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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 societal 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 paper, 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 (50%), whereas two-dimensional sets complement the environmental issues with economic indicators (34%). Moreover, even the sets encompassing all three sustainability dimensions (16%) 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.

KEYWORDS

Biobased economy, green chemistry, biobased chemicals, sustainability indicators, environmental indicators, economic indicators, social indicators

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% of chemicals are hazardous to human health or the environment in the EU [1]. Legislations like REACH (Registration, Evaluation and Authorization of Chemicals) and RoHS (Restriction on Hazardous Substances) have been introduced to stimulate the use of less hazardous chemicals. The concept of 'green chemistry' corresponds to these policies and is defined as "the design of chemical products and processes that reduce or eliminate the use and generation of hazardous substances" [2]. The definition of green chemistry is based on twelve principles, designed to help achieve sustainability, formulated by Anastas and Warner (1998) [3]. One of these principles is the use of renewable feedstocks, which can be translated into practice by the use and production of biobased chemicals, such as bioplastics and specialty chemicals.

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 [4]. The focus in the biobased economy is currently shifting from bioenergy and biofuels to the production of high value biobased products, including biobased chemicals [5]. 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 [6]. In 2014, the EU turnover of manufacturing biobased chemicals, pharmaceuticals, plastics and rubber was 130 billion euros, compared to 30 billion euros for liquid biofuels and 10 billion euros for biobased electricity [7].

The emerging biobased economy is often associated with increased sustainability [8]. 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 [9, 10]. To ensure that biobased products become or remain more sustainable than their fossil fuel based counterparts, a systematic and interdisciplinary assessment approach is needed [8]. 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 [11]. Criteria and indicators can be used as flexible and user-friendly techniques to evaluate and integrate environmental, economic and societal impacts. Sustainability indicators are needed to translate sustainability into a practical set of measures and are frequently used for policy- and decision-making [12–14].

International attempts to provide and stimulate sustainability within the general bioeconomy started with the development of criteria and indicators for sustainable forest management [5]. These first environmental assessments were designed as a result of the concerns about tropical deforestation. Later, sustainability frameworks for biofuels and bioenergy followed [5]. 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 [15, 16]. 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 [12,17]. 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) agree with these concerns regarding inadequate sustainable management [18–22]. 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 this paper 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 [23]. 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 [24,25]. 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 [26]. Moreover, a standardized set of sustainability indicators enables comparisons between biobased chemicals and facilitates policy recommendations. This paper 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 [27].

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, followed by an extensive discussion and conclusion.

2. Method

This 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) (Fig. 1). 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.

The decision for inclusion of articles is 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 are selected based on the use of sets of indicators aiming for a sustainability evaluation of a biobased chemical. Research about stand-alone indicators is 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 are not necessarily included, only if applied on a biobased chemical case study or considered relevant by other biobased chemical research applications. Second, the included indicator-sets are all developed for assessment on the product level of the chemical. Research that explores sustainable development more broadly, like on a company- or country-level, was excluded from the dataset.

The 38 papers that are included in this analysis to discuss a comprehensive selection of indicators is provided in Appendix A. The indicators are classified within the corresponding sustainability domain and assigned to a sustainability criterion. In the analysis, 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.

(Insert Figure 1)

The studies included for the gap analysis are 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 B).

3. Results

The included pool of articles consists of 20 method papers and 18 application papers. 70% of the 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) [3] (Fig. 2). Between 2004 and 2007, no relevant publications were found. From 2010 onwards, the first actual applications of the method articles emerge.

(Insert Figure 2)

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) confirm the interchangeability between metrics and indicators and specify metrics as only referring to quantitative measures, whereas indicators can also encompass qualitative descriptions [13]. In this paper the approach of Tanzil et al. (2006) where indicators can be both quantitative and qualitative is followed.

When screening the pool of indicators, a differentiation is 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 are marked as 'available' when explicitly described as part of the proposed framework developed or used in the paper. Indicators are 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 (RBE) is an available indicator in the framework of Sacramento-Rivero (2012) (Fig. 3), which is calculated using the constituent indicators global warming potential (GWP), ozone depletion, photo-oxidant formation, eutrophication, toxicities and acidification [28]. 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.

(Insert Figure 3)

Overall, 85 different indicators are proposed or used, with 59% of the indicators reflecting a variety of environmental impacts, 26% reflecting economic impacts and 15% reflecting social impacts (Fig. 4). 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 (i.e. 20%) developed in method papers explicitly tackle all three sustainability dimensions, whereas nine of the method papers (i.e. 45%) only assess the environment. On top, even if all three pillars are mentioned, the environmental dimension represents the majority of indicators in all papers. This lack of comprehensive and complete sets of indicators is even more explicit when examining the existing case studies (i.e. the application papers). For the biobased chemical application papers, 56% of the included papers only evaluate the environmental aspects. On top, these application papers often apply generic indicator-sets like ReCiPe or CML2 Baseline 2000, where the specific characteristics of biobased products, like renewability, are not taken into account [31, 32]. Over time, there is no trend noticed as for the inclusion of all three sustainability domains. The first authors that explicitly deal with economic and social impacts within biobased chemistry are Sugiyama et al. (2008), introducing the Net Present Value (NPV) and the 'Environment, Health and Safety Index (EHSI)' within the assessment. In 2016 and 2017, there were no publications including social impacts, except for some including human toxicity as an environmental indicator.

(Insert Figure 4)

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

(Insert Table 1)

3.1. Environmental indicators

The selected sustainability assessments provide 49 different environmental indicators (Appendix B.1.). Frequently used indicators like eutrophication, acidification and Global Warming Potential appear already in the first publications included in this review study [29–31]. 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.

Climate change is widely included as an impact category when assessing the environmental performance. 84% of the sets consider climate change as a constituent indicator, which makes it the number one used indicator in biobased chemical sustainability assessment. Nguyen et al. (2015) describe greenhouse gas (GHG) emissions as "all sources of CO_2, NH_4 and N_2O released from the production process, less any amount of CO_2 absorbed by the biobased feedstock during growth" [32]. GHG emissions operate as a useful indicator for climate change because the atmospheric concentrations of CO_2, NH_4 and N_2O have been proven to be the dominant cause of global warming (IPCC report) [33]. Often, the emissions are expressed in CO_2 equivalents in reference to their global warming potential (GWP), which measures the impact of greenhouse gasses on climate change by combining radiative forcing and the atmospheric lifetime of a gas molecule [34].

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 [32]. Huijbregts et al. (2010) found that CED serves as a relevant screening indicator for environmental performance [15]. 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 [35]. 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 [30]. 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 [36]. All other indicator-sets neglect the topic of renewable resources and the corresponding environmental impacts. 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 [37]. Land use is included in 50% (as a constituent indicator) of the existing indicator-sets. 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 [37]. 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 urban and agricultural land occupation as well as natural land transformation to calculate the full land use impact [29]. Because the land use indicator is often not well specified, different definitions of 'land use' are used interchangeably. Sheldon et al. (2015) define 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) highlight the resulting ecosystem damage [37–39]. 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 (45% as a constituent indicator), which includes the midpoint indicators, and 'ecosystem damage' indicators (13% as a constituent indicator), which includes 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 [40].

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 (55%), photo-oxidant formation (47%), marine eutrophication (53%) or freshwater eutrophication (59%), 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 4 method papers [16]. 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) [41].

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 B.2.). 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 (EC), economic index (EI) or investment value indicators like Net Present Value (NPV) or Minimum Selling Price (MSP). Although the listed economic indicators use mostly cost-related measures, 74% of the indicator-sets tackling economic impacts additionally try to estimate the profitability or calculate the investment value. The other 26% of the indicator-sets only calculate the costs related to the biobased chemical. 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, societal 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 analysis shows 13 different indicators evaluating the social sustainability of biobased chemicals (Appendix B.3.). 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 [28]. Human toxicity, accounting for the impact of toxic substances on human environment, is by far the most included social indicator currently existing for biobased chemicals, included in all the three-dimensional indicator-sets of this review study. Most publications consider human toxicity as an environmental indicator instead of a societal indicator. In this analysis 'human toxicity' is 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) [42].

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 biobased chemical indicator-sets are still 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 [43]. With demand for food increasing and climate change impacting agricultural yields, the impact of the biobased economy on food security and prices raises concerns [44]. 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 [44,45]. However, policy makers should stimulate good governance and should facilitate synergies between the different biomass uses [46].

3.4. Indices

Finally, indices are 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 [47]. Only two 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 societal impacts [48]. The lack of these interdisciplinary indices points to the availability of multidisciplinary indicator-sets without accounting for sufficient integration.

4. Discussion

This analysis finds that 50% of the included indicator-sets (n=38) consider only one sustainability dimension, 34% include two sustainability dimensions and another 16% emphasize all three dimensions. Environmental impacts are included in 100% of the sustainability sets, economic impacts in 50% of the sets and the social impacts in 16% of the sets (Fig. 5) (left axis). A close relationship is found between the number of dimensions included and the content of the sustainability indicators. Analysing the proportion of indicators used in biobased chemical assessment, again the environmental indicators predominate (Fig. 5) (right axis). A hierarchy of sustainability dimensions is found. If an assessment includes one sustainability dimension (1D), only the environmental impacts are considered. When two dimensions (2D) are included, economic and environmental issues are estimated. The social dimension only appears whenever environmental and economic aspects are also included in the indicator-set (3D).

(Insert Figure 5)

Considering the 12 most-used indicators for biobased chemical sustainability, environmental indicators clearly predominate the ranking (Fig. 6). 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 [49]. 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 [50]. LCA is widely applied in practice and might also be included in future European legislation like the Product Environmental Footprint method (PEF) [51]. However, the challenge remains to define a relevant set of indicators and include all components of sustainable development [52]. The fixation on environment is in stark contrast with the poor inclusion of social indicators [53]. Most assessments justify this lack of societal consequences by addressing its subjectivity and pointing to the lack of current scientific research related to the topic of social sustainability.

(Insert Figure 6)

This study shows that many indicators are still divided into the classic three-pillar sustainability dimensions (*i.e.* environment, economy and society). Some articles provide other classification schemes as well. For example, Sacramento-Rivero (2012) groups indicators into five categories (i.e. feedstock, process, products, environment and corporate) and Tabone et al. (2010) establish a link between indicators and the green chemistry principles [30, 43]. Multidisciplinarity within sustainability research is accepted and the importance of all three sustainability fields is recognised. 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 [54]. Moving to interdisciplinarity or transdisciplinarity can provide a solution by incorporating insights from the different fields and generating integration between the sustainability domains [8].

There is no consensus on a set of indicators for biobased chemical assessment and gaps, mostly concerning the assessment of economic and societal impacts, are present in current literature. To move towards a comprehensive and well-accepted list of indicators for the industry, government and academics, we advise using the framework provided in Fig. 7. This framework is developed based on the results of this study and the 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 B) 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, for example, the Delphi method, which gathers feedback from different stakeholders to deal with the complexity of the topic of sustainability [55]. 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 (e.g. the analytical hierarchy process) 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 is derived for use in a standardized sustainability assessment.

Future research might follow up on this framework to create a set of sustainability indicators specifically for biobased chemicals. In order to do so, some obstacles need to be overcome first. The inclusion of social indicators together with environmental and economic indicators means that qualitative and 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.

(Insert Figure 7)

5. Conclusion

This research reviews 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 reflected in an increasing rate of publications pertaining to the topic. For the existing body of literature we find 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 greenhouse gas 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, like for example ‘renewability’ or ‘food security’.

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 (Fig. 7), starting from the list of indicators constructed in this review study. If companies and governmental bodies assess their activities by applying the same criteria and indicators, consistent evaluations and comparisons between biobased chemicals will become possible. Future research should aim for adequate sustainability assessments that establish and promote biobased chemicals that “meet the needs of the present without comprising the ability of future generations to meet their own needs” [56].

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APPENDIX A

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

APPENDIX B

B.1. Environmental indicators included in sustainability assessments for biobased chemicals

		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 [32]. GWP represents the global warming potential, which is a combination of radiative forcing and atmospheric lifetime, for a time horizon 100 years (IPCC) [29,34]
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 [32]. 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 FEC (Fossil Energy Consumption), calculated based on CED of raw material and utilities [32]
		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 [38]
		Energy loss index (ELI)	estimates energy-related efforts in the process using reaction information only, aggregating 5 indicators: water in reactor outlet, product concentration, boiling point, MLI and reaction enthalpy [41]
		Non-renewable energy share	measures how much fossil energy is displaced by the new process/product [28]
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 [28]
		Land use: occupation and transformation	serves as an umbrella covering all land use indicators covering land transformation and land occupation
		Agricultural land occupation	calculates the amount of agricultural area occupied (in m^2) [29]
		Natural land transformation	calculates the amount of transformed area per year. 'Natural land' represents the type of land that arises without human distortion [29]
		Urban land occupation	calculates the amount of urban area occupied (in m^2) [29]
		Soil organic matter (SOM)	calculates the impact on fertile land use as it influences properties like buffer capacity, soil structure and fertility [57]
		Indirect land use change	calculates greenhouse gas emissions caused by land use change [58]
	Materials	Renewable sources	represents the % of material from biological sources in the final product, by mass [36]
		Use local sources	accounts for the categorical distance of the furthest feedstock location: international, national and regional [36]
		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 [28]
		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 [59]
		Material efficiency	gives the total weight of useful products, divided by the total weight of useful products and waste [38]
		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 [36]
		Design products for recycle	can be measured by the % recovery of a material in the U.S. municipal recycle stream [36]
	Abiotic depletion	Abiotic depletion potential (ADF)	calculates each extraction of minerals and fossils based on concentration reserves and rate of de-accumulation [30]
		Mineral depl.	indicates the extraction of mineral resources in kg [29]
		Fossil fuel depl.	indicates the extraction of fossil resources in kg [29]
		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 [31]

	Water	Freshwater-use reduction (WR)	indicates the water-use reduction achieved by a product or a biorefinery [28]
	Water	Water depletion/ water use	gives an estimation of the potential amount of water embodied inside a bio-based chemical [29,35]
ECOSYSTEM CARE	Air	Acidification	represents the decrease of pH by calculating at the base saturation [29]
ECOSYSTEM CARE	Air	Ionising radiation	calculates the level of exposure related to releases of radioactive material to the environment [29]
ECOSYSTEM CARE	Air	Particulate matter formation	gives an indication of the air quality and the presence of PM10 in the air [29]
ECOSYSTEM CARE	Air	Photo-oxidant formation	estimates the formation of reactive substances, also indicated as summer smog" [29,30]
ECOSYSTEM CARE	Air	Stratospheric ozone depletion	calculates the stratospheric ozone concentration [29]
ECOSYSTEM CARE	Eutrophication	Eutrophication	includes all effects due to excessive levels of macronutrients in the environment caused by emissions of nutrients to air, water and soil [60]
ECOSYSTEM CARE	Eutrophication	Freshwater eutrophication	refers to the eutrophication of fresh water with phosphor and nitrogen [29]
ECOSYSTEM CARE	Eutrophication	Marine eutrophication	refers to the eutrophication of marine water with phosphor and nitrogen [29]
ECOSYSTEM CARE	Eutrophication	Terrestrial eutrophication	refers to the enrichment of terrestrial ecosystems with phosphor and nitrogen [30]
ECOSYSTEM CARE	Ecotoxicity	Ecotoxicity	refers to the impact on ecosystems caused by emissions of toxic substances
ECOSYSTEM CARE	Ecotoxicity	Freshwater ecotoxicity	refers to the impact on freshwater systems caused by emissions of toxic substances to air, water and soil [30]
ECOSYSTEM CARE	Ecotoxicity	Marine ecotoxicity	refers to the impact on marine ecosystems caused by emissions of toxic substances to air, water and soil [30]
ECOSYSTEM CARE	Ecotoxicity	Terrestrial ecotoxicity	refers to the impact on terrestrial ecosystems caused by emissions of toxic substances [60]
ECOSYSTEM CARE	Waste	Atom economy (AE)	accounts for a rough estimate of the amount of waste that will be generated by different processes [61]
ECOSYSTEM CARE	Waste	Design biodegradable products	is measured by categorical classifications: non-biodegradable, biodegradable in an industrial facility and biodegradable in typical backyard conditions [36]
ECOSYSTEM CARE	Waste	E factor	accounts for the actual amount of waste produced in the process, defined as everything but the desired product [61]
ECOSYSTEM CARE	Waste	Environmental quotient (EQ)	takes into account not only the amount of waste (E factor), but also the nature of the waste [61]
ECOSYSTEM CARE	Waste	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 [41]
INDICES		Reduction of baseline emissions (RBE)	aggregates abiotic depletion, GWP, ozone depletion, photochemical oxidation, human- and eco-toxicities, acidification, and eutrophication [28]
INDICES		EI of raw materials	relates to the environmental impacts (EI) of raw materials per unit of product represented by GHG and CED [47]
INDICES		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 [62]
INDICES		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 [48]
INDICES		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 [29]

B.2. Economic indicators included in sustainability assessments for biobased chemicals

		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 [28]
		Transportation cost (TC)	calculates the cost of fuel consumption, capital recovery of transportation equipment and (un)loading [32]
	Production	Production cost/ Conversion cost (CC)	calculates the costs of raw materials, utilities, depreciation and others (including labor, maintenance, supplies and taxes) [32]
		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. [32]
		Taxes	calculates the taxes
		Energy cost	calculates the cost of energy
		Maintenance activities	calculates the cost of maintenance activities
		Total production cost (PC)	calculates the sum of TC and CC [32]
	End of Life	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 [28]
		Economic constraint (EC)	provides information about the raw material cost (feedstock) relative to the market value of the products [48]
		Fraction of revenue for feedstock (FRF)	represents the quotient of costs of the feedstock and the economic value of the product [28]
	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 [36]
		Economic index (EI)	calculates the ratio between the product price and the cost of synthesis (i.e. utilities and raw materials) [35]
		Modified gross margin (GM)	a financial ratio that relates the gross profit (GP) to the net sales (NS) [28]
	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 [63]
		Minimum selling price (MSP)	calculates the selling price that would bring the NPV to zero at a defined number of years [64]
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) [26]

B.3. Social indicators included in sustainability assessments for biobased chemicals

	Indicator name	Description
HEALTH	DALY (Disability-adjusted loss of life years)	calculates the sum of years of life lost and years of life disabled [29]
	Human toxicity	accounts for the effects of toxic substances on the human environment, usually not focused on the working environment [30]
	Human health: criteria air pollutants	accounts for human health effects due to exposure to ambient particulates [31]
	Human health: cancer	is the potential for toxicological impacts related to cancer effects [31]
	Human health: non-cancer	is the potential for toxicological impacts related to non-cancer effects [31]
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) [32]
	Process inherent safety (IPI)	aggregates: inventory of chemicals (II), process temperature (IT) and pressure (IP), type of equipment (IEQ), and structure of process (IST) [32]
	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 (2000 hours worked per employee per year) [28]
	Rate of fatal work injuries (RFWI)	calculates the number of recordable incidents for each 100 000 full-time employees per year (2000 hours worked per employee per year) [28]
SOCIAL CARE	Social investment (SI)	accounts for the contribution through employment and philanthropic and community development projects [28]
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) [48]
	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 [28]
	Health and safety compliance (HSC)	represents the degree of compliance with the normative OHS (Occupational Health and Safety) [28]

FIGURES

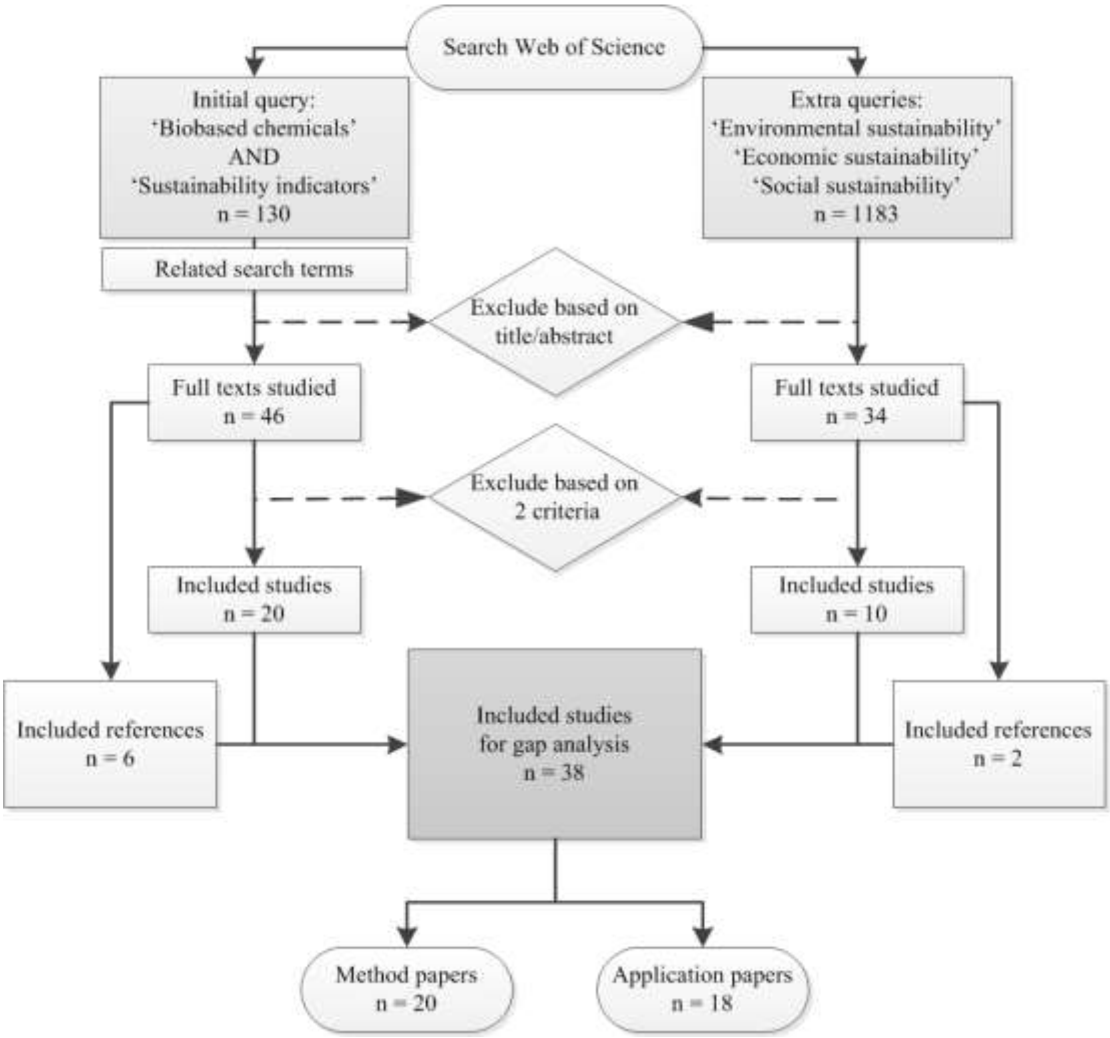

Fig. 1. Flowchart of article search and –selection

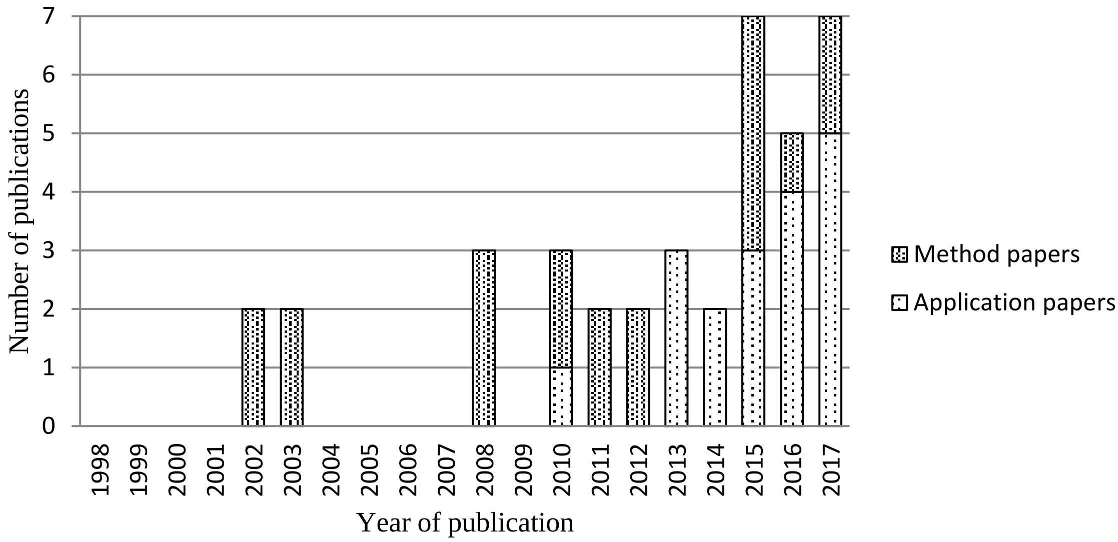

Fig. 2. Number of included publications 1998-2017 (n=38)

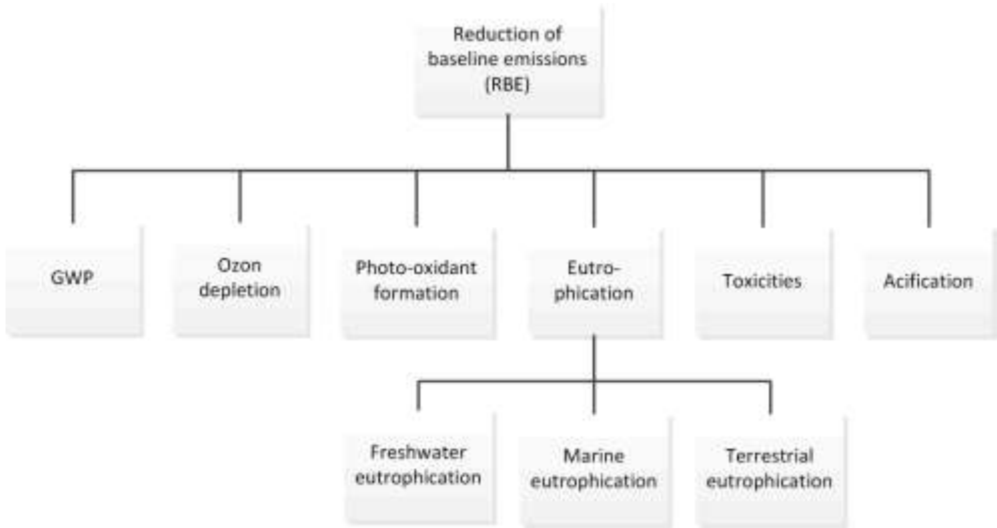

Fig. 3. Example of interlinkages between indicators [28]

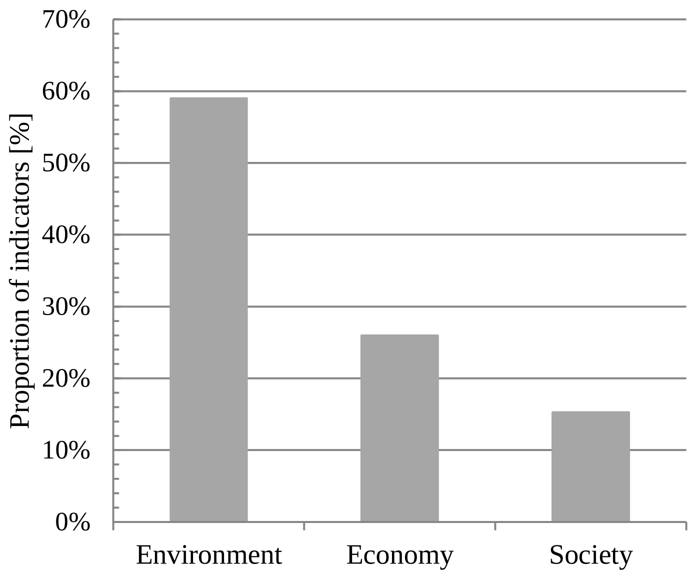

Fig. 4. Sustainability dimensions explicitly available in pool of indicators (n=38)

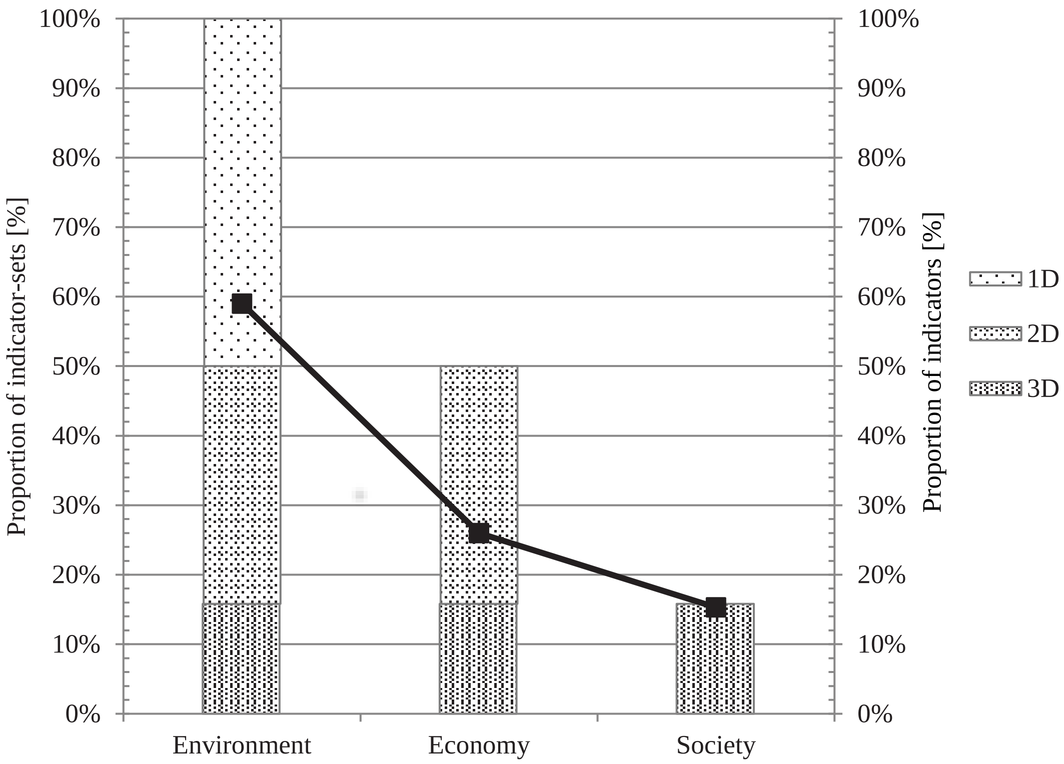

Fig. 5. Sustainability dimensions included in assessments of biobased chemicals
('Dimensionality' (1D, 2D, 3D) on left axis, 'Indicators' on right axis) (n=38))

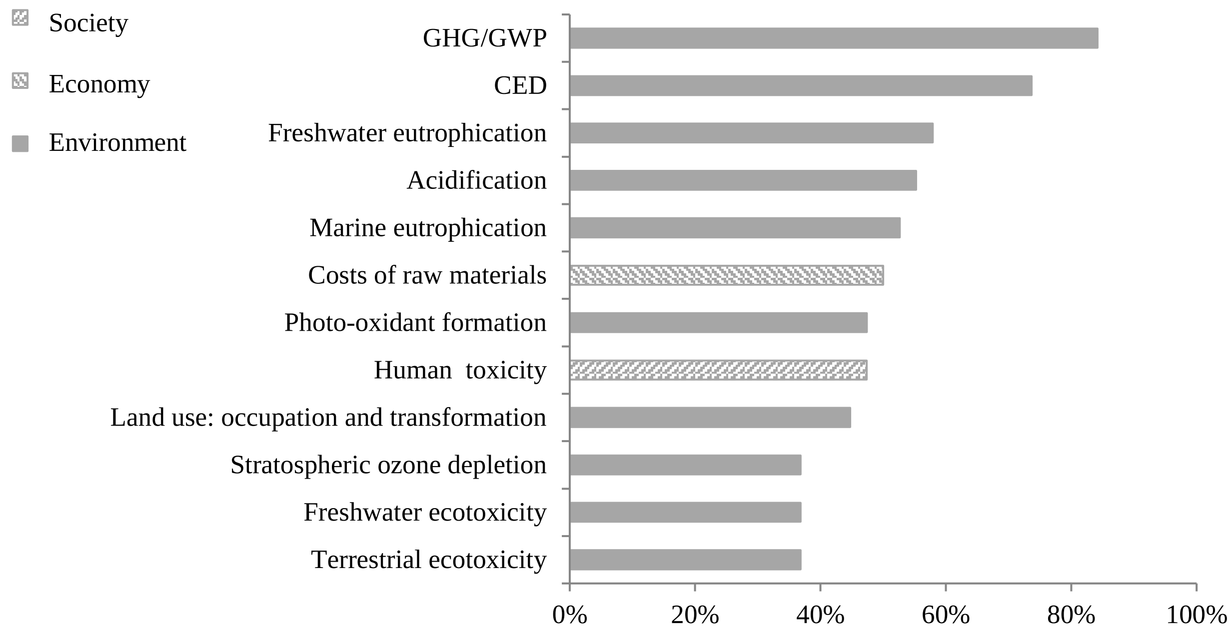

Fig. 6. Top 12 sustainability indicators used in biobased chemical sustainability assessments (n=38)

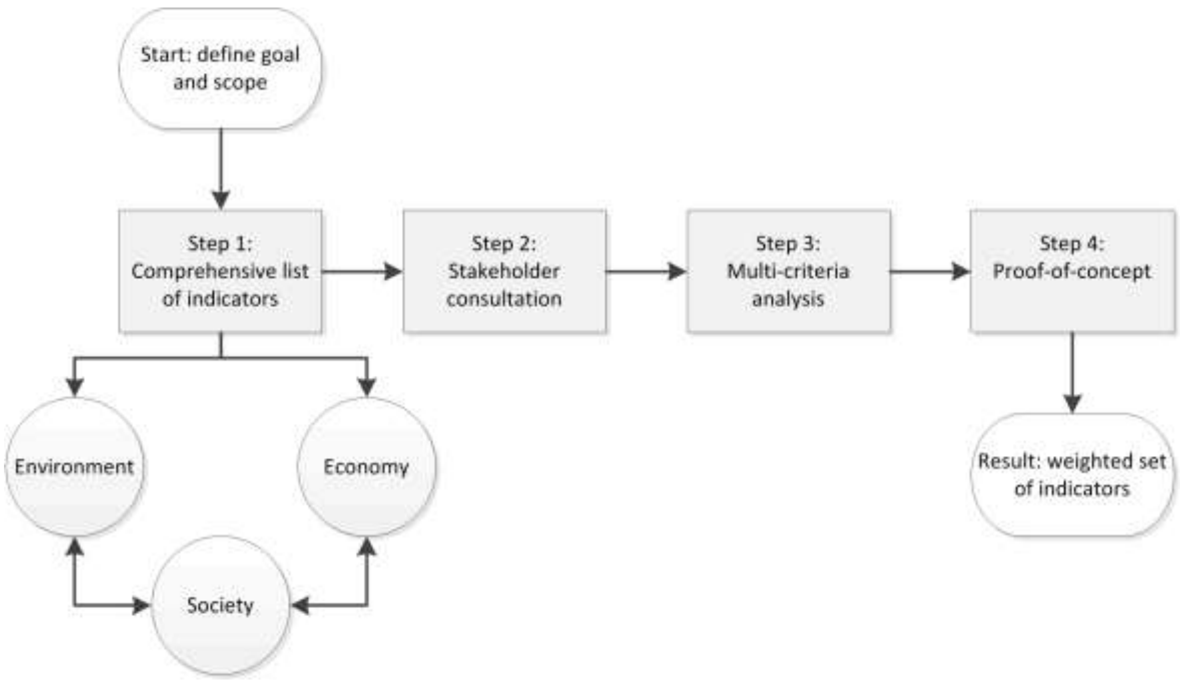

Fig. 7. Constructing an indicator-set to assess sustainability: a framework

TABLES

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

Dimension	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 process 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