	15	309	10	0.02	11	-1,584	-17	-0.1	0.25	107	2.13	1,787	8
Min	107	-310	23	212	0.07	8	-1.97	433	8	167	5	0.01	6	-1,728	-19	-0.12	0.25	53	0.88	1,012	4
Max	768	-25	192	1,053	0.35	40	-0.91	2,518	40	753	25	0.05	27	-1,440	-16	-0.08	0.25	296	7.4	3,965	25

SC3	**AFD**	**CP**	**EC**	**EF**	**FEP**	**FETP**	**FWP**	**GHG**	**HTP_C**	**HTP_{NC}**	**LUP**	**MEP**	**METP**	**PCI**	**PDI**	**PT**	**RA**	**RMC**	**SEC**	**TETP**	**WCP**
Base	33	-2	76	187	0.07	9	-0.82	188	12	216	6	0.02	12	-431	-22	-0.02	0.19	29	0.73	1,113	4
Mean	35	-2	81	257	0.09	10	-0.82	216	14	270	7	0.02	15	-474	-24	-0.03	0.19	37	0.78	1,315	5
Min	17	-7	36	50	0.03	4	-1.2	95	6	86	3	0.01	5	-517	-26	-0.04	0.19	11	0.35	523	2
Max	88	0	222	1,050	0.3	35	-0.56	628	45	956	22	0.07	49	-431	-22	-0.02	0.19	134	2.15	4,119	18

SC4	AFD	CP	EC	EF	FEP	FETP	FWP	GHG	HTP_C	HTP_{NC}	LUP	MEP	METP	PCI	PDI	PT	RA	RMC	SEC	TETP	WCP
Base	561	-2	150	904	0.22	23	-0.82	1,759	28	800	14	0.04	34	-1,440	-22	-0.02	0.12	153	7	2,783	12
Mean	599	-2	160	961	0.24	24	-0.82	1,872	29	851	15	0.04	37	-1,584	-24	-0.03	0.12	163	7	2,951	13
Min	283	-7	75	470	0.12	12	-1.2	905	14	414	8	0.02	18	-1,728	-26	-0.04	0.12	78	3	1,502	6
Max	1,533	0	412	2,394	0.59	60	-0.56	4,711	74	2,131	38	0.11	92	-1,440	-22	-0.02	0.12	413	18	7,088	32

List of abbreviations: SC = scenario; AFD = abiotic fossil depletion, CP = capital productivity, EC = energy cost, EF = E-factor, FEP/MEP = freshwater/marine eutrophication potential, FETP/METP/TETP = freshwater/terrestrial/marine ecotoxicity potential, FWP = fair wage potential, GHG = greenhouse gas emissions, HTP c/nc = human toxicity potential cancer/non-cancer, LUP = Land use potential, PCI = process innovation, PDI = product innovation, PT = product transparency, RA = risk aspects, RMC = raw materials cost, SEC = specific energy consumption, and WCP = water consumption potential.

2. Pseudocode MCDA model.

```
SMAA()
begin
    Initialize_via_user_input();
    Initialize: Result ← ∅; Rank ← ∅;
    foreach Monte Carlo iteration do
        Initialize
            InputArray ← Read_Monte_Carlo_iteration_from_file();
            listINDMatrixs ← ∅;
            listScoreMatrix ← ∅;
            listTScoreMatrix ← ∅;
        foreach indicator do
            Perform_a_pairwise_comparison_between_each_alternative_scenario();
        end
        Calculate_weighting_scheme();
        listSumWFlows ← Calculate_weighted_sum_of_flows();
        Result ← Result ∪⃖ {listSumWFlows};
        Ranking_of_alternative_scenarios ←
         Transform_listSumWFlows_into_ranking();
        Rank ← Rank ∪⃖ {Ranking_of_alternative_scenarios};
    end
end
```

```
Inititalize_via_user_input()
begin
    Number_of_scenarios;
    Number_of_indicators;
    Beneficial_vs_non_beneficial_character_of_indicators;
    Weighting_scheme;
    Prior_knowledge_or_not;
    if Prior_knowledge = true then
        Initial_ranking ← ∅;
        foreach indicator do
            Initial_ranking ← Initial_ranking ∪⃖ {rank_value};
        end
        if Weighting_scheme = Rank_Exponent_Weighting then
            Lower_limit_of_exponent_range;
            Upper_limit_of_exponent_range;
        end
    end
    Preference_structure;
    if Preference_structure = level_criterion then
        pLevel;
        qLevel;
    else
        if Preference_structure = linear_preference-indifference then
            pArray ← Beneficial_vs_non_beneficial_character_of_indicators ∗
             stan-
             dard_deviation_of_the_scores_of_the_alternative_scenarios_on_the_indicators
             /Number_of_alternative_scenarios;
            qArray ← pArray/2;
        end
    end
end
```

```
Perform_a_pairwise_comparison_between_each_alternative_scenario()
begin
    Initialize:
        initPairwiseArray ← matrix_of_zeros;
        initScoreArray ← matrix_of_zeros;
        initTScoreArray ← matrix_of_zeros;
    foreach h ∈ {1, ..., Number_of_indicators} do
        listINDMatrixs ← listINDMatrixs ∪ {initPairwiseArray};
        listScoreMatrix ← listScoreMatrix ∪ {initScoreArray};
        listTScoreMatrix ← listTScoreMatrix ∪ {initTScoreArray};
        foreach i ∈ {1, ..., Number_of_scenarios} do
            foreach j ∈ {1, ..., Number_of_scenarios} do
                listINDMatrixs_hij ← InputArray_jh  InputArray_ih;
                if ((Preference_structure = level_criterion) and
                 (Beneficial_vs_non_beneficial_character_of_indicators*listINDMatrixs_hij >
                 Beneficial_vs_non_beneficial_character_of_indicators* pLevel)) or
                 ((Preference_structure = linear_preference-indifference) and
                 (Beneficial_vs_non_beneficial_character_of_indicators*listINDMatrixs_hij >
                 Beneficial_vs_non_beneficial_character_of_indicators* pArray_h)) or
                 ((Preference_structure = true_criterion) and
                 (Beneficial_vs_non_beneficial_character_of_indicators*listINDMatrixs_hij >
                 0)) then
                    listScoreMatrix_hij ← 1;
                else if ((Preference_structure = level_criterion) and
                 (Beneficial_vs_non_beneficial_character_of_indicators*listINDMatrixs_hij ⩽
                 Beneficial_vs_non_beneficial_character_of_indicators*qLevel)) or
                 ((Preference_structure = linear_preference-indIfference) and
                 (Beneficial_vs_non_beneficial_character_of_indicators*listINDMatrixs_hij <
                 Beneficial_vs_non_beneficial_character_of_indicators*qArray_h)) or
                 ((Preference_structure = true_criterion) and
                 (Beneficial_vs_non_beneficial_character_of_indicators*listINDMatrixs_hij ⩽
                 0)) then
                    listScoreMatrix_hij ← 0;
                else if ((Preference_structure = level_criterion) and
                 (Beneficial_vs_non_beneficial_character_of_indicators* listINDMatrixs_hij >
                 Beneficial_vs_non_beneficial_character_of_indicators*qLevel) and
                 (Beneficial_vs_non_beneficial_character_of_indicators*listINDMatrixs_hij ⩽
                 Beneficial_vs_non_beneficial_character_of_indicators*pLevel)) then
                    listScoreMatrix_hij ← 1/2;
                else
                    listScoreMatrix_hij ← (listINDMatrixs_hij qArray_h) / (pArray_h qArray_h);
                end
            end
        end
        listTScoreMatrix_h ← listScoreMatrix^t_h;
    end
end
```

```
Calculate weighting scheme()
begin
    Initialize: ws ← ∅;
    if Weighting_scheme = equal_weight then
        foreach  i ∈ {1, ..., Number_of_indicators} do
            ws ← ws ⊎ { 1 / (Number of indicators) };
        end
    else if Weighting_scheme = stochastic_random_weighting then
        foreach i ∈ {1, ..., Number_of_indicators} do
            ws ← ws ⊎ {random ∈ [0, 1]};
        end
        sumws ← Σ_{i=1}^{Number_of_indicators} ws_i;
        ws ← ws / sumws;
    else if Weighting_scheme = rank_order_centroid_weighting then
        Initial_ranking ← ∅;
        foreach  i ∈ {1, ..., Number_of_indicators} do
            Initial_ranking ← Initial_ranking ⊎ {i};
        end
        InitRocwList= ∅;
        foreach j ∈ {1, ..., Number_of_indices} do
            total= 0;
            foreach i ∈ {j, ..., Number_of_indicators} do
                total ← total + 1 / Initial_ranking_i;
            end
            w ← total / Number_of_indicators;
            InitRocwList ← InitRocwList ⊎ {w};
        end
        foreach i ∈ {1, ..., Number_of_indices} do
            foreach j ∈ {1, ..., Number_of_indices} do
                if Initial_ranking_i = (j + 1) then
                    ws ← ws ⊎ {InitRocwList_j};
                end
            end
        end
```

else
$exp \leftarrow$ uniform random in $[Lower\_limit\_of\_exponent\_range,$
$Upper\_limit\_of\_exponent\_range]$;
$ws \leftarrow \emptyset$;
$total \leftarrow 0$;
foreach $i \in \{1, \ldots, Number\_of\_indicators\}$ **do**
$total = total + (Number\_of\_indicators - i)^{exp}$;
end
foreach $i \in \{1, \ldots, Number\_of\_indicators\}$ **do**
$w \leftarrow (Number\_of\_indicators - Initial\_ranking_i + 1)^{exp}$;
$ws \leftarrow ws \overleftarrow{\cup} \{w\}$;
end
end
end

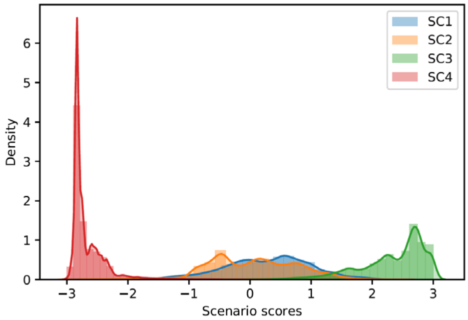
Calculate_weighted_sum_of_flows()
begin
Initialize: $listSumWFlows \leftarrow \emptyset$;
foreach do
scenario
end
$listSumWFlows \leftarrow listSumWFlows \overleftarrow{\cup} \{0\}$;
foreach $h \in \{1, \ldots, Number\_of\_indicators\}$ **do**
foreach $i \in \{1, \ldots, Number\_of\_scenarios\}$ **do**
$sumTScore \leftarrow \sum_{j=1}^{Number\_of\_scenarios} listTScoreMatrix_{hij}$;
$sumScore \leftarrow \sum_{j=1}^{Number\_of\_scenarios} listScoreMatrix_{hij}$;
$listSumWFlows_i \leftarrow listSumWFlows_i + (sumTScore -$
$sumScore) * ws_h$;
end
end
end

3. Average SMAA scores per sustainability dimension for different weighting schemes. SC = scenario, ROCW = rank order centroid weights, REW = rank exponent weights, and SRW = stochastic random weights.

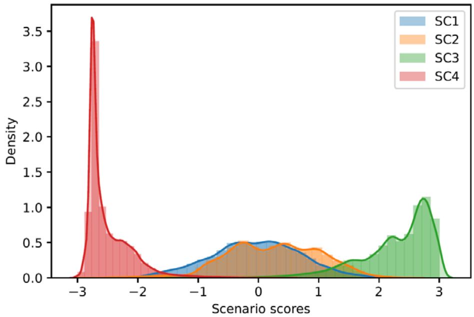
		SC1	SC2	SC3	SC4
Environmental	**ROCW**	0.284	0.048	2.334	-2.666
	REW flat	-0.048	0.253	2.292	-2.496
	REW steep	0.219	0.118	2.285	-2.622
	SRW	-0.199	0.331	2.297	-2.428
Economic	**ROCW**	-0.652	-0.157	0.952	-0.143
	REW flat	-0.993	0.150	0.600	0.243
	REW steep	-0.825	-0.140	0.796	0.170
	SRW	-1.080	0.417	0.517	0.146
Social	**ROCW**	1.152	1.899	-0.892	-2.159
	REW flat	0.961	1.871	-0.644	-2.188
	REW steep	1.047	1.887	-0.755	-2.179
	SRW	0.976	1.872	-0.667	-2.181

4. Histograms and Kernel density plots of environmental SMAA results for different weighting schemes. SC = scenario, ROCW = rank order centroid weights, REW = rank exponent weights, and SRW = stochastic random weights.

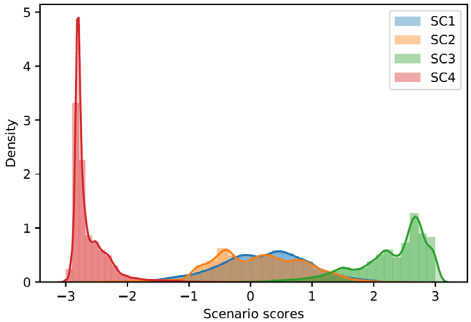
ROCW



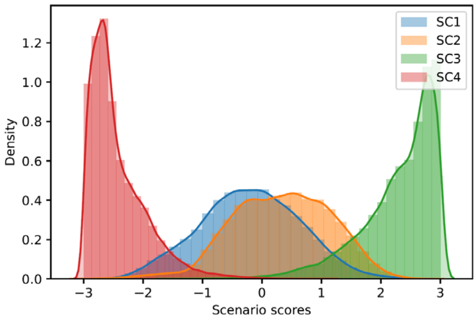
REW flat



REW steep



SRW



5. Average integrated SMAA scores for different weighting schemes and preference structures. SC = scenario, EW = equal weights, and SRW = stochastic random weights.

		SC1	SC2	SC3	SC4
Integrated sustainability	**EW, TYPE 1**	0.627	-1.060	-1.465	1.899
	EW, TYPE 2, p=1 q=0	0.650	-1.240	-1.628	2.219
	EW, TYPE 2, p=2 q=1	0.469	-0.695	-1.028	1.254
	SRW, TYPE 1	0.628	-1.059	-1.468	1.898
	SRW, TYPE 2, p=1 q=0	0.646	-1.241	-1.625	2.220
	SRW, TYPE 2, p=2 q=1	0.469	-0.694	-1.029	1.253

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