Monitoring Bioeconomy Transitions: Development of Indicators and Measuring Bioplastics in Germany, Using an Extended Hybrid IO-LCA Model

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von
Wiebke Jander, M.Sc., geb. Wodni

Präsidentin
der Humboldt-Universität zu Berlin:

Prof. Dr. Julia von Blumenthal

Dekan der Lebenswissenschaftlichen Fakultät
der Humboldt-Universität zu Berlin:

Prof. Dr. Dr. Christian Ulrichs

Gutachter:

1. PD Dr. habil. Philipp Grundmann
2. Prof. Dr. Harald Grethe
3. Prof. Dr. Justus Wesseler

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Extended Summary

Background and motivation

The relationship between bioeconomy transitions and sustainable development is not straightforward. Although bioeconomies rely on biomass inputs and biotechnologies, their contribution towards improving socio-economic and environmental conditions has been a subject of much debate. For policymakers it is often difficult to keep track of bioeconomy developments and formulate appropriate bioeconomy-related policies that are also conducive towards sustainable development. Consequently, bioeconomy monitoring systems have recently been initiated to provide more reliable sources of information, especially for policy purposes. With this thesis, I strive towards refining such systems by exploring the development of bioeconomy transition indicators from a theoretical, methodological, and practical point of view.

Research needs and design

There is a clear mismatch between visions of bioeconomy transition and available indicators. In particular, the transition from fossil-based to bio-based economies is often assumed as a good in itself but, due to missing data, has not been measured precisely using reliable indicators. I aim here to enhance current bioeconomy monitoring systems by developing and applying a set of appropriate indicators and providing insight into three key issues: 1) how indicators can be systematically developed, 2) what dimensions of an economy need to receive attention while monitoring transition from a fossil-based to a bio-based one, and 3) what kinds of quantitative models are suitable for this purpose. I address these issues in each of the main chapters, 2 through 5. In Chapter 2, I explore how available indicators can be improved and data gaps filled in the short term using low-cost and high-benefit options to measure key environmental indicators for the German surfactant industry in 2015, taken as an example. In Chapter 3, I adapt a bioeconomy framework, derive a relevant indicator for it from a theoretical point of view, and compare bottom-up and top-down approaches to modelling this indicator for the German biofuels and bioplastics industries in 2011. In Chapter 4, I adopt a hybrid modelling approach for developing an economic input-output (IO) model, apply it to the plastics industry in Germany in 2016, and measure related economic and environmental indicators. To my knowledge, this is the first time a model has integrated data and information on bio-based and fossil-based plastics production, trade, resources, prices, and technologies at a disaggregated sectoral and regional level into economy-wide monetary supply and use tables. In Chapter 5, because the use of bio-based plastics data involved some uncertainty, I check the robustness of the developed indicators by combining results of Monte Carlo simulations with qualitative data analysis.

Key research results

The *Substitution Share Indicator (SSI*), developed in this study to quantify the transition from a fossil-based to a bio-based economy, measures the percentage of fossil resource savings due to replacement of functionally very similar production outputs that use fossil resources with those using biogenic resources compared to the fossil resource use that would be required if no substitution took place. Measurement of the *SSI* and related economic and environmental indicators in this study has revealed that substitution of bio-based plastics for fossil-based plastics in Germany in 2016 reduced fossil resource use by 16% and required less water (-9%) but emitted more greenhouse gases (+34%) throughout the chosen cradle-to-gate system. Higher emissions in this case were due to higher process-energy use for bio-based plastics compared to fossil-based plastics. Employee compensation was 11% higher, but effects on value added were not noteworthy (-1%).

The *SSI* was systematically developed specifically for assessing bioeconomy transitions, rather than being based on available data. Its measurements, consequently, revealed considerable data gaps that had to be filled through modelling. This approach resulted in trade-offs between indicator assessment criteria. While the *SSI* is relevant – being closely linked to tracking transition processes – it has some limitations concerning its credibility, ease of use, and robustness. By contrast, indicators for economic and environmental pressures were easily measurable with available data, but their relevance is questionable.

Aspects requiring special attention in monitoring transition from a fossil-based to a bio-based economy are the supply chain and sectoral levels chosen for matching functionally similar production outputs that are assumed as substitutes, because they influence results significantly. For example, choosing a downstream supply chain level of bio-based plastics rather than biopolymers as substitutes for fossil-based plastics accounts for the use of fossil-based materials in bio-based plastics production and reduced net fossil resource saving. Meanwhile, choosing the level of industries focused on enables a differentiation between bio- and fossil-based plastics.

A suitable quantitative model for this study was found to be an extended hybrid input-output life-cycle assessment (IO-LCA) model. In this model, process-based (LCA) data for bio-based plastics was integrated into a national input-output (IO) table for Germany in 2016 and extended with sectoral economic and environmental data. The model enables matching of substitute products at the level of industries, which is more plausible than matching the highly aggregated sectors provided by official statistics. Even though a new source of uncertainty was introduced by using process-based data, indicator values can be considered relatively robust to changes in such data. Probabilities that conclusions from the deterministic model need to be corrected were low, even though uncertainty ranges were considerable and data quality was mixed.

Discussion and conclusions

This study shows that it is possible to quantify the transition from a fossil-based to a bio-based economy and measure it with systematically developed indicators. Taking into account the results of this research and a review of the current literature, I draw the following conclusions:

1. Developing bioeconomy indicators should be a process that is goal-oriented rather than data-driven, iterative rather than linear, and inclusive rather than

exclusive. The findings of this study are in line with studies emphasizing the superiority of goal-oriented approaches in which indicator development is preceded by a thorough planning phase. They can also be improved by more closely considering methodological and practical factors in order to achieve a good balance between monitoring cost and benefits. Frequent interaction between indicator developers, data providers, and potential users is likely to increase acceptance and feasibility.

2. Bioeconomy indicators need to exhibit advancement in the circular use of biomass and in sufficient consumption behavior, which is to some extent possible with the indicators developed here. A rather narrow meaning of the concept of substitution, focusing on similar functions of substitutes, technological innovation, and the replacement of resource inputs, is less suited for revealing transition processes, as conceptualized in the literature, than a broader meaning of substitution, which focuses on the replacement of systems fulfilling societal needs.
3. The model developed here can be integrated into bioeconomy monitoring systems but requires further methodological advances, especially regarding carbon flows and post-production processes. Carbon flows can be better represented by extending the system boundary from primary plastics production to plastic goods production, or even further, and by including carbon sequestration as credits in the direct GHG emissions data of agriculture, forestry, and food sectors in the model. Consumption patterns and end-of-life options can be represented through further augmentation of supply and use tables and adjustment of final demand and input coefficients.

Recommendations and outlook

The thesis closes with recommendations to developers of bioeconomy monitoring systems and policymakers wishing to design even more relevant systems. Developers should revisit underlying frameworks, sharpen the focus of their efforts, and develop new indicators, if necessary, through stronger involvement of carefully selected stakeholders. Policymakers need to participate more actively in designing bioeconomy monitoring systems and enable further development through greater and more stable funding. I also provide an outlook for further research regarding 1) an integrated monitoring system focusing on sectoral strategies to reduce environmental impacts through resource substitution, circularity, and sufficiency and 2) the relevance of monitoring design for increasing the impact of indicators on political decision-making.

Zusammenfassung (German)

Titel: Monitoring des Übergangs zu einer Bioökonomie: Indikatorenentwicklung und Messung am Beispiel der Biokunststoffproduktion in Deutschland mit einem um Prozess- und Umweltdaten erweiterten Input-Output-Modell

Zahlreiche Hoffnungen sind mit einer auf Pflanzen basierenden Wirtschaft, einer Bioökonomie, verbunden. Sie soll zu einer nachhaltigen Entwicklung mit sauberer Energie, besseren Material- und Abfallkreisläufen und gesünderen Ökosystemen beitragen. Aus diesem Grund haben viele Regierungen Strategien zur Förderung ihrer Bioökonomien beschlossen. Ob die Herstellung einer Vielzahl von bio-basierten Produkten und Bioenergie den Zustand der Umwelt und die Wohlfahrt eines Landes verbessern kann, bleibt jedoch fraglich. Die Einsparung fossiler Energieträger könnte dem Klimawandel entgegenwirken, doch der Anbau von Pflanzen für die Bioökonomie kann auch Probleme wie Landnutzungsänderungen, regionale Wasserknappheit und Arbeitslosigkeit nach sich ziehen. Bioökonomie-Monitoring-Systeme haben die Aufgabe, politischen Entscheidungsträgern und -trägerinnen Informationen über diese Art von Zielkonflikten zu liefern und somit eine erkenntnisgestützte Politikgestaltung im Bereich der Bioökonomie zu ermöglichen. Derartige Systeme befinden sich derzeit im Aufbau. Das Ziel dieser Doktorarbeit ist es, Erkenntnisse für die Weiterentwicklung solcher Systeme zu gewinnen.

Bioökonomie-Monitoring-Systeme erfordern Indikatoren-Sets, welche Bioökonomie-Transformationen korrekt abbilden können. Bisher entwickelte Bioökonomie-Indikatoren sind ungeeignet, bestimmte Transformationen, beispielsweise den Übergang von einer fossil-basierten zu einer bio-basierten Wirtschaft, in Zahlen auszudrücken. Das liegt unter anderem auch an einer unzulänglichen Datenbasis. In der vorliegenden Arbeit werden deshalb entsprechende Indikatoren entwickelt und am Beispiel der Biokunststoffproduktion in Deutschland gemessen. Damit können die Erkenntnisse meiner Untersuchungen einen Beitrag dazu leisten, wie Indikatoren für Bioökonomie-Transformationen systematisch entwickelt werden können, welche Aspekte für dieses Beispiel einer Bioökonomie-Transformation relevant sind und welches quantitative Modell für die Messung der Indikatoren geeignet ist. Die Kapitel 2 bis 5 im Hauptteil der Arbeit befasst sich mit diesen Themen in unterschiedlichem Maße.

Kapitel 2 führt in das Thema ein, indem gezeigt wird, wie vorhandene Indikatoren durch eine kostensparende Verbesserung der Datenlage kurzfristig angepasst werden konnten, um die Bioökonomie-Transformation in der Tensidherstellung sichtbar zu machen. Es wurde deutlich, dass neue Indikatoren für den Übergang zu einer bio-basierten Wirtschaft erforderlich sind und dass diese mit höheren methodischen und datenbezogenen Anforderungen verbunden sind, weil Substitutionsmöglichkeiten identifiziert werden müssen. Modelle auf Basis von Produkt- und Prozessdaten, sogenannte Ökobilanz (LCA)-Modelle, erweisen sich zwar als geeignet für den Vergleich von fossil- und bio-basierten Produkten, sind jedoch mit einem zu hohen Aufwand für ein Monitoring auf nationaler Ebene verbunden.

In Kapitel 3 wird ein neuer Indikator, der *Substitution Share Indicator (SSI),* vorgestellt. Er zeigt an, wie viele fossile Rohstoffe sich einsparen lassen, wenn fossil-basierte durch bio-basierte Produkte ersetzt werden, verglichen mit einer Entwicklung ohne Substitution. Der Indikator bezieht sich auf die Ebene von Industrien, sodass ein für die Politikgestaltung relevanter Vergleich fossil- und bio-basierter Industrien möglich ist, ohne dass die detaillierte Modellierung der Lebenswege aller Produkte erforderlich wäre. Hierfür erwies sich ein Input-Output (IO)-Modell-Ansatz als geeignet, da alle Vorketten und Wechselwirkungen in der gesamten Wirtschaft einbezogen werden und die zugrundeliegenden Daten regelmäßig in Input-Output (IO)-Tabellen zusammengefasst werden. Die Messung des Indikators war für die Transformation in der Kraftstoffindustrie einfacher als in der Kunststoffindustrie. Zum einen sind Kraftstoffe Endprodukte, denen deshalb bio-basierte Alternativen genau zugeordnet werden können. Zum anderen ist der Sektor für Kraftstoffe in den IO-Tabellen homogener. Auf Grund erheblicher Datenlücken im Bereich der Biokunststoffindustrie in Deutschland mussten restriktive Annahmen getroffen werden, welche eine glaubwürdige Messung verhinderten.

Kapitel 4 beschreibt daher ein neu enwickeltes Biokunststoff-Modell, in welchem Prozess-, Produktions- und Preisdaten für Biokunststoffe in eine IO-Tabelle integriert wurden. Somit war es möglich, den *SSI* sowie die Indikatoren Wassernutzung, Treibhausgasemissionen, Arbeitnehmerentgelte und Wertschöpfung, welche die mit der Transformation in der Kunststoffindustrie verbundenen sozioökonomischen und umweltrelevanten Auswirkungen sichtbar machen, zu messen. Die Ergebnisse der Modellierung für die Substitution mit Biokunststoffen im Jahr 2016 in Deutschland zeigen, dass 16% der fossilen Rohstoffe eingespart, 9% weniger Wasser verbraucht und 34% mehr Treibhausgase durch eine höhere Nutzung von Prozessenergie in der Biokunststoffproduktion, verglichen mit der fossil-basierten Kunststoffproduktion, emittiert wurden. Arbeitnehmerentgelte waren 11% höher und die Wertschöpfung war 1% geringer.

Im abschließenden Kapitel 5 wird die Belastbarkeit der Indikatorenwerte für die Transformation in der Kunststoffindustrie bewertet. Da die genutzten Biokunststoff-Daten teilweise mit großen Unsicherheiten verbunden sind, wurde die Belastbarkeit unter Verwendung von Monte-Carlo-Simulationen und einer qualitativen Datenanalyse überprüft. Die Ergebnisse zeigen, dass auch eine nachträgliche Korrektur unsicherer Daten die wesentlichen Aussagen der Indikatoren nicht verändert und diese somit relativ belastbar sind. Eine Verbesserung könnte erreicht werden, wenn Daten zur Biopolymerproduktion und –importen regelmäßig zur Verfügung gestellt würden. Die mit der Integration von Prozessdaten verbundenen Unsicherheiten sind weniger erheblich im Vergleich zu Unsicherheiten, die mit der Verwendung monetärer IO-Tabellen einhergehen. Preisschwankungen beeinflussen die Indikatorenwerte, ohne dass physische Änderungen stattfinden.

Aus den Ergebnissen der Forschung und der anschließenden Diskussion in Kapitel 6 können folgende Schlussfolgerungen zu den eingangs benannten Themen gezogen werden. Erstens könnten Bioökonomie-Monitoring-Systeme davon profitieren, wenn

die Indikatorenentwicklung noch stärker als Prozess verstanden wird. Eine umfassende Auseinandersetzung sowohl mit den angestrebten Zielen als auch mit deren Messbarkeit auf der Basis vorhandener Daten ist ratsam. Des Weiteren ist ein sich wiederholender Prozess wichtig, in welchem die wichtigsten Akteure einbezogen werden. Zweitens ist ein stärkerer Monitoring-Fokus auf nachhaltige Bioökonomie-Transformationen erforderlich, die sich an einem kreislauf- und suffizienzbasierten Wirtschaften orientieren. Dafür könnte der Substitutionsbegriff weiter gefasst werden als bisher, indem er nicht nur auf die Substitution von Rohstoffen oder Technologien bezogen wird, sondern auf die Substitution von Systemen, die gesellschaftliche Bedürfnisse erfüllen. Drittens könnte das hier entwickelte Biokunststoff-Modell in Monitoring-Systeme integriert und als Beispiel für weitere Modelle genutzt werden. Zuvor sind methodische Weiterentwicklungen im Bereich von Kohlenstoffflüssen und Post-Produktionsprozessen erforderlich. Kohlenstoffflüsse könnten besser dargestellt werden, wenn nicht nur die Kunststoffproduktion, sondern auch nachgelagerte Prozesse wie die Herstellung von Kunststoffprodukten einbezogen würden. Die Bindung von Kohlendioxid könnte den vorgelagerten Agrar- und Forstsektoren gutgeschrieben werden. Durch die Erweiterung der IO-Tabellen könnten Konsum- und Abfallverhalten besser repräsentiert werden.

Diese Erkenntnisse sind in besonderem Maße relevant für Entwickler und Entwicklerinnen von Bioökonomie-Monitoring-Systemen und politische Entscheidungsträger und -trägerinnen, die eine Förderung der Bioökonomie vorantreiben möchten. Weiterer Forschungsbedarf besteht vor allem hinsichtlich eines Monitoring-Systems, welches gesellschaftliche Bedürfnisse stärker in den Fokus rückt. Weiterhin kann Forschung zur Gestaltung von Monitoring-Systemen deren Wirksamkeit erhöhen, wenn Faktoren für die tatsächliche Nutzung von Indikatoren in der Entscheidungsfindung identifiziert werden.

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List of Abbreviations

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BTF – Bioeconomy Transition Framework

CGE – Computable General Equilibrium

DMC – Direct Material Consumption

DMI – Direct Material Intensity

DPSIR – Driver-Pressure-State-Impact-Response

EC – European Commission

EE-IO – Environmentally Extended Input-Output

EU – European Union

EW-MFA – Economy-Wide Material Flow Accounting

GDP – Gross Domestic Product

IO – Input-Output

IO-LCA – Input-Output Life Cycle Assessment

JRC – Joint Research Center

LCA – Life Cycle Assessment

MFA – Material Flow Analysis

NACE – Nomenclature statistique des activités économiques dans la Communauté européenne

PA – Polyamide

PE – Polyethylene

PEF – Polyethylene furanoate

PHA – Polyhydroxyalkanoate

PLA – Polylactide acid

PP – Polypropylene

PS – Polystyrene

PVC – Polyvinyl chloride

RACER – Relevant, Accepted, Credible, Easy, Robust

RMC – Raw Material Consumption

SAM – Social Accounting Matrix

SDG – Sustainable Development Goal

SEEA – System of Environmental Economic Accounting

SNA – System of National Accounts

SSI – Substitution Share Indicator

SUT – Supply and Use Tables

TPS – Thermoplastic starch

Chapter 1. Introduction

1.1 Monitoring bioeconomies for effective policymaking

Bioeconomy transitions can be viable trajectories for sustainable development. Bioeconomies enable the production, distribution, trade, and consumption of goods and services based on biological resources, technologies, and knowledge and can support a transition towards healthier environmental and human systems (Lewandowski et al. 2018). They can contribute towards achieving some of the United Nations Sustainable Development Goals (SDGs), such as affordable and clean energy, recycling, and ecosystem preservation (Ronzon and Sanjuán 2020).

Most prominently, expectations are high that bioeconomies can reduce dependence on the fossil resources (Pietzsch 2020) – mineral oil, natural gas, lignite, and hard coal – that all economies rely strongly on. For example, 76% of German primary energy use was based on fossil resources in 2020 and 24% of mineral oil was used for non-energy purposes (AGEB 2020). Bio-based substitutes are commercially available, especially for replacing fossil-based energy sources. In Germany in 2021, biofuels had a share of 7% of transport fuels, bioelectricity of 8% in gross electricity production, and bio-heat of 13% in final energy consumption for heating and cooling (BMWK 2022). Substitutes for fossil-based materials are also emerging on the market. In particular, bio-based plastics are being promoted as a solution for addressing problems of fossil-based plastics consumption, such as marine and terrestrial plastic pollution. Compared to business-as-usual development, substitution could reduce fossil-based plastic pollution by about 20% in 2040 (Lau et al. 2020).

For these reasons, some countries have developed bioeconomy strategies (Staffas et al. 2013; Besi and McCormick 2015; Meyer 2017a), supported by employing a variety of measures, from research and development, subsidies, and industrial policy to educational strategies (Dietz et al. 2018). The EU bioeconomy employed 9% of the entire labor force and generated 5% of gross domestic product (GDP) in 2017. The agriculture and food, beverage, and tobacco industries are currently the most significant ones involved, with bio-based materials and energy still playing a subordinate role (Ronzon et al. 2020).

However, trade-offs between some bioeconomy and sustainable development goals are likely as, for example, a growing bioeconomy may threaten sustainable biomass production and conservation of biodiversity (Fritsche and Rösch 2020). Because bioeconomy development is not a goal in itself but, rather, one possible instrument for achieving sustainable development, diverging trajectories need to be detected early on to enable steering towards the best possible alignment. Comprehensive monitoring of bioeconomic developments, associated impacts, and related policies are essential sources of information for political decision-making and accountability (Wesseler and Braun 2017). Some bioeconomy strategies provide for the establishment of bioeconomy monitoring systems, such as those of the European Commission (EC) and Germany:

> A comprehensive monitoring is needed in order to provide policy makers with transparent and harmonised (across the EU and over time) descriptions of status and trajectory of change in the environmental, social and economic dimensions of the bioeconomy. (EC 2018a, p. 89)
>
> Observing, measuring and evaluating the process of transformation towards a sustainable, bio-based and natural cycle-oriented economy are an important prerequisite in ensuring that we do not achieve individual goals at the expense of others. […] This requires reliable data, comprehensive balance sheets and meaningful indicators that can provide guidance for all involved. (BMEL 2020, p. 54)

Bioeconomy monitoring systems have recently been under development by different groups of researchers representing a variety of approaches. Significant advancements have been made by continuous research of the EC's Joint Research Center (JRC), the project "Design of a systems analysis tools framework for the EU bio-based economy strategy" (SAT-BBE, 2012-2015), three independent German projects "Dimension 1: Resource Base and Sustainability / Production of Biomass", "Dimension 2: Determination of Economic Indicators and Indicators for Monitoring the Progress of the Bio-Economy", and "Dimension 3: Systemic Monitoring and Modelling of the Bioeconomy (Symobio)" (2016-2021), and the EU project "BioMonitor" (2018-2022). There is also ongoing investigation into the topic by the Food and Agricultural Organization (FAO) and the United States Department of Agriculture (USDA). All of these efforts have in common the goal of establishing a comprehensive, systemic representation of interlinkages between new and more traditional bio-based sectors and of possible trade-offs. Challenges to monitoring arise from 1) the crosscutting nature of the bioeconomy, because it is difficult to separate bioeconomic sectors from other economic sectors, and 2) vague ideas about bioeconomy goals. Monitoring systems have progressed much in defining sectoral boundaries of bioeconomies and developing methods for measuring a bioeconomy's contribution to a nation's overall GDP. However, measuring a bioeconomy's contribution towards solving global challenges has received less attention so far, and methods to do so need to be developed. In the following, I summarize the main challenges to measuring and assessing national bioeconomies and promising solutions.

Challenge 1: Bioeconomic sectors. An unresolved issue in monitoring is that bioeconomy researchers typically choose sectoral boundaries ad hoc, depending on study objectives, rather than agreeing "on a common definition, classification, and representation of the bioeconomy" (Wackerbauer 2020). Daystar et al. (2020) and previous studies for the USDA measuring the "biobased products industry" take a practical approach by including all products that participate in the US' BioPreferred Program, thus excluding bioenergy, livestock, food, feed, and pharmaceuticals. Vandermeulen et al. (2011) also focus on "non-traditional applications of biomass", including bioenergy. By contrast, more sectors are included in the JRC's monitoring concept. Ronzon et al. (2017) and Ronzon and M'Barek (2018) propose that all sectors producing or processing biomass belong fully or partially to the bioeconomy. A similar approach is followed by Heijman (2016). Efken et al. (2016) by including bio-based services extend the sectorial boundary to even more downstream sectors, and Cingiz et al. (2021) also consider upstream industries meaning inputs from "partly bioeconomic industries to fully bioeconomic" ones, such as agrochemicals and machinery. One solution to accommodate different monitoring objectives is a flexible system that allows for inclusion or exclusion of bioeconomic sectors depending on their relevance to a particular research question, employing for example innovation or substitution "filters" (Wackerbauer et al. 2019). In addition, questions regarding levels of sectoral and regional disaggregation are important to stakeholders but have not been answered to date (Kardung et al. 2021; Robert et al. 2020).

It is a particular methodological challenge to separate partly bioeconomic sectors and determine their bio-based share because official statistical classifications are not conceived for that aim and, thus, a coherent database is missing. While data is available for fully bioeconomic sectors, and indicators can be easily quantified, modelling of emerging sectors requires new methods and forms of data collection (van Meijl 2015). Output-based approaches estimate the physical or monetary output of bio-based products (Daystar et al. 2020) or their biomass content (Ronzon et al. 2017; Ronzon and M'Barek 2018; Wackerbauer et al. 2019). They rely on a mix of statistical data and expert interviews. Input-based approaches generally rely on statistical input-output data only and estimate bio-based shares based on the input of fully bioeconomic sectors to partly bioeconomic sectors (Efken et al. 2016; Heijman 2016; Iost et al. 2019) and also vice versa (Cingiz et al. 2021). A combined approach has also been suggested, which averages input- and output-based shares (Kuosmanen et al. 2020).

Challenge 2: Economic and environmental impacts. Measurement of bioeconomy goals is difficult, because expectations regarding a bioeconomy's contribution towards sustainable development are formulated rather vaguely in strategies and by stakeholders (Zeug et al. 2019; Robert et al. 2020). SDGs that are associated with bioeconomies in the literature have been identified and may be an indicator for setting priorities in national monitoring systems (Egenolf and Bringezu 2019; Ronzon and Sanjuán 2020; Calicioglu and Bogdanski 2021). The economic indicators GDP, turnover, and employment within the bioeconomy have been repeatedly measured (Ronzon and M'Barek 2018; Iost et al. 2019; Wackerbauer et al. 2019; D'Adamo et al. 2020; Capasso and Klitkou 2020; Daystar et al. 2020; Ronzon et al. 2020; Schweinle et al. 2020; Bringezu et al. 2021; Cingiz et al. 2021; Kilsedar et al. 2021b). The need for further economic indicators that reveal innovation, investment, comparative advantage, and trade relations has already been acknowledged (Wackerbauer et al. 2019; Wydra 2020; Kardung et al. 2021), but social and environmental impacts have received less attention so far (Bracco et al. 2018). Environmental indicators in use refer mostly to primary sectors (Kilsedar et al. 2021b, see Annex 2; Bringezu et al. 2021), a bioeconomy's impact on climate change (Schweinle et al. 2020; Daystar et al. 2020), and pressures on biomass, land, and water resources (O'Brien et al. 2015; O'Brien et al. 2017; Egenolf and Bringezu 2019) because data is available for these areas. Whilst a more complete set of environmental indicators is envisioned (Kardung et al. 2021; Kilsedar et al. 2021b), "the main challenge for monitoring the bioeconomy sustainability is associated with the lack of methodologies for attributing a specific impact to the bioeconomy and related value chains, and consequently, for data collection" (Bracco et al. 2019). A dominant approach for economic indicators that can also be used for environmental indicators is the connection of bio-based shares to available economic data (see for example Ronzon and M'Barek, 2018; Iost et al., 2019; Wackerbauer et al., 2019). Another suitable approach for both economic and environmental indicators seems to be (environmentally extended) input-output modelling that links domestic consumption to global impacts (Daystar et al. 2020; Bringezu et al. 2021).

Summing up, monitoring of sustainable bioeconomies has advanced significantly, and some important challenges have been identified and resolved. A comprehensive monitoring system should include all relevant sectors of the bioeconomy and provide information in sufficient sectoral and regional detail so that it can serve as a basis for a large number of decisions. One important methodological question – How can sectoral detail be achieved in monitoring bioeconomies? – has been adequately addressed by measuring bio-based shares of partly bioeconomic sectors. By contrast, an important conceptual question – What is the purpose of developing bioeconomies? – and its resulting implications for measuring bioeconomy transitions towards predefined goals requires comparatively more research. Thus, in this doctoral thesis I seek to contribute towards advancing bioeconomy monitoring systems conceptually, methodologically, and empirically by exploring indicators for transitioning from a fossil- to a bio-based economy.

Before outlining the research presented in this thesis in more detail in section 1.3, I provide more detailed answers to the questions "Why monitor a bioeconomy?" in 1.2.1, "What to monitor about a bioeconomy?" in 1.2.2, and "How to monitor a bioeconomy?" in 1.2.3.

1.2 The state of bioeconomy transition indicators: development, relevance, and measurement

1.2.1 Development of relevant indicators from bioeconomy frameworks

Monitoring is an activity that provides "regular feedback on the progress being made towards achieving […] goals and objectives" (UNDP 2009, p. 8). It can be situated in the wider context of New Public Management, which applies private sector management methods to the public sector (Lane 2002). Analogous to the use of quantitative indicators such as company profit for gauging a company's overall long-term performance, GDP has been used to show the health of a nation's economy and has been influencing economic policies at least since the mid-twentieth century (van Bergh 2009). Use of such indicators has accelerated from the 1980s onwards, even though they have been important since at least the start of industrialization (Rottenburg and Merry 2015). Other forms of information, be it conventional wisdom or individual experience, have become much less influential in modern times (Porter 2015; Espeland 2015), whereas quantitative indicators have become essential in evidence-based policymaking, in which scientific findings inform policy decisions (Parkhurst 2017) and have an instrumental use, meaning a linear relationship between indicators and decisions (Hezri and Dovers 2006). Such findings are intended to support justifiable and objective arguments in the process of coming to decisions and, in the process of evaluating such decisions, they should transparently present their possible and likely effects. This has been quite observable during the ongoing COVID-19 pandemic, as the daily number of people infected with the Coronavirus has significantly influenced formulation of policy measures (Saltelli and Di Fiore 2020). Poorly designed indicators, in turn, can have adverse effects on management, as the example of forest biodiversity indicators shows (Failing and Gregory 2003).

Monitoring a sustainable bioeconomy requires a set of performance indicators. Measuring performance rather than just describing developments has been envisioned for the EU and German bioeconomy monitoring systems, which should "track […] progress towards a sustainable bioeconomy" (EC 2018a, p. 18) and measure "the process of transformation towards a sustainable, bio-based and natural cycle-oriented economy" (BMEL 2020, p. 54). Measuring performance via a set of indicators is necessary because many goals are pursued through implementation of the bioeconomy concept, and a sustainable bioeconomy cannot be represented by a single indicator, as it is related to a variety of natural resources, processes, products, regions, and themes[1] as well as other broad concepts such as well-being and sustainable development (Stiglitz et al. 2009).

In the following paragraphs I lay the theoretical foundation for choosing relevant bioeconomy transition indicators by presenting, first, what indicators are and, second, what criteria can be distilled from available bioeconomy frameworks. The present study begins from the proposition that indicators should be first and foremost relevant and that other criteria for good indicators, such as their acceptability, credibility, ease of use, and robustness[2], can be subsequently ensured.

An indicator is an observable measure linked with a logical "rule of correspondence" to an abstract, non-measurable, theoretical construct (Meyer 2017b, p. 17, 2011, p. 196). In other words, it "cannot measure the very thing of interest, but in its place something whose movements show a consistent relationship to that thing" (Porter 2015, p. 34). The European Commission (EC) specifies that indicators are relevant to policymaking if they are "closely linked to the objectives to be reached" (EC 2021, p. 360). But how can such a close link be established? A systematic and transparent quantification process can lead to more relevant indicators (Dietz and Hanemaaijer 2012). Quantification is "to convert into numerical existence what was previously expressed in words and not in numbers […] involving comparisons, negotiations, compromises, translations, registration, encoding, codified and replicable procedures, and calculations" (Desrosières 2015, p. 333). A central part of this conversion involves designing a conceptual framework that proposes relationships between key concepts and themes of a theoretical construct, thereby supporting development of a common understanding. In such a "thematic approach" (Dietz and Hanemaaijer 2012, p. 34), problems and solution strategies are clustered in themes, long-term goals and related targets determined, and synergies and

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[1] The bioeconomy concept is further explained and discussed in 1.2.2.

[2] The European Commission summarizes these criteria with the acronym RACER (EC 2021, p. 360).

trade-offs identified. From such a framework, indicators can be formulated (Dietz and Hanemaaijer 2012). Quantification differs from measurement, which "implies that something exists already in a form that is physically measurable" and is a "rule-based implementation of […] conventions" (Desrosières 2015, p. 333). Quantification presupposes a formal procedure that can be filled with data to yield indicator values. Hence, properly speaking, theoretical constructs are quantified with indicators, which can then be measured. If a measured value is not connected to a theoretical construct, it is not an indicator but just a parameter, for example.

Indicators do not provide an explanation for achieving goals or not. As they do not show causal relationships, indicators may support evaluation of progress but cannot replace an assessment that, in addition, considers contextual information (Porter 2015; EC 2021, p. 356). Furthermore, indicators must not be confused with the theoretical construct that they make visible because this bears the risk that, if the indicator is steered in a desired direction, goals will not be attained (Desrosières 2015; EC 2017b).

In sum, a relevant indicator is the result of quantifying a theoretical construct by making assumptions regarding the relationship ("rule of correspondence") between a construct and an indicator (Meyer 2017b). Information on these three basic elements, depicted in Figure 1-1, is necessary so that users can assess whether indicators are relevant for their decision-making contexts.

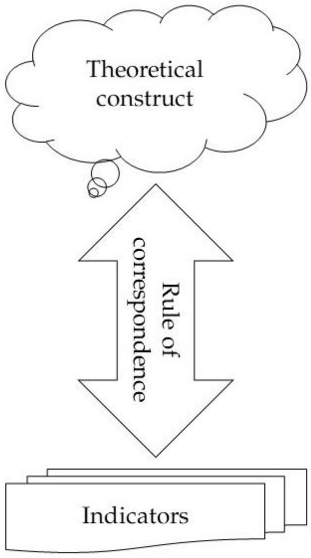

Figure 1-1. Elements of an indicator. Source: Based on definition in Meyer (2017b).

Conceptual bioeconomy frameworks can support the process of developing relevant bioeconomy transition indicators because they include the explicit goals of a particular bioeconomy and hint at regional and sectoral levels that are appropriate for monitoring. An initial conceptual framework was developed in the SAT-BBE project, mentioned in Chapter 1.1, "to a) monitor the evolution of the bioeconomy in the EU, and b) to analyse the socio-economic and environmental impacts of the bioeconomy and its relevant policies" (van Meijl 2015). This "systems analysis framework for the bioeconomy" seeks to quantify the theoretical construct "bioeconomy", defined as "the production of renewable biological resources and the conversion of these resources and waste streams into value added products" (EC 2012, p. 9). Figure 1-2 depicts these products within food and feed, biomaterials, and bioenergy groups and connects them to impacts (right), drivers (left), constraints (bottom), and responses (top). Impacts refer to goals, as stated in the EU's bioeconomy strategy (EC 2012). These are particularly important when developing performance indicators because they specify the overall purpose of developing bioeconomies. Drivers and constraints, influencing supply and demand for bio-based products, and responses, referring to political influences on supply and demand, can be part of a monitoring and evaluation system because they explain performance, though they are considered less important than impacts.

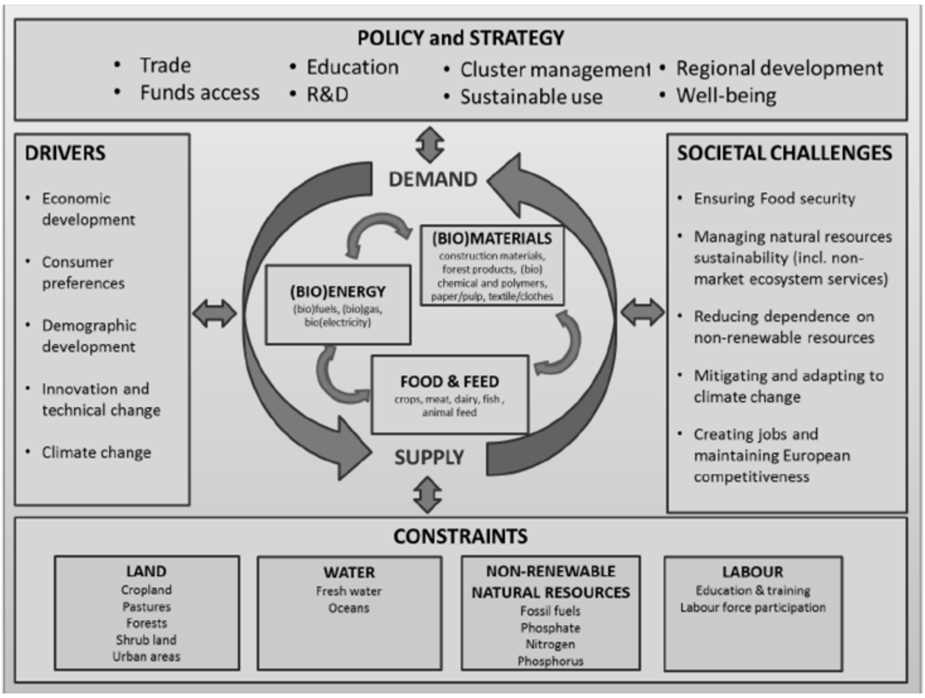

Figure 1-2. Example of a conceptual bioeconomy framework. Source: van Meijl (2015).

O'Brien et al. (2017) extend this Drivers-Impacts-Response (DIR) framework to a Drivers-Pressures-States-Impacts-Response (DPSIR) framework, placing more emphasis on the interaction between economic and environmental systems by including environmental pressures and environmental states caused by economic activity that lead to environmental, economic, and social impacts. Pressures have been categorized into extraction from environment ("input") and release to environment ("output") (Bringezu 2015).

Building their framework on an updated definition of bioeconomy, researchers from the JRC also emphasize environmental systems, especially terrestrial and marine ecosystems. They further specify bioeconomies by adding primary, biomass supplying sectors (agriculture, forestry, fisheries, aquaculture, waste) and service sectors (Robert et al. 2020) and clustering impacts along economic, social, environmental sustainability dimensions. Similarly, Egenolf and Bringezu (2019) emphasize sustainability, basing their framework on the German Bioeconomy Council's definition, which focuses on a bioeconomy as a contribution to a "sustainable economic system" (Egenolf and Bringezu 2019, p. 1); but they also specify related objectives, calling food security, sustainable production and consumption, and sustainable infrastructures "integrative key objectives" related to all three dimensions of sustainability. They also emphasize impacts of domestic production and consumption on other regions (Egenolf and Bringezu 2019).

All of the frameworks presented here have in common that they are oriented towards high governance levels because they were derived from (supra)national strategies, which include several enabling and constraining governance mechanisms (Dietz et al. 2018). Thus, one purpose of a monitoring system is to provide information on the effect of policy implementation on achieving sustainability goals with a bioeconomy. Relevant indicators inform policymaking on a national level. There are also regional and industrial strategies, analyzed in Besi and McCormick (2015), but they are likely to be different for different actors. For example, useful indicator sets for the agricultural sector are different for policy-makers and farmers (Hřebíček et al. 2013). Nevertheless, it would be ideal if data permitted disaggregation to inform local policymaking and business decisions as well.

A focus on higher governance levels implies that industries should be compared and their interlinkages should become visible through monitoring. Interlinkages are important because all direct and indirect impacts of a bioeconomy need to be included for the most comprehensive monitoring of its status. This means moving towards life cycle thinking, considering the impacts of a product over its entire life cycle: from natural resource extraction to disposal (Horne 2009). Developments in single products or small product groups are not very relevant here, but indicators enabling sectoral aggregation for a whole economy are desirable for international comparisons.

In conclusion, a relevant bioeconomy transition indicator

- links the developments within a bioeconomy to policy goals,
- is focused on the national level,
- and provides information at the level of industries and their interlinkages.

In the following, I present visions of bioeconomy transitions, what policy goals they emphasize, and which currently available bioeconomy indicators are linked to them (in 1.2.2). Available data and models for the relevant regional and sectoral levels identified here are introduced thereafter (in 1.2.3).

1.2.2 Bioeconomy transitions and corresponding indicators

Frameworks for bioeconomy monitoring systems very much depend on the underlying definition of bioeconomy chosen, as there is no uniformly agreed-upon definition of the term. So let us take a brief look at how the term has been conceived. First, it evolved from "bioeconomics" in the 1960s to "bioeconomy" in the 1990s. In the European Union, the term was chosen deliberately as a policy concept to stimulate economic growth by advancing biotechnologies and to replace fossil with biological resources (Birner 2018). Lately, there has been a stronger focus on "circular" rather than "linear" bioeconomy, emphasizing the efficient use of biological resources within biological and technical cycles (D'Amato et al. 2017; Giampietro 2019). "Circular bioeconomy" is a much-debated concept without an agreed-upon definition (Leipold and Petit-Boix 2018), but central elements of all concepts include the use of residues and wastes, biorefineries, and cascading use (Stegmann et al. 2020; Tan and Lamers 2021).

Positive and normative views of the bioeconomy have been suggested (Gawel et al. 2019), which can be used to distinguish between the terms "bioeconomy" and "bioeconomy transition". From a positive perspective, bioeconomy is defined by including certain sectors of the economy (Gawel et al. 2019), for example as in the EU strategy's definition:

> The bioeconomy covers all sectors and systems that rely on biological resources (animals, plants, micro-organisms and derived biomass, including organic waste), their functions and principles. It includes and interlinks: land and marine ecosystems and the services they provide; all primary production sectors that use and produce biological resources (agriculture, forestry, fisheries and aquaculture); and all economic and industrial sectors that use biological resources and processes to produce food, feed, bio-based products, energy and services. (EC 2018a)

This definition includes many sectors but excludes medical and health biotechnologies. A bioeconomy is often seen as a sector of the whole economy and part of the broader "carbon" (van Beeck et al. 2014) and "green" (D'Amato et al. 2017) economy. As depicted in Figure 1-3, it usually refers to primary sectors (agricultural, forestry, and fishery industries), food and feed industries, and the bio-based economy. The term bio-based economy is sometimes used interchangeably with bioeconomy but has also been found to emphasize more strongly the biological raw material base of industries (Staffas et al. 2013; Hausknost et al. 2017) as it "relates to the conversion of biological resources into products and materials" (Kardung and Wesseler 2019, p. 282) rather than their production. Defined in this way, a bio-based economy includes secondary rather than primary or tertiary sectors. The term has been defined even more narrowly relating to "non-food applications such as components, chemicals, materials, transport fuels, electricity, and heat" (van Beeck et al. 2014, p. 285).

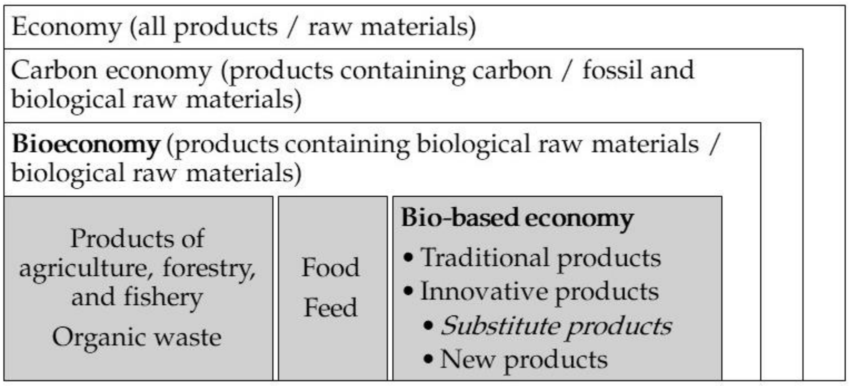

Figure 1-3. Definition of bioeconomy and bio-based economy used in the present thesis.

Products of the bio-based economy have been further divided into "traditional" products, such as textiles and paper, and "innovative" ones, meaning for example biofuels and bioplastics (Kardung and Wesseler 2019, p. 282). This distinction can be misleading, as innovation also occurs in more traditional sectors, and it may thus be more useful to differentiate between innovation types. Innovative, bio-based products fulfill the same functions as more traditional ones ("substitute products") or have a new function ("new products") (Bröring et al. 2020). Although substitute products can also be more traditional, for example a cotton or a nylon shirt, I focus on innovative substitute products for reasons that are explained in Chapter 3. Thus, in the context of this work bio-based economy will be rather narrowly defined, referring to innovative bio-based industries replacing fossil-based ones, including bio-based products with very similar functions to those of fossil-based products (Figure 1-3, in italics). I use the term bio-based economy in its resource-centered, innovative, substituting meaning, which is in line with the observation that "the term BBE [bio-based economy] is often used in documents where the focus is on an economy which is based on the use of biomass resources rather than fossil-based products and systems" (Staffas et al. 2013, p. 2756).

This setting of boundaries to the term bioeconomy illustrates that, by selecting certain sectors and ignoring others in a monitoring system, some normativity is introduced, as some sectors are thus considered to be more important than others. A normative view of bioeconomy becomes even more explicit if a transition towards objectives is specified (Gawel et al. 2019). The second part of the EU strategy's definition can be taken as an example:

> To be successful, the European bioeconomy needs to have sustainability and circularity at its heart. This will drive the renewal of our industries, the modernisation of our primary production systems, the protection of the environment and will enhance biodiversity. (EC 2018a)

In the broadest sense, the bioeconomy can be described as a strategy for supporting sustainable development. More narrowly, bioeconomy can refer to several kinds of transition. Discussions about bioeconomy transitions as visions or narratives for example are rare, even though their implications for society can be significant (Hausknost et al. 2017; Urmetzer et al. 2022; Birch 2019). In the context of monitoring, however, bioeconomy transitions are theoretical constructs that can be quantified with indicators.

Based on a similar grouping already used in the literature, I distinguish three broad types of bioeconomy transition in Table 1-1. *Transition Type 1: Transition from a fossil-based to a bio-based economy* is the most dominant vision in EU policymaking (Veraart and Blok 2021; Asada et al. 2020b; Scordato et al. 2017; Bracco et al. 2018). Schutter et al. (2019, p. 1) have remarked that "bioeconomy strategies in high income societies focus at replacing finite, fossil resources by renewable, biological resources to reconcile macro-economic concerns with climate constraints". Stakeholders taking part in a workshop for the EU bioeconomy monitoring system considered "tracking trade-offs in the transition from a fossil to a bio-based economy" as one of their top priorities (Robert et al. 2020, p. 13). At the beginning of the German bioeconomy strategy, it is stated that

> [t]he German Federal Government supports the transition from an economy largely based on fossil raw materials to a more resource-efficient and circular economy based on renewable resources. (BMBF, p. 6)

and

> [a]n expansion of the bioeconomy will bring about […] a replacement of fossil raw materials. (BMBF, p. 10)

When asked about their opinion on bioeconomy monitoring in an online survey, most of the invited German stakeholders agreed that "substitution of fossil fuel materials by a sufficient and efficient circular economy" should be part of a sustainable bioeconomy (Zeug et al. 2021, p. 10). Transition Type 1 incorporates the implicit expectation that bioeconomy development will lead to economic growth – or at least avoid stagnation caused by unavailable resources – and reduced greenhouse gas emissions as well as pollution (Stark et al. 2022).

Bioeconomy studies have generally been oriented towards Transition Type 1 when analyzing the Swedish (Bennich and Belyazid 2017; Bennich et al. 2018), Finish and Dutch (Bosman and Rotmans 2016), and Brazilian (Bastos Lima 2021) cases, to name just a few. By contrast, LCA studies have hardly considered this type in their goal statements as summarized in a recent review (Talwar and Holden 2022).

In the literature, several terms are associated with Transition Type 1. For example, Dietz et al. (2018) calls this type "Fossil fuel substitution", which is one of their four transformation paths, taking biofuels as a prominent example. Meyer (2017a) found a "transformation-centred vision", which means a shift from a fossil- to a bio-based economy, in bioeconomy strategies. Other references to this type are the terms "life sciences vision", "bio-resource vision", and "biomass-based economy" (Bugge et al. 2016; Vivien et al. 2019; Levidow et al. 2013). However, these perspectives are not exactly congruent with Transition Type 1 and need to be distinguished from it. The transition from a fossil-based to a bio-based economy focuses on resource substitution as a guiding principle, whereas the other visions emphasize growth in biological raw materials and their conversion. For example, increased wheat production may or may not reduce fossil resource use. On the one hand, more mineral fertilizer and diesel are likely to be used as inputs. On the other hand, wheat may replace fossil-based gasoline if it is fermented into ethanol and used as transport fuel.

Table 1-1. Three dominant visions of bioeconomy transitions found in the literature.

Transition type	**Transition Type 1: Transition from a fossil-based to a bio-based economy**	**Transition Type 2: Bioeconomy transition securing economic growth**	**Transition Type 3: Ecological bioeconomy transition**
Main goal	Reduce dependence on fossil resources	Economic prosperity	Stay within ecological boundaries
Guiding principle	Substitution	Innovation/Efficiency / Productivity	Sufficiency
Economic paradigm	Economic growth/avoid stagnation	Economic growth	Degrowth
Biosphere	Considered to some extent (climate change and pollution)	Not primarily considered	Economic system is part of ecosystem
Related concepts in the literature			
(Levidow et al. 2013)	"life sciences vision"		"agro-ecology vision"
(Bugge et al. 2016)	"bio-resource vision"	"bio-technology vision"	"bio-ecology vision"
(Meyer 2017a)	"transformation-centred vision"	"biotechnology-centred vision"	
(Hausknost et al. 2017)	"capitalist growth"		"sufficiency"

(Dietz et al. 2018)	TP 1 “Fossil fuel substitution”	TP 2 “Boosting primary sector productivity” TP 3 “New & more efficient biomass uses” TP 4 “Low-bulk & high-value applications”	
(Vivien et al. 2019)	“Bioeconomy III: a biomass-based bioeconomy”	“Bioeconomy II: a science-based bioeconomy”	“Bioeconomy I: Considering the limits of the biosphere”
(Veraart and Blok 2021)	“Type III – biomass-based economy”, “biomass-centric”	“Type II – science-based bioeconomy”, “techno-centric”	“Type I – degrowth conceptualisation”, “eco-centric”

The focus of *Transition Type 2: Bioeconomy transition to secure economic growth* is less resource- and more technology-oriented (Bugge et al. 2016). Technological innovation and associated efficiency and productivity gains are assumed to reduce environmental pressures (Veraart and Blok 2021) and increase economic growth, competitiveness, and jobs (Meyer 2017a). Start-ups and knowledge are important components of this transition (Vivien et al. 2019). Three transformation paths related to increased productivity in the agricultural sector, more efficient use of biomass and organic waste, and development of new products can be considered sub-types of Transition Type 2 (Dietz et al. 2018). This transition type is compatible with a definition of circular bioeconomy that focuses on the technical cycle of secondary flows, which are “produced and consumed inside the technosphere and transformed under human control” (Giampietro 2019, p. 148). The aim is to keep materials within the economic sphere by maintaining, reusing, and recycling them as often as possible (Ellen MacArthur Foundation 2015).

While Transition Types 1 and 2 follow a “capitalist growth” logic (Hausknost et al. 2017), *Transition Type 3: Ecological bioeconomy transition* supports an economy that stays within boundaries defined by nature. It grounded in the field of “doughnut economics” (Raworth 2018) and associated planetary boundaries (Rockström et al. 2009; Steffen et al. 2015) and “based on the intrinsic limits and possibilities of the biosphere” (Veraart and Blok 2021, pp. 170–171). This alternative degrowth economic paradigm implies consumption oriented towards sufficiency with low-input agriculture (Levidow et al. 2013; Hausknost et al. 2017; Vivien et al. 2019; Veraart and Blok 2021). The vision of a circular bioeconomy is concordant with this transition if primary flows crossing the technosphere and biosphere, i.e. biological cycles, are considered. Giampietro (2019) argues that a bioeconomy transition is irreconcilable with economic growth.

None of these three bioeconomy transition types can be considered sustainable in an all-encompassing manner, and they emphasize quite different bioeconomy goals. Transition Type 1 is in line with the goal of “reducing dependence on non-renewable, unsustainable resources”, as specified in the EC’s bioeconomy strategy (EC 2018a, p. 9); Transition Type 2 is connected to economic objectives, “strengthening European competitiveness and creating jobs” (EC 2018a, p. 10); and Transition Type 3 is geared towards "managing natural resources sustainably" (EC 2018a, p. 9). In the same vein, further types bioeconomy transitions are also conceivable, such as transitioning towards a sustainable food system ensuring food security (Herrero et al. 2020). For any transition type, trade-offs between goals are likely and need to be analyzed.

Available bioeconomy indicators are more or less oriented towards these different bioeconomy transition types. Most bioeconomy indicators measure the contribution of a bioeconomy to overall economic development represented by GDP, turnover, and employment (Bracco et al. 2018), thereby aligning with Transition Type 2. For example, Ronzon and colleagues measure these indicators for specific bioeconomic sectors in order to assess whether EU Member States have made a "transition to an innovative, resource-efficient, and competitive economy" (Ronzon et al. 2020, p. 10) or are on a "transition path to higher productivity" (Ronzon and M'Barek 2018, p. 2; Ronzon et al. 2022). Others measure similar socio-economic indicators that could be interpreted as fitting under Transition Type 2, but clear references to a particular transition type are missing (Capasso and Klitkou 2020; D'Adamo et al. 2020; Iost et al. 2019; Alviar et al. 2021; Lazorcakova et al. 2022). In some studies, there is a dissonance between transition as a theoretical construct and the indicators proposed. For example, in one study the bioeconomy was seen as "a new economic paradigm founded on the use and recycling of biological resources *in place of fossil resources* to help achieve multiple policy objectives" (Ronzon et al. 2022, emphasis added), yet how the developed labor productivity indicator is linked to this construct with a rule of correspondence is not explained.

Transition types 2 and 3 have been partly quantified with bioeconomy footprints (Bringezu et al. 2021), although the transition types were not explicitly mentioned. Socioeconomic and environmental consumption footprints show how much input is required or output generated due to domestic final demand. Value added and employment indicators might be said to come under Transition Type 2, whereas agricultural biomass use, agricultural area, roundwood equivalents, water withdrawals, and GHG emissions might belong to Transition Type 3 if they are related to global reference values for sustainable resource use (Egenolf and Bringezu 2019).

Transition Type 1 is currently being assessed for industries of the bio-based economy using the indicators value added, gross value added per person employed, and turnover (Giuntoli et al. 2020; Kilsedar et al. 2021a). These indicators are related to that part of the bioeconomy where substitution is expected but, as explained above, are not specific enough. Increasing value added is not necessarily related to reduced fossil resource use if (1) process fossil energy use is high or (2) fossil-based products are not replaced. A new indicator – the share of renewable energy in energy consumption of bio-based industries (Melim-McLeod et al. 2022) – is more specific in addressing the first point. However, existing databases do not enable making a distinction between some bio-based and non-bio-based industries, so values for the chemicals, pharmaceutical, and plastics industries have not been reported (Melim-McLeod et al. 2022). The second issue has been addressed by measuring production, turnover, consumption, net trade, import dependence, and land use of the bio-based chemical sector, reasonably assuming that this sector replaces the fossil-based chemical sector (Baldoni et al. 2021). However, net impacts on fossil resource use have not been considered. In a different effort, six indicators[3] derived from analysis of the literature were proposed for Transition Type 1 (Lier et al. 2018). How these indicators are linked to this type, individually or as an index, and how they were calculated based on which database(s) was not, however, explained.

Current monitoring approaches have fallen short of providing a comprehensive picture of progress (Golembiewski et al. 2015; Bracco et al. 2018). As this section has shown, links between developed bioeconomy indicators and stated (or unstated) theoretical constructs have rarely been discussed. In particular, the most dominant vision, Transition Type 1, has not undergone a thorough quantification process. Thus, one of the criteria for relevant bioeconomy transition indicators developed in 1.2.1, the link between the bioeconomy and its goals, remains to be met.

One important reason for the current focus on economic and biomass growth rather than substitution is the challenge of developing indicators from available data, because sectors in official databases are not distinguished according to their biogenic and fossil inputs. In the following section, I discuss potential modelling approaches to filling data gaps for measuring Transition Type 1, which I will simply call "bioeconomy transition" for the remainder of this thesis, as types 2 and 3 will no longer be mentioned.

1.2.3 Modelling approaches and available databases

Different model families have been suggested for analyzing bioeconomies (O'Brien et al. 2017). Pauliuk et al. (2015a) show that the underlying system structures and accounting frameworks of these model families have been similar. On the most general level, life cycle assessment (LCA), material flow analysis (MFA), input-output (IO), and computable general equilibrium (CGE) models all connect flows and distribution and transformation processes, which can be presented in physical or monetary supply and use tables (SUTs). Resource, product, and waste flows occur within the economic system and interact with the environment. Distribution processes are product, waste, factor, resource, and emissions markets. Transformation processes refer to production industries, final use, and waste treatment sectors (Pauliuk et al. 2015a). However, specific model structures and available data make some more suitable than others for monitoring and, consequently, for the purposes of this research. By comparing model families, I argue below for combining IO and MFA modelling for measuring bioeconomy transition indicators.

Modelling is necessary because available indicators and data do not sufficiently meet criteria for relevant bioeconomy transition indicators, as summarized in 1.2.1. More

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[3] The six key indicators were: 'Production of renewable energy', 'Production of biofuels and biogas', 'Material and waste recycling and recovery rates', 'Material replacing non-renewable resources (bio-materials)', 'Public financial support and private investments for reducing dependence on non-renewable resources', and 'Investment in research and innovation' (Lier et al. 2018, pp. 17–18).

specifically, models are required to 1) enable comparative assessments, i.e. substitution of bio-based for fossil-based industries; 2) reveal changes in fossil resource and other resource flows; 3) provide information at regional and sectoral levels relevant to policymaking; 4) include life cycle impacts; and 5) keep continuous monitoring efforts on a low level. Table 2 summarizes how well basic forms of LCA, MFA, IO, and CGE models fulfill these requirements.

Table 1-2. Comparison of model families with criteria for relevant bioeconomy transition indicators.

	LCA	EW-MFA	IO	CGE
1) Output substitution	+	-	+	+
2) Resource flows	+	+	-	-
3) Macro-level	-	+	+	+
4) Life cycle impacts	+/-	-	+/-	+/-
5) Relative simplicity	+	+	+	-

LCA models depict environmental pressures and impacts of products or processes, from resource extraction to waste disposal. To this end, life cycle inventory data is used, collected according to EN ISO 14040 and 14044 standards. Also, EN ISO 16760 provides specific guidance for bio-based products on how to handle carbon storage in products, land use, and allocation, which are controversial issues (Pawelzik et al. 2013). LCA modelling is facilitated by large databases that contain many products and processes, such as Ecoinvent (2018). By representing specific technologies, LCAs enable direct comparison of fossil- and bio-based substitute goods with respect to their fossil resource use and other environmental pressures and impacts. The number of such comparative LCAs for bioplastics and petrochemical plastics has increased recently, and many include fossil depletion as a mid-point impact category (Bishop et al. 2021). Schweinle et al. (2020, p. 4) propose monitoring sustainable bioeconomies with "core products that represent the major material flows of the bioeconomy", such as their example of an EUR/Epal 1 pallet, using LCA models. If such LCA modelling results were aggregated for leading substitute pairs, this could inform sectoral and national-level indicators.

However, aggregation of LCA results is a major challenge, apart from the difficulty of selecting representative, innovative, bio-based products. Since LCAs require a system boundary that cuts off some direct inputs, such as services, and indirect inputs, such as upstream inputs of direct inputs (Weinzettel et al. 2014), they may be prone to truncation errors. Although the magnitude of such errors is currently under debate, results can be significantly affected (Ward et al. 2018). Full coverage of all products in an economy would reduce this error but also increase the effort involved to an unreasonable level if double-counting is to be avoided (Suh and Huppes 2009; Schaffartzik et al. 2014).

MFA models refer to the input and output of substances or materials along processes in physical terms. Six major types have been identified (Bringezu and Mriguchi 2002), including one type that is relevant to the present study because it corresponds to the macro-level: economy-wide material flow accounting (EW-MFA). Describing an economy in physical terms, that is, input, accumulation, and output of raw materials, EW-MFA indicators are suitable as highly aggregated indicators (Fischer-Kowalski et al.

2011). They are based on a standardized methodological framework for data collection in Europe (EC 2018b) and are part of the System of Environmental Economic Accounting (SEEA) (United Nations 2014), which is an international standard established to make environmental statistics consistent with economic ones by using the same concepts, structures, rules, and classifications as national accounts. Modules within SEEA range from pollution and environmental protection expenditures, natural resources and raw materials, and linkage of environmental indicators to macroeconomic indicators such as GDP (Hecht 2007). Within SEEA, EW-MFA is used to focus on material flows, while physical flows of air and water are presented separately (Fischer-Kowalski et al. 2011). Environmental accounts can be used to show biological and fossil raw material flows and environmental pressures such as air emissions or water use by industries. Common indicators relevant to a transition away from fossil resources are Direct Material Input (DMI) of fossil-based energy materials, consisting of imports added to domestic extraction, and Direct Material Consumption (DMC) of fossil energy materials, which is DMI less exports (Fischer-Kowalski et al. 2011).

However, these indicators neither show the causes and effects of changing fossil resource use nor measure life cycle impacts of products or industries. Only a combination with input-output or LCA models would establish a cause-effect link between consumption, raw material use, and impacts (Lutter et al. 2016). For example, the Raw Material Consumption (RMC) indicator measures globally extracted raw materials required for final domestic consumption by using IO and LCA inventory data (Schoer et al. 2012; Asada et al. 2020b).

IO models represent changes in the total output of all sectors due to changing final demand or supply within a country (Miller and Blair 2009, 10-21; 541-555), based on empirically observed SUTs showing monetary transaction flows between industries. Here, data collection is standardized with the System of National Accounts (SNA) (United Nations 2009). Supply tables include a production matrix matching products with the industries that produce them, an import matrix for these products, and a valuation matrix with margins, taxes and subsidies so that supply of products at basic prices can be transformed into purchase prices. This is necessary to combine supply and use tables in an IO model because transactions in the use table are valued at purchase prices. Use tables include intermediate and final consumption of products and value added (Eurostat 2008). Their main purpose is to show production structures, that is, the ratio of each product in the output for each industry. These technical coefficients are fixed, which means that changes in fossil-based inputs are not automatically linked to substitution of bio-based for fossil-based industries.

Output substitution can be determined exogenously in open IO models, not depending on other outputs produced or transactions between industries (Miller and Blair 2009, pp. 34–41). Thus, a bioeconomy transition indicator could show economy-wide monetary impacts of increasing final demand in one sector and decreasing final demand in a sector that can be considered a substitute. Asada et al. (2020a), for example, suggest a scenario in their IO model where products of mineral and metal industries are replaced by products of the wood industry in the construction industry. This means that IO models can cover a large part of a product's life cycle and, thereby, avoid the truncation errors found in LCA models. However, standard IO models neither include life cycle impacts beyond consumption, such as those occurring in the use or disposal phases, nor environmental impacts in physical terms.

CGE models are based on Social Accounting Matrices (SAMs), which are extended national SUTs and include more information on households, factors of production, and government activities. Results show price-mediated effects by balancing supply and demand in an economy. For example, CGE models have been developed for assessing the medium- to long-term effects on prices and fossil fuel demand of some substitute products, such as bioplastics (Escobar et al. 2018) and bioenergy and biomaterials production (van Meijl et al. 2018; Schuenemann and Delzeit 2022). In contrast to IO models, input ratios are not fixed, and substitution elasticities between the production factors capital, labor, energy, and materials are specified in nested productions functions. Nesting implies that a change in one input group, such as materials, does not influence the input composition of another input group, such as capital. For example, using biomass instead of fossil raw materials does not necessarily require changing the technologies used (Nakamura and Nansai 2016).

Thus, CGE models, just as IO models, can represent output substitution, life cycle impacts to some extent, and economy-wide effects, but are less suited for showing substitution between intermediate inputs, environmental impacts, and effects of downstream life cycle stages. They can better show medium- to long-term effects due to their flexibility but require much more data than IO models, which is associated with greater uncertainties (Lenzen 2014; O'Brien et al. 2017). Econometrically estimated elasticities are frequently not available for the case analyzed or require improvement (Antoszewski 2019; Lagomarsino 2020). In short, CGE models entail considerable effort due to their complexity and high data requirements.

With their macro-level orientation and relatively lower mathematical complexity, IO models linked with EW-MFA models showing resource flows can be considered well suited for modelling bioeconomy transition indicators. When combined, they have been known in the literature as **EE-IO models** (environmentally extended input-output models) and can link physical data to interindustry flows in an economy (Lutter et al. 2016). Thus, IO models have been "extended" to show changes in fossil raw material use and other environmental pressures, such as land and water use and greenhouse gas emissions, throughout supply chains (Feng et al. 2011; Schoer et al. 2013; Wiedmann 2009; Castellani et al. 2019). Such an extension implies that all products in one industry have the same intensity, meaning environmental impact per unit of output (Miller and Blair 2009). The more aggregated sectors are, however, the less credible this assumption becomes. An advantage is that EE-IO models are based on systematically collected data being rooted in compatible SNA and SEEA. The statistical offices of many countries already produce SUTs as well as environmental accounts on a regular basis.

Past research has addressed three shortcomings of standard EE-IO models: 1) imports have the same production structures as domestic products, 2) monetary flows correspond to physical flows, and 3) products of an industry have homogenous production structures. The first point has been increasingly addressed since about 2012 by construction of multi-regional databases. By linking national SUTs, import intensities can be distinguished by country of origin. The databases Asian International Input-Output Table (AIIOT), EXIOBASE, Eora, Eora, GTAP, and WIOD differ with regard to their geographical, sectoral and temporal coverage, and their structures lead to different results (Owen 2017; Tukker and Dietzenbacher 2013; Wiedmann et al. 2011), though standardization is strived for in the Figaro project (Remond-Tiedrez and Rueda-Cantuche 2019). Since it will be important later in this study, it is worth noting that the incipient German bioeconomy monitoring system relies on EXIOBASE (Bringezu et al. 2021). The second point, which is critical if prices for purchasing industries vary, can be addressed with physical SUTs and has become the focus of a very novel field of research (Wieland et al. 2020). The Food and Agricultural Biomass Input Output (FABIO) model provides SUTs with flows of agricultural, forestry, and food products in physical units on a global level (Bruckner et al. 2019). At the same time, FABIO and other multi-regional input-output databases contain more detailed representation of sectors than previous data sources, addressing the third shortcoming of national input-output data collection. There is also now a general tendency to build more disaggregated information in virtual laboratories (VL), "shared digital workspaces offering a high-performance computing architecture" (Geschke and Hadjikakou 2017, p. 143), and a special effort is being made to represent the bioeconomy in so-called BioSAMs. VL enable data collection of multi-regional IO tables, with some countries being represented with high regional and sectoral resolution, in particular Australia. Data for Eora, EXIOBASE, WIOD can be integrated with VL platforms (Lenzen et al. 2017). In BioSAMs, agriculture, forestry, food, petroleum, coal, chemicals, rubber and plastics, wood products, and electricity and gas industries have been further disaggregated, providing more detail on bio-based sectors and their links to the rest of the economy (Mainar-Causapé et al. 2021). Nevertheless, a major challenge is development of appropriate methods and statistics with sufficient detail for measuring innovative bio-based industries that may play a major role in bioeconomy transitions (Kardung and Wesseler 2019; Mainar-Causapé et al. 2021).

1.3 Enhancing bioeconomy monitoring systems

1.3.1 Research objectives

Transitioning from fossil-based to bio-based economies has become a salient vision in political and scientific discussions but has, up to now, not undergone a systematic process of quantification, mainly due to unavailability of adequate models and data. Thus, at the moment it is difficult to measure bioeconomy transition progress and possible trade-offs.

The work presented here seeks to contribute towards a better understanding of how transitioning from a fossil-based to a bio-based economy could be more precisely monitored, thereby building the foundation for comprehensive analysis, assessment, evaluation, and, ultimately, more effective policymaking. In doing so, I seek to answer the following overarching question:

> What enhancements in bioeconomy monitoring systems are necessary to support evidence-based policymaking oriented towards sustainable bioeconomy transition?

Enhancements suggested by this study refer to three levels of abstraction, as depicted in Figure 1-4, which should be valuable to researchers on sustainable transition, developers of bioeconomy monitoring systems, and policymakers.

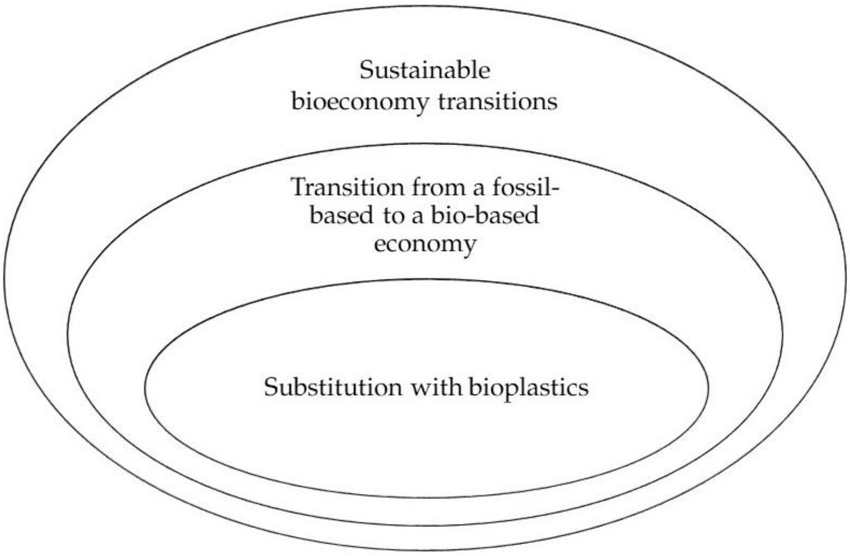


Figure 1-4. Thesis research topics, focalizing from broad (outer circle), to medium (middle circle), to specific (inner circle) levels of abstraction.

Regarding sustainable bioeconomy transitions (Figure 1-4, outer circle), I suggest here a general approach for developing indicators. Insights generated through this study into indicator development processes may be useful to developers of bioeconomy monitoring systems and bioeconomy researchers in general because a major gap in sustainability transitions research is still "the quest for appropriate indicators" (Köhler et al. 2019, p. 19). Thus far, transition progress has often been measured through technological change rates, and discussion of more comprehensive indicators is needed (Köhler et al. 2019). Many criteria for assessing indicators have been suggested and applied (Donnelly et al. 2007). The EC's RACER concept is a rather small and simple set of criteria suitable for assessing indicators informing policymaking and has previously been used to assess resource-efficiency indicators (Eisenmenger et al. 2016). An indicator is RACER if it is relevant, accepted, credible, easy, and robust (EC 2017a). With this in mind, the first of three general research questions (RQ) guiding the present study is:

> RQ1: How can indicators for bioeconomy monitoring systems be developed so that they adequately fulfill indicator assessment criteria?

Focalizing one specific transition (Figure 1-4, middle circle), in this work I present new indicators for its monitoring and assessment, at the level of industries. Reconciling micro and macro levels has been identified as a particularly important research gap in sustainability transitions research (Köhler et al. 2019). Thus, the envisioned indicators need to be relevant for bioeconomy transitions researchers wishing to connect and analyze different levels. They also need to be usable by developers of bioeconomy monitoring systems to measure transition in important industries. Consequently, answers to the following research question have informed the design of these new indicators:

> RQ2: What are relevant considerations for monitoring transitions from fossil- to bio-based economies?

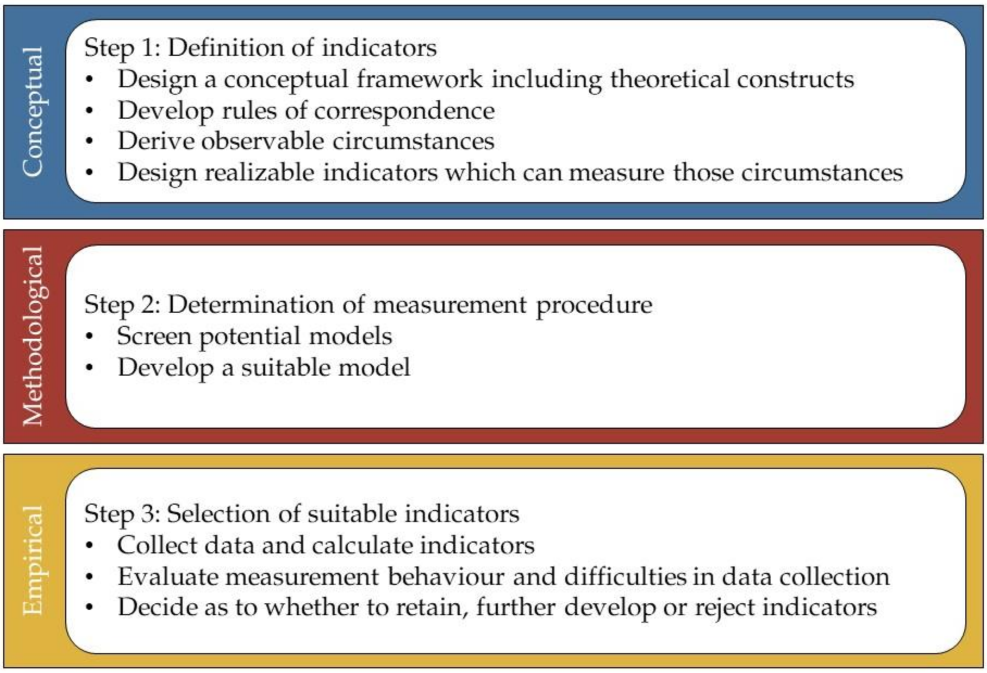
Specifically to the German plastics industry (Figure 1-4, inner circle), I seek to provide new insights by measuring developed indicators. In doing so, I fill some data gaps for the German bio-based plastics industry, addressing one of the main challenges in monitoring, which is data availability for emerging bio-based industries. Developers of monitoring systems should be able to integrate these data and modelling results into existing systems. Meanwhile, policymakers can use the results to explore extension of official data collection and to design policies that support plastics substitution. As filling these data gaps requires modelling, the following question has been considered:

> RQ3: What quantitative model could be suitable for informing indicators for monitoring transitions from fossil- to bio-based economies?

More specific RQ of Chapters 2 through 5, which relate to these three general RQ, are presented in section 1.3.3.

1.3.2 Research design

In this thesis, I approach RQ 1 to 3 by following a process of indicator development that is suggested in the literature and depicted in Figure 1-5.



Step 1: Definition of indicators

- Design a conceptual framework including theoretical constructs
- Develop rules of correspondence
- Derive observable circumstances
- Design realizable indicators which can measure those circumstances

Step 2: Determination of measurement procedure

- Screen potential models
- Develop a suitable model

Step 3: Selection of suitable indicators

- Collect data and calculate indicators
- Evaluate measurement behaviour and difficulties in data collection
- Decide as to whether to retain, further develop or reject indicators

Figure 1-5. Approach to indicator development. Source: Own content, based on Meyer (2011, p. 200).

The process starts by considering theoretical aspects first, as recommended by Meyer (2011, p. 199):

> Researchers must start […] by clarifying the measurement objective, that is, occupy themselves with the question of why a thing is to be measured and, indeed, what it actually is in the first place […] Without an appropriate clarification of the contents and the various different dimensions of the construct, no suitable indicators can be developed to depict it.

Here I adapt an existing conceptual bioeconomy framework – the DIR framework presented in 1.2.1 (Figure 1-2) – to emphasize more strongly the specific transition from a fossil-based to a bio-based economy. Current bioeconomy monitoring systems in the EU (Kardung and Wesseler 2019) and Germany (O'Brien et al. 2017) have also built on this framework. In a subsequent quantification process, I link the transition to a set of indicators expressing important assumptions about the transition. This step aims at making the indicators relevant to the theoretical concept to be observed, meaning that they include unique characteristics of the bioeconomy transition.

In the second major step, I compare and assess some of the models presented in 1.2.3, revealing key methodological shortcomings and data gaps in present practice by exemplarily measuring the indicators for the surfactant, transport fuels, and primary plastics industries in Germany. I then explore options for filling such data gaps through advanced modelling. Next, I propose a suitable formal model such that these indicators can be measured in ways that fulfill methodological requirements. This step is necessary to obtain credible indicators that are "unambiguous and easy to interpret" (EC 2021, p. 360).

Third, the indicators are measured for the plastics industry in Germany in 2016 in order to assess their practicality. Official statistics serve as a database for showing the transition in this industry. Potential data gaps are filled with data from secondary sources, including scientific or technical studies or, when necessary, with primary data from expert interviews. This should help to show how easily indicators can be monitored and how robust they can be.

The plastics industry is one out of several options for a case study. In a comprehensive monitoring system, many more industries should be included. There is a specific focus on the plastics industry in the EC's strategy:

> The action will […] mobilise the key actors in the plastics value chain to support the development of substitutes to fossil resources, in particular bio-based, recyclable and marine biodegradable substitutes for plastic. (EC 2018a, p. 12)

In 2020, the German government also wished to monitor bioplastics to make evaluation of policy measures possible but noted that data is currently unavailable (BMBF 2020). Apart from the apparent interest in a plastics transition in the two strategies, the selection of plastics was based upon two considerations: 1) the industry currently uses a great amount of fossil resources and 2) bio-based substitution possibilities can be identified. Figure 1-6 shows that 20% of the fossil resources coal, lignite, crude oil, and natural gas were used by the electricity and heat industries in Germany in 2014, and 63% were used to manufacture coke and petroleum products. The output of this industry mainly consists of transport fuels and other materials (17%) that are further processed into chemicals and chemical products. Bio-based substitution possibilities are available in increasing number (IEA Bioenergy 2020). Bioplastics are a prominent example, with four out of the "top 20 emerging bio-based products" being bioplastics (Fabbri et al. 2018) and two out of 15 "success stories" being associated with bioplastics (EC 2019).

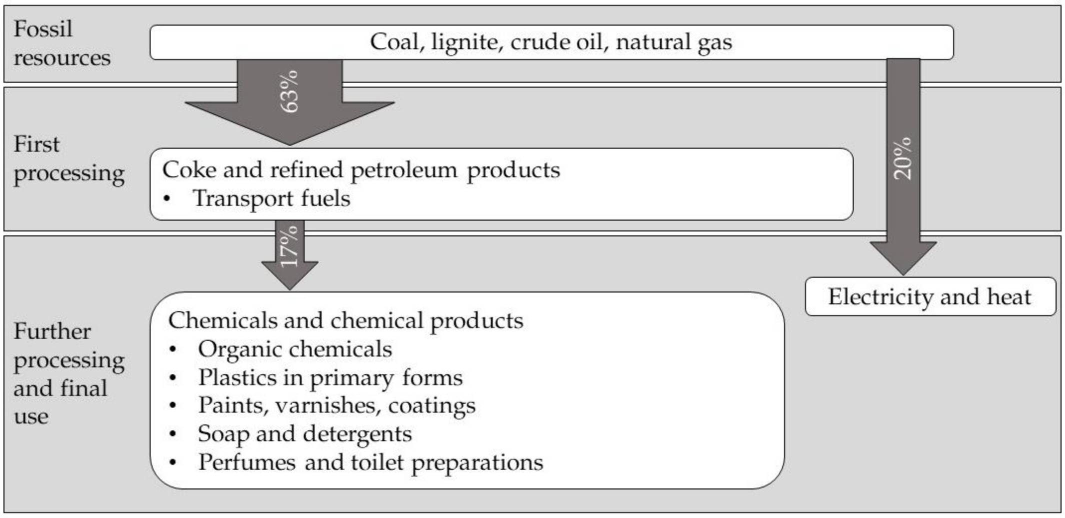


Figure 1-6. Shares of fossil resource use in the German economy, from extraction to intermediate production, in 2014. Source: Own empirical content, based on Destatis (2015).

1.3.3 Thesis structure

This thesis is organized along three general themes that are addressed in Chapters 2 through 5 in varying degrees. As Figure 1-7 illustrates, I examine the overarching research question from different angles by answering research questions related to three central themes: *Theme A:* Indicator development (RQ1), *Theme B:* Bioeconomy transition (RQ2), and *Theme C:* Social-ecological systems modelling (RQ3). Research in Chapters 2 through 5 was guided by more specific RQ, which are summarized towards the bottom of Figure 1-7. The strength of relationships between themes and chapters is indicated with thin and bold arrows in Figure 1-7. Chapters 2 through 4 are included exactly as they were published in peer-reviewed journals between 2019 and 2022, except for the titles, which I have modified in order to emphasize each chapter's purpose within the thesis as a whole.

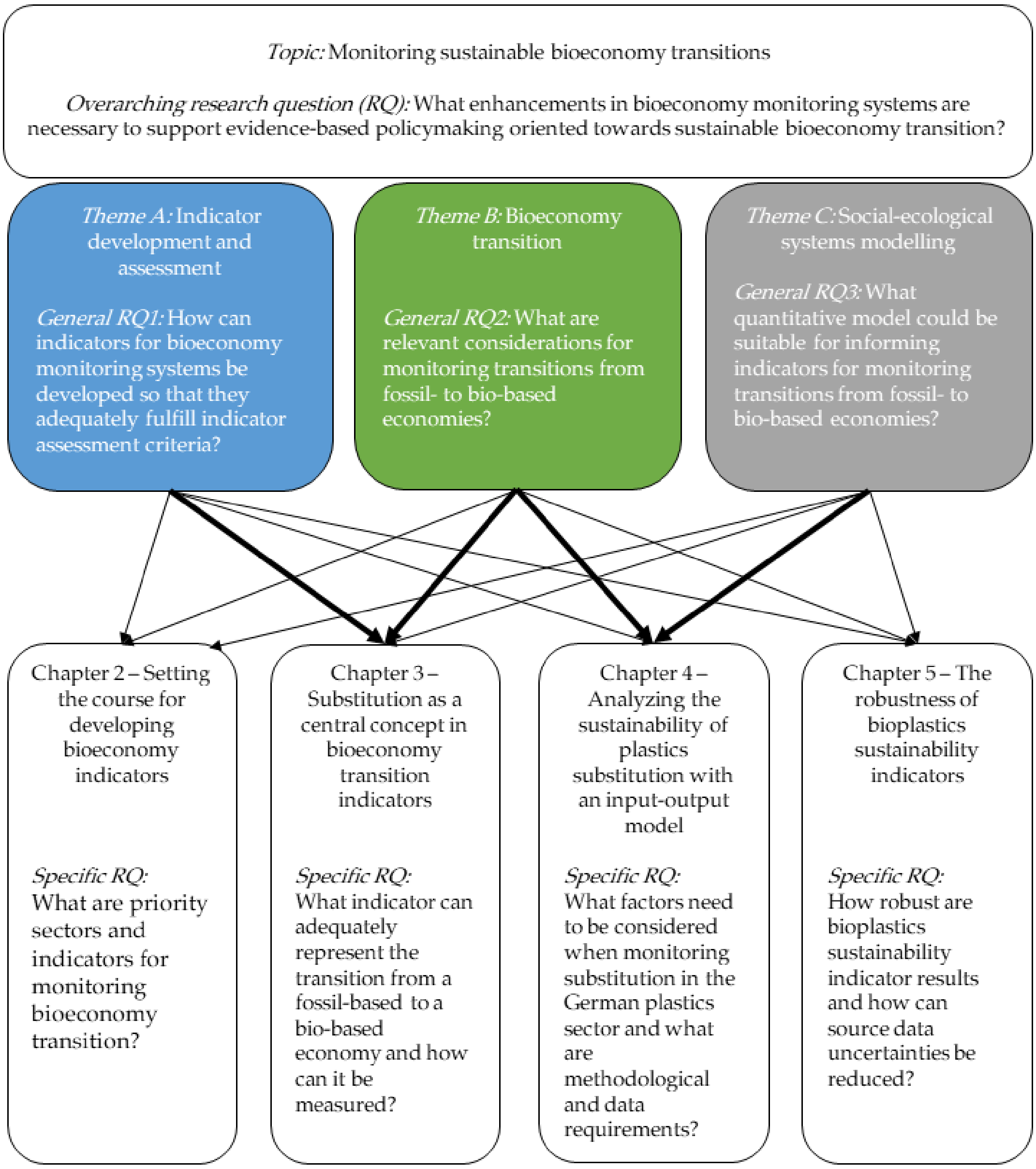


Figure 1-7. Relationships between the overarching research question, general research questions relating to themes, and research questions specific to chapters of this thesis. Bold arrows indicate special focus of chapters on particular themes.

In **Chapter 2**, I identify solutions for addressing the missing distinction between "bio-based" and "non-bio-based" industries in official statistics. Assuming that systems of data collection are not extended or changed to include information on resource bases of products in the short to medium term I, together with former project partners, identify priority areas – indicators and industries – for monitoring. By measuring the German surfactant industry in 2015 using key economic, environmental, and innovation indicators, we show how indicators can be improved and data gaps can be filled in the short term with low-cost and high-benefit options. This chapter serves as an extended introduction into the difficulties faced by developers of monitoring systems and outlines a basic understanding for developing more relevant bioeconomy transition indicators, which is the main purpose of chapters 3 and 4.

In **Chapter 3**, I develop a new indicator that is intended to help make the transition from a fossil-based to a bio-based economy visible. It is based on a previously existing framework that I have adapted to reflect specific theoretical considerations regarding basic elements of the transition. In contrast to the indicator development approach pursued in Chapter 2, which is based on available data, I derive the indicator theoretically before exploring methodological and practical issues by comparing two modelling approaches as applied to two German industries, transport fuels and primary plastics, for the year 2011.

In **Chapter 4**, I develop a new model that makes it possible to apply the indicator presented in Chapter 3 to the plastics industry with a higher degree of credibility. In this model, I integrate process-based data into German SUTs from 2016. The model itself is described in a different article and included here as a **Research Methods Annex**. This step required further data collection from market studies and expert interviews that I conducted because appropriate data and information on the German bioplastics market was not available from official statistics. Furthermore, I suggest and measure economic and environmental indicators for assessing bioeconomy transitions.

In **Chapter 5**, I assess indicators regarding the indicator criterion “robustness” in more detail. Serving as an important addition to Chapter 4, I suggest a method for a robustness check of bioeconomy transition indicators that have been derived with the new model, involving Monte Carlo simulations and data quality analysis. If process-based data is uncertain, it might have to be corrected, making indicator values less robust. The influence of process-based data and options to reduce uncertainties are analyzed, as they are necessary if such modelling of the ongoing transition in the German plastics industry is to be integrated into continuous bioeconomy monitoring.

In **Chapter 6**, I summarize results from the main chapters 2 through 5, taking them as a starting point for discussing themes A, B, and C against the background of current scientific debates. In **Chapter 7**, I draw conclusions by considering the results of my research and the discussion from the previous chapter. In **Chapter 8**, I provide recommendations to developers of bioeconomy monitoring systems and policymakers as primary users of such systems, closing with a statement on further research needs.

Chapter 2. Setting the course for developing bioeconomy indicators

Chapter 2 has been published as Jander et al. (2020) and is the result of a research collaboration between 2016 and 2019 within the project "Dimension 2: Determination of Economic Indicators and Indicators for Monitoring the Progress of the Bio-Economy", in which we focused on indicators for innovative aspects of the bioeconomy (Wackerbauer et al. 2019).

The published research paper has been added to this thesis in the next pages.

sustainability

MDPI

Article

Monitoring Bioeconomy Transitions with Economic–Environmental and Innovation Indicators: Addressing Data Gaps in the Short Term

Wiebke Jander [1,*], Sven Wydra [2], Johann Wackerbauer [3], Philipp Grundmann [1,4] and Stephan Piotrowski [5]

[1] Technology Assessment and Substance Cycles, Leibniz Institute for Agricultural Engineering and Bioeconomy e.V. (ATB), 14469 Potsdam, Germany; pgrundmann@atb-potsdam.de
[2] Business Unit Bioeconomy and Life Sciences, Fraunhofer Institute for Systems and Innovation Research ISI, 76139 Karlsruhe, Germany; sven.wydra@isi.fraunhofer.de
[3] ifo Center for Energy, Climate, and Resources, ifo Institute, 81679 München, Germany; wackerbauer@ifo.de
[4] Department of Agricultural Economics, Humboldt-Universität zu Berlin, 10099 Berlin, Germany
[5] nova-Institute GmbH, 50354 Hürth, Germany; stephan.piotrowski@icloud.com
* Correspondence: wjander@atb-potsdam.de

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Abstract: Monitoring bioeconomy transitions and their effects can be considered a Herculean task, as they cannot be easily captured using current economic statistics. Distinctions are rarely made between bio-based and non-bio-based products when official data is collected. However, production along bioeconomy supply chains and its implications for sustainability require measurement and assessment to enable considered policymaking. We propose a starting point for monitoring bioeconomy transitions by suggesting an adapted framework, relevant sectors, and indicators that can be observed with existing information and data from many alternative sources, assuming that official data collection methods will not be modified soon. Economic–environmental indicators and innovation indicators are derived for the German surfactant industry based on the premise that combined economic–environmental indicators can show actual developments and trade-offs, while innovation indicators can reveal whether a bioeconomy transition is likely in a sector. Methodological challenges are discussed and low-cost; high-benefit options for further data collection are recommended.

Keywords: Bioeconomy monitoring; transition framework; surfactant industry; bio-based share; fossil resource substitution; diffusion of innovations

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Highlights

- Findings indicate growth in innovative, bio-based products and possibly a beginning transition from a fossil-based economy to a bio-based economy.
- Despite considerable innovation potential, stagnating patent indicators reflect declining market optimism.
- Limitations in data for monitoring the bioeconomy can be overcome in the short-term by integrating diverse data sources.
- A modified Driver-Pressure-State-Impact-Response framework is proving beneficial for the analysis of high-resolution sectors and indicators for an initial monitoring of the bioeconomy.
- Fossil-resource saving may be in the order of 29 MJ per € of production costs.

1. Introduction

Monitoring the bioeconomy is becoming increasingly important, as the demand for products based on biogenic resources, including biomass from agriculture, forestry, fishery, and organic waste, is increasing and new bio-based technologies (e.g., gene editing) are being explored in various sectors. There is, consequently, a growing interest among governments in setting up bioeconomy monitoring systems that can enable the measurement and assessment of bioeconomy supply chains—from biomass extraction to consumption and recycling—and their implications for sustainability in order to facilitate considered policymaking [1,2]. Quantification of bioeconomies, as for example in [3,4], enables comparative analyses of bioeconomies' performances and promote sustainable transitions. Measuring bioeconomy sectors has the advantage that biomass input can be channeled to those sectors that use it most efficiently and effectively in terms of sustainability.

However, monitoring bioeconomies and their economic, environmental, and social effects can be seen as a Herculean task. Each bioeconomy can be considered a cross-sectoral economy (i.e., an economy spanning various sectors), similar to the environmental economy or health care industry. A key problem for bioeconomy monitoring is that when data is collected by governments for official economic statistics, distinctions are rarely made between bio-based and non-bio-based products. Consequently, bioeconomy contributions are not clearly delineated in official statistics, making their complete depiction difficult and presumably costly.

One result of this lack of sufficient and reliable data is that those responsible for implementing coherent and continuous monitoring are faced with many different and often conflicting statements concerning the bioeconomy, because varying sectoral demarcations are assumed. Sectors included in various studies and the monitoring systems employed by countries differ widely because they—especially the latter—are oriented towards differing objectives [5–8]. The European Commission describes the bioeconomy in terms of three sectors, called "core," "partial," and "indirect" bioeconomy [1]. Meanwhile, the German Ministry of Education and Research (BMBF) and the German Ministry of Food and Agriculture (BMEL) distinguish ten economic sectors that are relevant for the bioeconomy but do not fully belong to it [9], whereas the German Bioeconomy Council includes all value chains—from the production of biomass in the agricultural and forestry sectors, fisheries and aquaculture, culture media (microbial production), and waste management, to the end products derived from them [10].

While the primary sectors of agriculture and forestry are always included and the chemical sector, for example, is at least partly considered in most monitoring systems internationally [6], methods and results generally differ (see Table 1). Following the definition of the German Bioeconomy Council, for example, [11] consider all sectors that have some biomass input as part of the German bioeconomy. In their study, the agricultural biomass input share of each 4-digit level sector, according to the NACE Rev. 2 code, is estimated in terms of value, based on a regular survey called "Materials and Goods Received." NACE is the acronym used to designate the statistical classification of economic activities in the European Community. It is a framework for collecting and presenting statistical data. From the survey, however, it is not discernible whether biomass input is actually used in the production process or if some input of processed goods is bio-based but not declared as such. Another approach has been to estimate bio-based shares at the product level (8-digit according to the Combined Nomenclature, a tool for classifying goods: https://ec.europa.eu/taxation_customs/business/calculation-customs-duties/what-is-common-customs-tariff/combined-nomenclature_en) with the support of experts [12]. This kind of data has been used for the calculation of socioeconomic indicators for the EU's bioeconomy [3,4] and in an input–output model of the Polish bioeconomy [13]. Meanwhile, [14] do not include bio-based chemicals in their estimation of Japan's bioeconomic GDP. In short, the sectors that belong to the bioeconomy and the determination of the bio-based shares of partially bio-based sectors are still under discussion.

Furthermore, either economic or environmental performance is measured, but not both [15]. Already, existing monitoring systems emphasize economic targets [5], and, thus, a number of studies rely on the results from economic indicators—above all, employment and value added [3,11,13,14]. Others, however, focus on environmental sustainability [16–18]. This divide indicates that a holistic framework and appropriate indicators that can display trade-offs between two or more objectives are missing.

Table 1. Overview of bioeconomy sectors and indicators suggested in this study compared with current literature.

Literature	Bioeconomy Sectors Covered	Economic Indicators	Environmental Indicators	Innovation Indicators
This study	Bio-based manufacturing sectors with substitution potential (case here: bio-based surfactants. More sectors in [19].	Number of employees, gross value added, turnover, foreign sales, investment	Energy consumption, land footprint, fossil-resource saving	Publications, patents
Biber-Freudenberger et al. 2018 [17]	Primary and high-tech bioeconomy sectors	Value added, employment, exports	Selected indicators linked to SDGs	Patent applications
Capasso and Klitkou 2020 [20]	Sectors with a bio-based share	Value added, employment, productivity	-	-
D'Adamo et al. 2020 [4]	Sectors with a bio-based share	Employment, turnover, value added	-	-
Efken et al. 2016 [11]	Sectors with bio-based inputs	Employment, gross value added	-	-
Egenolf and Bringezu 2019 [18]	Not specified	-	Agricultural land, forest, water, material, climate footprints	-
Frietsch et al. 2016 [21]	Sectors with bio-based related patents	-	-	patents
Fuentes-Saguar et al. 2017 [22]	Selected bioeconomy sectors	Output and employment multipliers	-	-
Iost et al. 2019 [23]	Sectors with bio-based inputs	Employment, gross value added, turnover	-	-
Jander and Grundmann 2019 [24]	Bio-based substitute products	Substitution share, fossil-resource saving	-	-
Loizou et al. 2019 [13]	Sectors with a bio-based share	Output, employment, income multipliers	-	-
Ronzon and M'Barek 2018 [3]	Sectors with a bio-based share	Number of persons employed, turnover, value added, labor productivity, location quotient	-	-
Wen et al. 2019 [14]	Selection of mainly bio-based sectors + bioenergy	Value added	-	-
Wydra 2020 [25]	Sectors with a bio-based share	-	-	R&D expenditures, patents

Given the limited financial resources for upcoming bioeconomy monitoring needs, no agreement has been reached so far among scholars on what priority areas should be for monitoring in the short term, or appropriate overall boundaries for the long term. Taking a practical approach, we recommend aiming first at monitoring the most important sectors and indicators in depth and, then, gradually including them in a larger monitoring framework. In the present article, we propose a feasible starting point for such bioeconomy monitoring efforts based on two kinds of indicators. First, economic–environmental indicators can reveal actual transition developments and trade-offs, while, second, innovation indicators show where further contributions to bioeconomy transition may be expected. Innovations have been found to be core to a bioeconomy transition [26]. By proposing these as core indicators, we seek to contribute towards the ongoing debate regarding what should be measured during bioeconomy transitions. To tackle the problem of separating out the bioeconomic components of an industry and showing how they can be unambiguously described, we focus here on a case from manufacturing—the German surfactant industry—chosen for this study as a priority area for monitoring.

Below, we provide details on calculating our selected indicators, combining existing data and information in novel ways. Our analysis is based on economic classifications and relevant indicators that can be observed with information and data from many alternative sources, based on the assumption that current classification schemes and official modes of data collection will not be appropriately modified in the near future. Because of the scale of this challenge, we have set our main focus for now on a few selected indicators and sectors, but it is clear that this initially limited scope needs to be extended by including more indicators and sectors in the medium and long term. In the conclusion, we discuss methodological limitations and data gaps and provide hands-on options for improving the suggested indicators that can hopefully close the most important gaps with relatively few additional resources.

2. Analytical Framework

The currently existing definitions of the term bioeconomy are not completely congruent and offer scope for interpretation. Against this background, we adopt a broad definition for building an objective, comprehensive, and value-neutral bioeconomy monitoring system. This means including all value chains that use biological resources. Both already quantitatively relevant industrial sectors, such as the timber industry or the food and beverage sector, should be taken into account, as well as emerging sectors that have not yet reached significant production volumes but hold high innovation potential, such as bio-based polymers and plastics. All biological resources need to be considered, including all types of biomass: vegetable, animal, and waste streams, as well as processes in which biological resources, such as living organisms (plants, animals, microorganisms) or parts thereof (e.g., DNA, enzymes, etc.), are used in the production process.

This study is further guided by an extended version of the Bioeconomy Transition Framework (BTF) described in [24]. When investigating bioeconomy transitions, such a framework becomes indispensable to achieve a common understanding between the indicator developers and users on broad and dynamic constructs with numerous objectives, drivers, constraints, and possible responses. The BTF is developed further here (Figure 1) in order to include not only the transition from fossil-based to bio-based economies, but also other kinds of "transformation paths" [27], such as towards greater food security, or "visions," such as more ecologically sound ways of producing goods [28]. "Drivers" are now taken to include all bioeconomy sectors following the above definition, and not only bio-based substitute goods (i.e., biomaterials and bioenergy) as in the original framework. However, with our case study, here we suggest an initial focus for bioeconomy monitoring on the transition towards innovative bio-based products that not only may generate economic growth, but also often have a substituting function. We emphasize showcasing this kind of transition rather than increasing agricultural production or imports, which may not be directly connected to improving sustainability. Bioeconomy sustainability objectives, as formulated in [29], are termed "societal challenges" in the framework (Figure 1). The bioeconomy is expected to have a positive impact on these objectives, and we derive indicators for the challenges in the grey boxes (Figure 1) in this article.

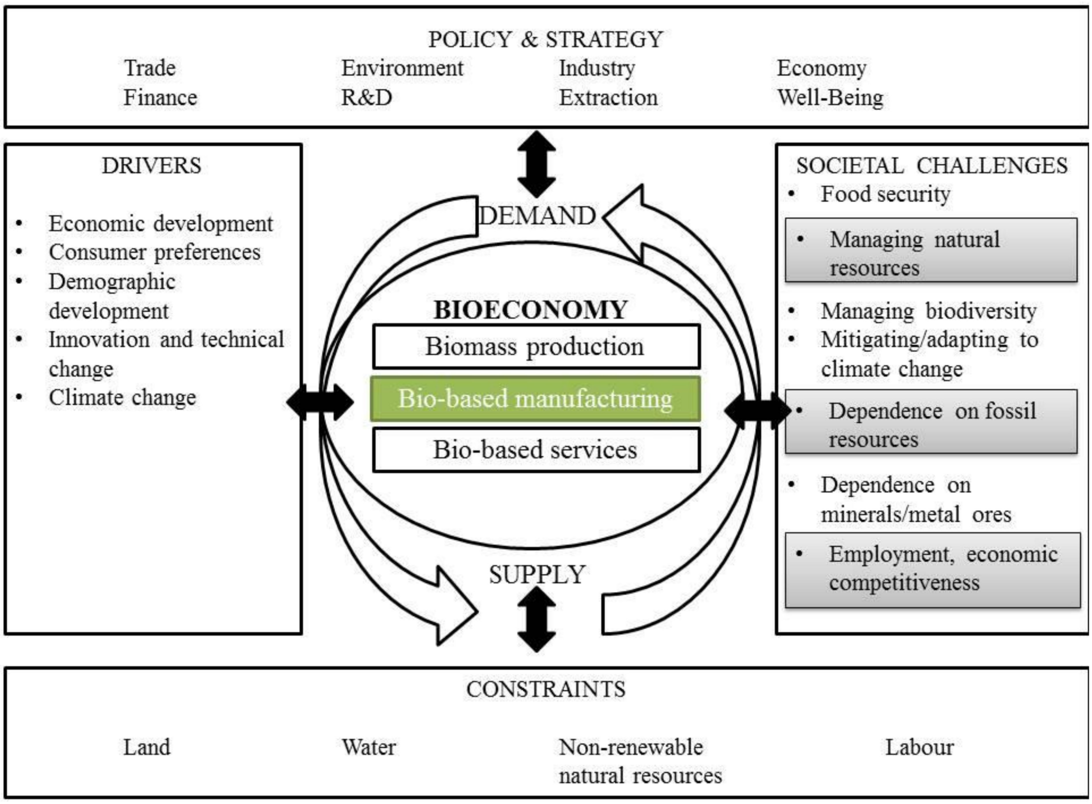

Figure 1. Bioeconomy Transition Framework (green represents the bioeconomy sector examined and gray the societal challenges, for which indicators are developed in this study). Source: Own illustration, adapted from [30].

2.1. Administrative and Sectoral Boundaries

As is common for economic classifications, the bioeconomy can be subdivided into three broad sectors: biomass production (primary sector), bio-based manufacturing (secondary sector), and related services, such as trade (tertiary sector). While in principle, all of these should be well represented in a monitoring system, the focus in this article is only on the manufacturing sector in Germany, which was chosen so as to investigate the complexity of value chains in the bioeconomy. Biomass production and the food sector have already been better covered by existing statistics than manufacturing because they are well delineated within economic classifications. The processes after first-stage processing are, however, more difficult to measure, as product and sectoral statistics do not list the types and amounts of resources used. Thus, in order to investigate the possibilities and limitations of indicators for such processing sectors, our case study deals with the manufacturing of surfactants, which is part of the chemical industry. We find that transitioning from a fossil- to a bio-based economy is a central objective in most bioeconomy strategies and that relevant substitution processes are occurring in the chemicals industry. Consequently, we examine this sector in our case study because, beside energy industries, chemical industries have been relying strongly on fossil fuels. The tertiary sector of trade and services related to bio-based products is not covered in this article but certainly deserves attention in any monitoring scheme. We focus our case study on Germany, because several ministries there are making a concerted effort to set up a bioeconomy monitoring scheme, taking the lead in this regard in Europe.

Bioeconomy developments are taking place at different levels, which define the boundaries of the analysis of monitoring systems. Depending on concrete monitoring goals, relevant levels may include the local, sectoral, national, regional, or global levels. For our empirical analysis, the level of the NACE classes was chosen because of our specific interest in comparing bioeconomy developments in different sectors. A class is defined as a group of products that are included in the NACE classification system on the 4-digit level, which we selected because activities that are clearly attributable to the bioeconomy should be recorded there. While some industries are completely bio-based at the 2- or 3-digit levels—for example, the food, paper and pulp, and printed matter industries—others, such as the pharmaceutical or chemical industries, clearly have bio-based subsectors at best at the 4-digit level or even lower, meaning that bio-based shares have to be estimated. This study also provides a detailed assessment of the related 9-digit product codes. Most economic indicators are available at the 4-digit level but not lower.

2.2. Indicator Selection

The European Commission has proposed its own relevant, accepted, credible, easy, and robust (RACER) criteria for evaluating the usefulness of indicators in policymaking [31] (p. 308), which have been applied to resource use, resource efficiency, and environmental impact indicators lately [32]. For a future monitoring scheme, given the current limitations of data availability, we suggest a narrow set of basic indicators covering the economic, environmental, and innovation domains—each with two to four indicators—aiming to provide an overview of key bioeconomy transition dimensions. The initial selection of indicators for this study has been based on their relevance and practicality, with relevance being determined by an explicit linkage to the phenomenon under observation, meaning the bioeconomy and its effects. The relevant indicators should contribute towards understanding problems and identifying solutions for them. Practicality, or "easiness," is taken here to mean that data and information collection is possible at low cost.

3. Indicator Methods and Data Sources

For our chosen economic indicators, "value added," "turnover," and "number of employees" were frequently mentioned and seemed to be of most interest to policymakers. To these, we added "foreign sales" and "investments." All economic indicators were linked to the bioeconomy through the "bio-based share" indicator that showed bioeconomic growth in physical terms.

The economic–environmental indicators were examined to reveal trade-offs between contrary objectives, as growth in the value added of bio-based products may increase energy consumption if bio-based processes are more energy-intensive than fossil-based ones, for example. Combined indicators are valuable because they provide much information at a glance. If one part of the indicator stagnated, for example, the other part could compensate for this development with a strong increase. The environmental indicators chosen here refer to the objectives "managing natural resources" and "reducing dependence on fossil resources" in our BTF (Figure 1). When combined with economic indicators, they were "energy productivity," "land productivity," and "cost effectiveness in terms of fossil-resource savings."

The innovation indicators for the bioeconomy should be useful for deriving information about whether and where innovation activities and outputs are likely to emerge and help to achieve desired positive impacts on societal goals. Hence, ideally, they should cover the whole innovation process, from inputs to outcomes/impact; however, the data availability for the latter is rather low [25], so we only included the indicators "publications" and "patents." Together with the other chosen economic indicators, they were intended to map the objective of "improving economic competitiveness" in the BTF (Figure 1).

3.1. Bio-Based Share

As mentioned above, there are several industries at the 4-digit NACE classification level that belong only partially to the bioeconomy. For such cases, we developed an estimation method to determine the bio-based shares of respective industries by combining information from production and industry statistics. For manufactured goods, the annual production survey of the Federal Statistical Office of Germany provided the value and quantity of products intended for sale at the 9-digit level. We multiplied the production value of each good by its estimated bio-based share, as obtained from the literature review and expert interviews, and summed the results up at the class level. Thus, the estimated bio-based production value results were given as a proportion of the total production value of a NACE class. Further economic indicators, such as employees and turnover, were only available in the official statistics at the NACE-class level. Under the simplifying assumption that production values per tonne are roughly the same within a NACE class, the same proportions for bio-based products could be assumed for these economic indicators as matches their share of the production values of the corresponding NACE class.

3.2. Number of Employees

The number of employees refers to the calculated labor force in the production of bio-based products. It is of high political interest, because it shows the contribution of the bioeconomy to the overall economic goal of full employment. The indicator was relevant for monitoring policy measures that aim at securing or creating employment opportunities, as well as measuring the impacts of new activities, such as technical innovation on the labor market. All economic data used for this study was collected from publications by the German Federal Statistical Office, and the number of employees can be found in the "Annual report for enterprises of manufacturing companies" [33].

3.3. Gross Value Added

Gross value added (GVA) was calculated as the total monetary value of the goods and services produced in the production process (production value) minus the value of the inputs used. At the macroeconomic level, it is included in the Gross National Product as the sum of all goods and services produced for final demand during a year. Related to individual economic sectors, such as the bioeconomy, it shows their overall economic importance. The indicator was relevant for the formulation and focusing of policies and other measures aiming at maximizing economic growth. The data for gross value added in the case study were taken from the publication "Cost structure survey in the manufacturing sector" [34].

3.4. Turnover

Turnover is the sum of the value of all products and services sold within a certain period of time and is a suitable indicator for representing the market share of a company or industry. It differs from production values due to changes in storage. The indicator may be used to better understand the economic importance of the various branches of the bioeconomy. Data for this indicator is available in the "Value added tax statistics" [35].

3.5. Foreign Sales

Foreign sales include goods and services sold to customers abroad or to exporters who export the goods without further processing. Foreign sales are an indicator of the international market share of a company or industry and, thus, also an indicator of its international competitiveness. The indicator was relevant for focusing policy measures and other activities related to export promotion. We drew data from the publication "Employment and turnover of enterprises in the manufacturing and mining industries and the extraction of stones and soils" [36].

3.6. Investment

Investment includes the outlay of financial funds for tangible investments (such as machinery), immaterial assets (such as software or patents), or financial investments (such as bonds or equity investments). It is decisive for both overall economic growth and the growth of individual companies, including those in the bioeconomy sector. As an indicator, investment statistics provide information about the development of medium- to long-term production capacities. Data for our case study came from the publication "Investment survey of companies in the manufacturing and mining industries and extraction of stones and soils" [37].

3.7. Energy Consumption

Energy consumption is considered one of the main drivers of climate change, even with renewable sources gaining importance. While it is important to save fossil-energy sources by using more and more biogenic resources in products, this transition should not come at the cost of employing more energy-intensive production processes. A contribution of the bioeconomy to climate change mitigation is indicated if less energy is consumed over time. We calculated the energy consumption of a bio-based sector for a given year by multiplying the annual energy consumption of the whole sector by its bio-based share, including the use of natural and associated gas, district heating, and electricity in one sector, but not the material use of energy carriers or energy use in upstream sectors. Bio-based share is derived as described above for economic indicators, with sectoral energy consumption taken from German energy statistics [38]. We suggested combining this indicator with GVA to obtain the indicator "energy productivity," which showed how much economic output could be generated from one energy unit, enabling the observation of relative and absolute decoupling. A growing GVA or decreasing energy consumption increased the energy productivity.

3.8. Land Footprint

Bioeconomy growth will very likely increase land usage compared to the current fossil-based economy. If such land is not used sustainably, however, it will become an indicator for a variety of environmental pressures, from biodiversity loss to soil degradation. We recommended including the land footprint of bio-based manufacturing sectors, showing how much land across the globe was used to produce biomass inputs. Our method started with an estimation of bio-based production on the 8-digit level and multiplied it by conversion rates for bio-based inputs, which were plant oils and animal fats in our case study. Based on the information from [39], we split the total amount into the demand for specific plant oils and, based on various literature sources, determined the amount of raw materials used. While material productivity might also be a valuable indicator in some contexts, we decided to go one step further by calculating land productivity based on global average factors for area required by FAOStat. We assumed that biomass was harvested due to producer demand in the selected sector and, thus, no allocation factors for by-products needed to be applied. The land footprint was also combined with the GVA, resulting in the indicator "land productivity."

3.9. Fossil Resource Saving

One of the main arguments for supporting the transition to bioeconomy is its potential to reduce the reliance on fossil resources by substituting bio-based products for fossil-based products. As bio-based products may also rely on fossil resources as energy carriers or additional inputs, net savings needed to be calculated. Fossil resource saving (FRS) in a sector (s) showed how much crude oil, natural gas, and coal, in energy units, were saved due to the production of bio-based substitute goods (X_b) within a year. Fossil resource equivalents ($FRE_{b,f}$) were factors for fossil resource use along the supply chain of fossil-based and bio-based products, which we extracted from the life-cycle database ecoinvent (2017). Bio-based production was estimated based on bio-based shares, as described above. A more detailed description can be found in Jander and Grundmann (2019).

$$FRS_s = \sum_{b,f=1}^{n} X_b * \left(FRE_f - FRE_b\right) \tag{1}$$

The FRS was combined with the value of intermediate consumption, which was the value of inputs to a sector (s) or, put differently, turnover minus value added. We assumed that substitution might come at the cost of higher input prices, especially if increasing the demand for biomass resulted in higher prices for these inputs, and value added might be reduced as a consequence. A growing FRS or decreasing value of inputs (i.e., costs) will cause an increase in FRS per €, which we called the "cost effectiveness in terms of fossil-resource savings" indicator.

3.10. Publications

The statistical analysis of scientific publications provided a means to monitor the performance of the science landscape over time. Here, we proposed the number of scientific publications in a sector of the bioeconomy in a country over time as an indicator, as data sources, literature, and citation databases were used, such as Scopus, Web of Science SciSearch, and Compendex. For our search strategy, we considered a combination of journals and books that could be completely attributed to the bioeconomy and a keyword search to identify further articles in other journals or books as appropriate.

3.11. Patents

Patent indicators are useful for monitoring the economically relevant results of innovation activities or measuring technological competitiveness in international comparison. Patent applications refer to inventions in the technical field that are new and for which an interest in industrial application is assumed. We proposed taking the absolute number of patents over time as an indicator for monitoring. Key questions arose here regarding the delineation of patent classes or keywords. In particular, it needed to be decided whether a patent search should solely focus on innovation for production or the use of biogenic resources or whether important input innovations, such as new agricultural machines, were to be included as well.

4. Results for Bio-Based Surfactants and Soaps

The manufacturing of surfactants and soaps is a core segment of oleochemicals that has seen an increase in bioeconomic activity in the past years, but for which little relevant information exists in comparison to other segments, such as biofuels. The indicators suggested in Section 3 were here applied to class 20.41 of the German Classification of Economic Activities (2008 edition), which is called the "Manufacture of soap and detergents, cleaning and polishing preparations." The year 2015 was chosen, as data from the Federal Statistical Office and other data sources were relatively complete for this year. We focused on organic surface-active substances (anionic, cationic, and non-ionic) and soaps, which made up 75% of the production volume for sector 20.41 in 2015.

4.1. Past Transition and Implications

Table 2 displays our derivation of the proportion of bio-based surfactants and soaps in the production values of the whole NACE class 20.41. As explained in Highlights section, first, the bio-based shares in the production of surfactants (33%) and soaps (90%) were determined from a literature analysis and expert interviews. These shares were multiplied with the respective total production values and volumes of surfactants and soaps and summed up for NACE class 20.41, with the bio-based share of surfactants and soaps accounting for about 31% of the total production volume and 13% of the total production value.

In a second step, the calculated bio-based share in the production value was applied to the sector's economic indicators. Based on the assumption that the bio-based share of production value was the same for all economic variables, the results shown in Table 3 were obtained for class 20.41. According to these estimations, 2782 people were employed in this sector in 2015, generating a gross value added of €470 m, a turnover of €904 m, and foreign sales of €355 m. At the same time, €45 m were invested in the bio-based part of NACE class 20.41.

Table 2. Derivation of the proportion of bio-based surfactants and soaps in the production volume and value of NACE class 20.41.

		Production Volume			**Production Value**		
Production Code NACE Code	**Designation**	**Total Production (t)**	**Bio-Based Production (t)**	**Calculated Bio-Based Share of Production Volume**	**Total Production Value (m €)**	**Bio-Based Production Value (m €)**	**Calculated Bio-Based Share of Production Value**
20.41.20	Surfactants	1,179,266	389,980	33%	1641	540	33%
20.41.31	Soaps	185,821	167,239	90%	198	178	90%
20.41	Manufacture of soap and detergents, cleaning and polishing preparations	1,828,060	557,219	31%	5356	718	13%

Source: Own calculations, based on [40].

Table 3. Results for economic indicators in the surfactant and soap industry.

Economic Indicator	**NACE Class 20.41**	**Bio-Based Surfactants and Soaps**
Number of employees	20,755	2782
Gross value added (m €)	3505	470
Turnover (m €)	6740	904
Foreign Sales (m €)	2646	355
Investments (m €)	333	45

Source: Own calculations, based on [40].

Whether bioeconomic growth is not only economically but also environmentally sound is shown here via the development of combined indicators, as explained in 3. One gigajoule used for the manufacturing of bio-based soaps and surfactants in 2015 generated, on average, €150 of value added. Meanwhile, energy consumption was 3,127 TJ, assuming a bio-based share of 31% and 10,238 TJ of process energy for the whole NACE class 20.41.

Regarding the resource of land, we found that the value added generated was €336 per ha. In total, the production of bio-based surfactants in 2015 required about 1.1 m ha for the cultivation of coconuts and palm oil fruits, whereas coconuts, palm oil fruits, soybeans, and sunflower seeds were grown on about 0.3 m ha for the production of soaps. The land requirements for soaps are much lower than for surfactants, because less palm kernel oil is used, which requires a much higher amount of raw materials per tonne of oil than the other raw materials. There is, however, much uncertainty in estimating the kinds of oils used. Anionic and non-ionic substances are produced from lauric and stearic acid, which can only be found in palm kernel and coconut oil [39]. We assumed a share of 50% of these oils. Other surfactants also have palm oil and animal fats as inputs. Soaps are produced from various oils [39], depending on the current market situation and desired product properties.

For every euro of input, 29 MJ were saved by producing bio-based surfactants and soaps in 2015. The most important bio-based substitute products in this sector were bio-based fatty alcohol ether sulfates, fatty alcohol sulfates, ethoxylated alcohol, and soaps. For fatty alcohol sulfates and ethoxylated alcohol, it was possible to determine the Fossil Resource Equivalents (*FRE*) for bio-based and fossil-based alternatives from ecoinvent, as well as for the coconut oil, palm kernel oil, and palm oil inputs. For fatty alcohol ether sulfates and fossil-based soaps, the same parameters as for fatty alcohol sulfates were used due to a lack of data. Based on our calculations, the Fossil Resource Saving (FRS) was 12,611 TJ in 2015. Assuming that soaps can also be produced from crude oil [39], bio-based soaps had the largest share in the savings, with 68%. Linear alkyl benzol acid is still completely fossil-based, and no bio-based alternative is currently being produced [39]. Cationic substances were not considered, as they always have been bio-based and do not substitute a fossil-based alternative. While soaps have been traditionally bio-based as well, synthetic detergents (syndets) from fossil resources could replace bio-based soaps in the future, contributing to an opposite trend. They already have a market share of about 8% [41]. It is worth observing this "negative" substitution, because one kg of bio-based soap saves more fossil resources (51 MJ) than anionic and non-ionic surfactants (about 20 MJ).

4.2. Prospective Transition

For the prospective analysis, we have used the innovation indicators described in 3. Although the actual data were ex-post, it may be important for developing a prospective outlook, as current activities are undertaken with the expectation of further transitioning towards the bioeconomy and future returns. For patents and publications, we used worldwide numbers, as relevant markets were rather globalized and country-specific numbers fluctuated more heavily. Moreover, as proxy information for innovation output, for which reliable indicators were available, we assessed market developments and expectations from market studies. While market developments were not necessarily driven by new innovations, they indicated the market environment for the introduction and adoption of new products.

Our results are shown in Table 4. The publication indicators revealed a considerable increase, whereas patents have stagnated in recent years. This may be related to rather stagnant market development for bio-based surfactants, leading to a general decrease in innovative activities. According to a study commissioned by the FNR [39], the quantity of oils and fats in detergents, care products, and cleaning agents in Germany rose from about 589,000 tonnes in 2011 to around 599,000 tonnes in 2016. However, global market expectations are rather optimistic, with a forecast of global growth rates of around 6%–7% in the next five years [42]. An additional analysis for the development in Germany in the years 2010–2015 revealed significant activities in patenting and publication, occupying a position among the leading countries in this sector.

Table 4. Transnational* worldwide patents and publications for biosurfactants.

Year	2005	2006	2007	2008	2009	2010	2011	2012	2013	2014	2015
Patents	1066	969	954	875	881	951	858	935	881	1067	890
publications	1854	1914	1961	2014	2150	2190	2292	2277	2315	2364	2433

Sources: WPINDEX (STN), SCISEARCH, COMPENDEX; * for the concept of transnational patents see [43].

5. Discussion and Recommendations

5.1. Findings

The selected indicators—developed and experimentally applied for measuring the progress of the bioeconomy in the sector of biobased surfactants—revealed a share of 13% of the production value of NACE class 20.41 and a share of 31% of the production volume for this sector. This finding indicated past and future growth in innovative, bio-based products and possibly the beginning of a transition from a fossil-based to a bio-based economy in this sector. A fossil resource saving of 12,611 TJ supported this observation. Linked to this development was a significant demand for biomass inputs and, ultimately, land, which was in line with previous research [44].

Our analysis of the innovation pipeline and market outlook indicated that there is considerable potential for future innovation that can fuel bio-based industries towards achieving higher growth rates and gaining market shares. However, such evolution cannot be taken for granted—an indication of which is the stagnation of patents filed, probably because of the declining market optimism among involved actors.

5.2. Methodological Challenges

We feel that our proposed indicators, as well as methods and data sources for calculation, provide an important step forward for monitoring bioeconomy progress. In order to guarantee sound and reliable monitoring, however, more work is needed to further develop methods that increase the reliability of the monitoring results. As methodological shortcomings are frequently the result of insufficient data, we recommend the extension of data sources in 5.3.

Clear delineation between the emerging bioeconomy and other parts of the economy is still missing with regard to relevant PRODCOM ("PRODuction COMmunautaire") codes, patents, or publication searches, for example. Although the setting of boundaries appeared to be rather straightforward in our case study, in terms of the identification of relevant statistical codes and estimating bio-based shares, the critical assessment of other research and harmonization with other studies is needed. In [24], for example, all products that use biogenic resources in order to substitute fossil-based products were considered in the analysis. For the case of surfactants and soaps, this approach omits cationic substances, as these do not have a substituting function. Meanwhile, [11] considered all industries that have biological inputs, whereas [45] did not further specify relevant bioeconomy sectors in their Driver-Pressure-State-Impact-Response framework.

The bio-based share of a smaller part of NACE class 20.41, meaning only surfactants and soaps, was much higher for us, at 13%, than as found by [11], who calculated a bio-based share of 4% of input value. This illustrates a range of results depending on the methods employed. [23], who further developed the method used by [11], underlined this possibly wide range by finding a bio-based share from 2.6% to 13.5% for this NACE class. Both methods, with one relying on official data and the other relying on expert estimates, currently suffer from non-transparent and arbitrary procedures in the derivation of bio-based shares.

One limitation of the current approach, as well as in many other economic assessments of the bioeconomy, is that all economic indicators are estimated proportionally to the bio-based share of resource use. However, there is uncertainty about whether the bio-based share is truly the same for all indicators. Some industries may, in general, be more export-oriented than others, especially with respect to foreign sales. Hence, the bio-based share could be different with respect to turnover, on the one hand, and foreign sales on the other. The same could be true for investment. The goal of developing bio-based production could require more investment than traditional production, meaning that the bio-based share of investment could be higher than investment in the traditional part of the industry. While this assumption can often be considered as a best guess for some indicators, such as turnover, the value added is probably correlated less with resource use. Bio-based products may have high value added in niches, such as high-price cosmetics, combined with relatively low resource use. This difference can be even more pronounced for environmental indicators. With top-down bio-based share assumptions, important characteristics may be overlooked, such as different energy usage for conventional and bio-based products. In our case study, additional information from ecoinvent regarding per-tonne energy consumption was not informative, as there was no significant difference between bio-based and fossil-based surfactants, whereas in other sectors, such as transport fuels, the proportionality assumption is untenable.

For the innovation indicators used in this article, the identification of bio-based relevant publications or patents is more straight-forward, as they can be identified on a much higher granularity level. Nevertheless, in some cases, bio-based patents can still be separately identified, as there is no reference to the feedstock in the international patent codes. Related to this, there are not yet any lists for codes or keywords for the bioeconomy for patents and publications that are widely accepted.

Overall, our case study shows that investigating the market and resource flows of bio-based products on a disaggregated level can be very informative and combines well with existing data sources. Nevertheless, great uncertainties still exist concerning biomass inputs and origins for surfactants and soaps. For example, for want of more specific information, we have assumed the shares of different oils and fats in terms of input volumes and we have used worldwide average values for area requirements. These uncertainties call for an analysis of the dependence of results on the kind of raw materials used and on production conditions in different regions.

5.3. Recommendations

A requirement for goal-oriented monitoring of the bioeconomy is that potential users agree and clearly define the objectives of the system. What are the boundaries of the bioeconomy, and which aspects of it should be observable through monitoring? The framework suggested in Section 2 includes many possible bioeconomy boundaries for scientific analysis, depending on the monitoring objectives. We recommend a focus on the most interesting and agreed upon objectives, such as fossil resource substitution, the use of natural resources, such as land and water by the bioeconomy, and the promotion of a certain biogenic resource for new bioeconomy monitoring schemes with limited financial resources. In the beginning, it would be useful from a methodological point of view to focus on the manufacturing sectors where bio-based (substitute) products are currently gaining market shares, instead of trying to coarsely outline the whole bioeconomy, however, it is defined with methods still in their infancy that rely on official data, which are not at all designed to unambiguously identify bio-based products. Analyzing sectors in depth allows targeted resource allocation and more sustainable production. From a resource economic and political point of view, it might be useful to focus first on sectors with a particularly high use of resources. Over time, as data collection becomes more refined and methods more mature and transparent, more indicators and sectors could be gradually introduced to the monitoring scheme. Regarding matters of consistency and feasible workload, more detailed official production statistics are needed to delineate bio-based products. However, this would require changes in laws and intensive coordination between statistical agencies at different levels (regional, national, European).

Regarding bio-based industry shares, we recommend refining the estimation methods before delivering indicators for the whole bioeconomy. We agree with [23] that, given insufficient official data for bio-based product groups, transparently presented expert estimates should play an important role. The identification and selection of experts and key informers is crucial in this regard and the use of participatory methods should be improved in future analyses. This would allow the monitoring of the dynamics of bioeconomy developments if regular and precise updates on bio-based inputs, the raw materials used, and their origins were available.

As long as no significant improvements in the quality and quantity of official data are achieved, analysis and monitoring activities have to rely on complementary data for bio-based products. Expert opinion may not only verify bio-based shares, but also assumptions, such as proportionality between bio-based shares and suggested indicators. Environmental indicators could be informed by lifecycle data from respective data bases. In our view, the data from the life cycle assessment (LCA) can only inform us about relative differences and not about absolute energy use because, first, not all processes in a sector are included in existing data bases, and, second, representative products, as analyzed in the literature, for a given year might overestimate efficiency. Statistical data based on annual surveys is more current, even though estimation procedures are also necessary. A combination of economic with environmental indicators is currently possible using LCA data, if no other information is available from surveys. In-depth material flow and market studies should be regularly commissioned along with further, regionally specific LCA studies of new bio-based processes. Given the resource bases of the bioeconomy and their rather decentralized production patterns, the local level should constitute the reference or basis of validation for nearly any analysis and monitoring effort, and any monitoring results should be validated via information on the local and product levels. In the long term, the German survey "Materials and Goods Received" could be extended to include more disaggregate input groups, meaning not just agricultural inputs, but, specifically, cereals and oil crops, and receiving industries could also be further disaggregated in some cases, such as chemicals. Including these steps and input groups would enable a more detailed input–output table for Germany—as it is common for Japan, Australia, and the USA—and more reliable analyses of the FRS indicator, for example. For innovation indicators, similar issues apply. While in the long term, it would be appropriate to further develop codes and classifications that enable the identification of bio-based innovations; in the short term, efforts towards a common list of keywords and patent codes based on current classifications would be helpful.

Additional indicators may be appropriate for obtaining a more comprehensive overview in the future, such as with social or further economic, ecological, or innovation indicators. As indicated above, we do not provide a complete list of useful indicators, but have instead focused on presenting those with rather good data availability. Nevertheless, it should be noted that in an extensive study, the authors of this article have empirically derived a total of seventeen economic indicators for surfactants and soaps, including indicators, such as gross production value and domestic sales [19]. This study also includes a list of further environmental sustainability indicators that could be linked to the bioeconomy. Two approaches were suggested: using "top-down" national sustainable development indicators, as measured by the German Statistical Office, such as air emissions and phosphorus in water, and using "bottom-up" product data from life cycle inventories, such as the use of pesticides and nitrogen fertilizer. More have been suggested in [18] (p. 10). A further interesting area of study is circular bioeconomy, which is increasingly studied but has hardly addressed indicator development and sectoral analyses so far [46]. Bioplastics, solvents, lubricants, fabrics, fine chemicals, and insulation material have been identified in a multi-criteria decision analysis as significant sectors in studying the circular economy [47]. Extensive combination options are also possible. For example, labor productivity can be calculated from the combination of gross value added and employed persons. A combination with environmental indicators would also be conceivable for individual economic sectors, such as the turnover achieved per hectare of forest land in the forestry sector. While we suggest comparing economic sectors within a country, applying spatially explicit indicators at the local, regional, and global level would provide important information on drivers and outcomes on the respective level.

Regarding the innovation indicators, the patent and publication indicators we used are only early stages of the innovation process. There are still clear data gaps in the outcome and impact indicators. Current government surveys do not provide adequate boundary setting for analyzing the bioeconomy. This could be improved in the future by, for example, conducting an explicit survey regarding the bioeconomy or through adding another item in the European Community Innovation Survey (CIS) asking whether responding firms are active in the bioeconomy or not or by adding questions similar to those concerning environmental innovation, which is a topic in the CIS every few years [48].

Furthermore, in order to provide more decision-relevant information for public and private actors, greater focus may be placed on the ex-ante assessment of innovation and innovation potentials. There have been some important studies in the past in this regard, but more comprehensive coverage beyond the lists of examples of single innovations is crucial. Moreover, certain impacts, including the potential prices and cost structure for actors, potential substitution rates of fossil-based products, or required land use, may be important information that can be gathered using a systematic approach. In addition, the integration of such indicators into a model-based forward-looking analysis (e.g., [49,50]) may provide further insights regarding the potential diffusion and economic and environmental impacts of the bioeconomy.

6. Summary and Conclusions

With this article, we wish to contribute towards the development and measurement of relevant indicators for the economic and environmental impacts of bioeconomies. We have discussed approaches, derived indicators, and applied them to monitor developments in surfactant production in Germany. New indicators and analytical frameworks for the investigation of transformations within and the monitoring of bioeconomy innovations have also been discussed. In summary, we suggest that our results contribute towards creating a basis for forecasting, future scenario analysis, and impact assessment of bioeconomy developments.

We have also identified shortcomings in the ways official statistics are generated that are jeopardizing the intention and relevance of transition-monitoring systems in general and of our proposed indicators in particular, including significant weaknesses in the existing data and information base regarding the bioeconomy in Germany. To our knowledge, the case of Germany is not unique, however, as the monitoring efforts in other parts of the world are also affected by such limitations. The identification and evaluation of options and strategies to improve information bases should be given high priority at all levels involved in the implementation of bioeconomy monitoring systems. A short-term strategy proposed here is the integration of further data sources, which can refine the results and extend the assessments to other areas of the economy. In addition to possibly having positive impacts on decision making in practice, this may also enable a more advanced ex-ante analysis, using them as tool models based on input–output tables, for example. Future research should also address the integration of indicators into monitoring systems that reveal otherwise largely neglected social impacts. The limitations of this study also make it necessary to further examine the validity and applicability of the indicators and frameworks for other sectors and the bioeconomy as a whole. This step must be accompanied by the review of the meaning of indicators for research activities and their relevance in view of the intentions of decision-makers in practice. The development of several bioeconomy monitoring systems can be expected in the medium term as a result of a number of national, European, and global initiatives. This calls for the proper coordination of activities and even the harmonization of approaches and tools at all levels to enable synergies and facilitate exchange and comparison of results.

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Chapter 3. Substitution as a central concept in bioeconomy transition indicators

Chapter 3 is called "Substitution as a central concept in bioeconomy transition indicators", deviating from the title in Jander and Grundmann (2019), because it identifies, explains, and operationalizes the concept of substitution in the context of a bioeconomy transition.

The published research paper has been added to this thesis in the next pages.

Nomenclature

A	technology coefficients matrix
$dFRC_i$	direct Fossil Resource Consumption of industry I (in MJ)
$dFRI_i$	direct Fossil Resource Intensity of industry I (in MJ/€)
$FRC_{i,b,f,o}$	Fossil Resource Consumption of industry i, bio-based substitute products b, fossil-based products f or other products o of i (in MJ/€)
$FRE_{bi,fi,oi}$	Fossil Resource Equivalents of bio-based substitute products, fossil-based products or other products of industry i (in MJ per t or €)
FRS_i	Fossil Resource Saving of industry i (in MJ/€)
I	unity matrix
L	Leontief coefficients matrix
RMI_f	Raw Material Input of fossil energy carriers (in MJ)
SF_i	Substitution Factor of industry i (dimensionless)
SSI_i	Substitution Share Indicator of industry i (dimensionless)
$tFRI_{bi,fi}$	total Fossil Resource Intensity of the bio-based or fossil-based part of industry i (in MJ/€)
w_i	weight (dimensionless)
$X_{bi,fi,oi}$	quantity of bio-based substitute products, fossil-based products or other products of industry i (in t or €)

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Monitoring the transition towards a bioeconomy: A general framework and a specific indicator

Wiebke Jander [a, b, *], Philipp Grundmann [a, b]

[a] *Leibniz Institute for Agricultural Engineering and Bioeconomy e.V. (ATB), Department Technology Assessment and Substance Cycles, Potsdam, Germany*
[b] *Humboldt-Universität zu Berlin, Faculty of Life Sciences, Albrecht Daniel Thaer-Institute of Agricultural and Horticultural Sciences, Germany*

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ABSTRACT

Monitoring schemes and indicators are currently under development to enable the assessment of the economic, social, political, and environmental impacts of bioeconomic transitions and better inform bioeconomic policy-making. Such transitions generally mean reduction in fossil resource use through innovative, clean technologies that can enable substitution of biogenic resources for fossil resources. The concept of bioeconomy transition is not yet well embedded in current monitoring schemes. Proper framing and a quantitative indicator for measuring the advancement and status of bioeconomy transitions has been missing up to now. This research aims to lay some groundwork for monitoring transitions from fossil-based to bio-based economies by adapting an existing bioeconomic framework and applying a newly developed indicator: the Substitution Share Indicator (SSI). This indicator relates bio-based substitute products to their fossil-based counterparts and accounts for indirect fossil resource flows, which are estimated using a bottom-up approach, based on life-cycle inventory data, and a top-down approach, based on input–output data. The innovative indicator is tested and validated for the first time in the case of transport fuels and plastics sector in Germany. The SSI in the German transport fuels sector is currently relatively low, at 3.1% (bottom-up approach) to 3.4% (top-down approach). It is even lower in the plastics sector, at 0.09% (bottom-up approach) to 0.6% (top-down approach). Major policy efforts need to be undertaken in Germany, focused not only on the growing bioeconomy but on substitution effects as well. Future policies should provide incentives for increasing production of innovative bio-based substitute goods, improving the fossil resource use efficiency of existing fossil- and bio-based products, and lowering consumption of fossil-based products. Such efforts should be reflected in the SSI and signal bioeconomy transition. Before the widespread use of the indicator for policy formulation and analysis, further advancement is recommended. A hybrid approach integrating process data into input–output data would be expedient for improving the SSI in terms of credibility, measurability and robustness. Linkage to relevant indicators for sustainability assessment of transitions is equally important for effectively monitoring sustainable bioeconomy transitions.

1. Introduction

Most economies still fundamentally depend on fossil resources for energy generation and production of a variety of products: from automobile fuels to zippers. More than 80% of the world's final energy consumption is currently based on crude oil, natural gas, and coal. About 10% of fossil resources are used for non-energy purposes, mainly in the chemical industry (OECD/IEA, 2017). In Germany, 94% of the final energy used for transportation is fossil-based (AGEB, 2018). A strong dynamic in petroleum-based plastics production, with output value rising from €50*10^9 in 2009 to more than €70*10^9 in 2017 (Destatis, 2017d), has led to increasing demand for fossil resources for non-energy purposes in Germany. It is fairly well known by now that fossil resource use is linked to many environmental, social, economic, and political problems along all supply chains: from extraction to use and disposal. Oil and gas drilling are associated with loss of biodiversity (Kadafa, 2012), displacement of indigenous peoples (Finer et al., 2008), violent conflicts (Mildner et al., 2011), and contamination of soils and groundwater (Wake, 2005). Improper disposal of petroleum-based plastics and unhindered release of microplastics are contributing to marine litter, having severe impacts on marine ecosystems (Andrady, 2011), and combustion of fossil fuels is considered a main

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* Corresponding author. Leibnitz Institute for Agricultural Engineering and Bioeconomy e.V. (ATB), Max-Eyth-Allee 100, 14469, Potsdam, Germany.
E-mail address: wjander@atb-potsdam.de (W. Jander).

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contributor to climate change (IPCC, 2014). In view of the finite nature of fossil resources, the dependence of large numbers of producers and consumers on it will, in the long run, affect the well-being of firms and individuals when it runs out.

Changing to economies based on biogenic rather than fossil resources has been proposed as an alternative to current economic processes that generate negative externalities. Moving in the direction of becoming bioeconomies is increasingly the preferred objective of countries with diverse and large industries that depend strongly on fossil resources, such as Germany, Japan and the US (Pietzsch, 2017). There is at present a felt need to monitor and evaluate bioeconomy transitions, requiring ways to track their progress, identify barriers, and manage trade-offs with other societal goals, such as food security and employment (EC, 2012). Monitoring is especially needed, since many bioeconomy developments depend to a large extent on public funding and policy support. “Bioeconomy” is an umbrella term for all economic processes and products that produce or use biogenic resources, meaning organic, non-fossil resources that are renewable in the sense that they can be potentially available on a recurrent basis, including products from agriculture, forestry, and fishing as well as organic residues and wastes (EC, 2012).

Monitoring systems are designed to “measure progress towards achieving […] objectives” (Frankel and Gage, 2007) and are often based on indicators that can support surveillance of not directly observable objectives. Such indicators must meet certain theoretical, methodological, political, and practical requirements (Meyer, 2017). An observable indicator needs to be linked to an unobservable construct through a correspondence rule, meaning a hypothesis regarding the relationship between indicator and construct. The rule can be derived via a causal model that makes assumptions regarding influences on a construct's development (Meyer, 2017). A bioeconomy transition indicator should include all key factors that influence transitioning from a fossil-based to a bio-based economy and must

A) make explicit the starting point and completion of the *transition*;
B) chart developments in *fossil* resource consumption within an economy;
C) show developments in the availability of substitute goods from *biogenic* resources; and
D) include all sectors of an *economy* that are important for the transition, to make entry points for steering it visible.

Transition, material flow, and bioeconomy indicators proposed in the literature only partly fulfil these requirements. Transition indicators should define clearly the beginning and end of a transition. An economy may shift from a centrally planned economy to a market economy (Myant and Drahokoupil, 2012), or from an agrarian economy to an industrial or service one (Silva and Teixeira, 2008). Sustainability transition indicators should chart development from economic processes considered unsustainable to more sustainable ones (Markard et al., 2012). From a macro perspective, transition indicators divide an economy into sectors in order to “analyse the dynamic properties of the economy as a whole” (Silva and Teixeira, 2008). There are currently no transition indicators that attempt to display progress towards fossil resource substitution, and sectors are not grouped to represent fossil-based or bio-based parts of an economy. The main focus of economic indicators has generally been to show the relative importance of land, labor, and capital (Machlup, 1991), rather than of fossil or biogenic resource inputs, within a very limited number of sectors (Silva and Teixeira, 2008). Sustainable development indicators generally refer to human needs (e.g. food security) and life-support-system (e.g. climate change) goals (Parris and Kates, 2003), showing possibly negative impacts on humans rather than describing raw material use. Sectors are grouped according to the logic of the respective transition to be analysed and transition indicators have only sought to show progress towards goals other than raw material substitution.

Material flow indicators emphasize the need to dematerialize production and substitute raw materials, with the indicators raw material consumption (Schoer et al., 2012) and raw material input (Kovanda and Weinzettel, 2017) making visible the amount of raw materials required as inputs for economic sectors. Imported intermediate and final products are assigned so-called raw material equivalents in order to estimate how much raw material from other regions was used in production chains. By tracing the share of fossil resource use in the total raw material use of a sector, a transition may be monitored. Yet it is not possible to easily link reduced fossil resource use to developments in fossil- and bio-based sectors. It would be misleading, for example, to claim that reduction in fossil energy use in the chemical sector is automatically related to substitution of bio-based chemicals for fossil-based ones, as it could also be induced by improved energy efficiency or declining sales. A newly proposed indicator, called SUB-RAW, seeks to establish such a link by showing changes in energy consumption and CO_2 emissions due to raw materials substitution (Bontempi, 2017). Although it is not suited to be an economy-wide transition indicator, as it is focused on the product level and only on the first part of a product's life cycle, it does provide a good impetus towards understanding how to link changes in fossil resource consumption to substitution of bio-based for fossil-based products.

Bioeconomy indicators have the advantage of charting developments in the production of bio-based products. Several authors have sought to quantify bioeconomies by selecting bio-based sectors and determining their share in value added or employment, such as the wood (Budzinski et al., 2017), forestry (Karvonen et al., 2017), and bioenergy, biomaterials, and biochemicals sectors (Vandermeulen et al., 2011). Shares for whole economies have also been determined (Ronzon et al., 2017). Bio-based sectors are distinguished by their reliance on biogenic resources as inputs to production processes (Efken et al., 2016). This implies that bioeconomy transition advances when the relative share of bio-based sectors increases but it is not usually possible to observe developments in fossil resource consumption with these indicators. Relative growth in paper production, for example, does not necessarily entail a reduction in fossil resource use and may actually lead to an increase if production processes are run primarily on fossil energy. Bioeconomy indicators need to be refined to include only bio-based products that explicitly substitute fossil-based products and exclude conventional bio-based products, such as food and paper. A first step in this direction could be indicators that show greenhouse gas emissions or fossil energy *avoided* due to the use of renewable energies or bio-based products (Memmler et al., 2017; Rogers et al., 2016). This would make clear the beginning (the production of bio-based substitute goods) and end (cessation of production of fossil-based alternatives) of a transition. Disadvantages of the indicators proposed by Memmler et al. (2017) and Rogers et al. (2016) include developments specific to bioenergy not being observed because all renewable energies are included and selection criteria for choosing specific bio-based products not being clearly explained. If a precise description of sectors relevant to an economy-wide indicator is missing, it may not represent national developments very well, especially if new bio-based sectors emerge.

This brief review of the current literature on relevant indicator groups demonstrates that none of the existing indicators can adequately represent the transition from a fossil-based to a bio-based economy, although they can provide good stimuli for a new indicator. Current transition indicators emphasize the importance of a baseline and a defined target (requirement A, listed above), but they are not linked to the goal of raw materials substitution. Existing material flow indicators suggest how fossil resource consumption may be monitored, supporting the setting up of a baseline (requirements A and B), but they do not establish connections for substituting goods from biogenic resources. Bioeconomy indicators chart developments in the use of bio-based products, hinting at the completion of a transition (requirements A and C), but leave fossil resource consumption unobserved. Transition, material flow, and bioeconomy indicators often assume a macro perspective, which is required if developments in an entire economy are to be monitored (requirement D), but they do not separate sectors that produce bio-based substitute products from other (bioeconomy) sectors. Either the whole economy is represented, without indicating fossil-based and bio-based substitute products, or selected substitute products are grouped into sectors. Only representing a small part of the economy leaves a chance that not all sectors relevant for substitution are included.

The Substitution Share Indicator (SSI) is developed in this paper. The SSI seeks to quantify economy-wide reductions in fossil resources, activated by bio-based production. Combining some advantages of existing transition, material flow, and bioeconomy indicators, the SSI makes explicit when a transition starts and is completed, links developments in fossil resource consumption to bio-based production, and seeks to represent all transition-relevant sectors of an economy at an appropriate level of aggregation.

The SSI is intended to become part of a comprehensive scheme for bioeconomy monitoring, as it seeks to reflect progress made regarding one of its pivotal objectives. Being able to compare bioeconomy developments to a baseline or reference point, such as current fossil resource use, would likely improve multi-criteria assessment and policy advice regarding possible trade-offs with other sustainable development goals. This indicator might be able to support, for example, assessment of land use or employment effects resulting from bioeconomy transition in a particular country. It may also enable research on the interplay between bioeconomy and circular economy (CE) transitions, the latter of which refers to increasing resource use efficiency through recycling of urban and industrial waste (Ghisellini et al., 2016). By applying the SSI to two sectors in Germany for the year 2011, the present work also reveals data gaps in official statistics that are currently impeding research and policy formulation based on bioeconomy transition analysis. The transport fuels and plastics sectors have been chosen as they reflect material and energy use strategies that have become the focus of much research.

This article is structured as follows: Section 2.1 starts by explaining the conceptual framework which has guided development of our indicator. In 2.2 and 2.3 the proposed substitution indicator (SSI) is described as well as two methods for calculating indicator values, from bottom-up and top-down perspectives. Section 2.4 presents the materials used for our empirical case studies of the German transport fuels and plastics sectors. Results of applying the SSI with the two methods to these sectors are presented and the suitability of the indicator for long-term bioeconomy monitoring is discussed in section 3. Limitations and recommendations are found in section 4.

2. Methods and materials

2.1. Conceptual framework

A coherent monitoring scheme that includes many indicators for various dimensions of a particular object of interest should generally be built upon a comprehensive conceptual framework (OECD, 2008). Such frameworks are expected to contribute to a common understanding of concepts, boundaries, and relations between their own elements among indicator developers and users. The Bioeconomy Transition Framework (BTF; Fig. 1) has been designed to derive and conceptualize transition indicators that can provide feedback for policy makers on transition progress, drivers, and impacts. It is based on a bioeconomy framework that seeks to describe interactions between the bioeconomy and the environment (van Leeuwen et al., 2015; O'Brien et al., 2017). Compared to other frameworks addressing social-ecological systems (SES), Driving forces-Pressure-State-Impact-Response (DPSIR) frameworks (Eurostat, 1999) are said to be particularly well suited for deriving “action-oriented strategies for reducing the impact of humans on the ecological system” (Binder et al., 2013), which is one of the aims of bioeconomy monitoring. Such policy frameworks focus on the influence of human activities on the environment (rather than vice versa) as well as on influences on the micro level from processes at the macro level, seen from an anthropocentric rather than an ecocentric perspective (Binder et al., 2013). The BTF includes the five original elements of van Leeuwen et al. (2015): drivers, constraints, the bioeconomy, societal challenges, and strategies and policies. The central element, that is the conceptualization of bioeconomy is adapted, which is a possible “driver” of increased or reduced dependence on non-renewable resources (“pressure”).

The concepts in Table 1 are key to understanding the BTF and our new indicator: the Substitution Share Indicator (SSI). These concepts belong to different systems, either the natural environment or the economy, and can be distinguished according to their availability. “Resources” means materials and substances that exist in the natural environment, with or without human interference (EC, 2005). “Products”, in contrast, have been extracted and processed in order to create economic value. This distinction between the economy and the natural environment is also maintained in official accounts (Fischer-Kowalski et al., 2011). Fossil resources are non-renewable within a time frame relevant for human beings, whereas biogenic resources may be renewable if extraction is lower than natural growth (Perman 2009). The term “ossil resources” includes crude oil, natural gas, lignite, and coal.“Fossil-based products” are produced from these resources after they have been extracted from the environment, from primary processing into coke or refined petroleum products to further processing into transport fuels and plastics. These products can be replaced in theory, but substitution possibilities are only technically mature at present in some cases. If they can be replaced, they are called “fossil-based substitute products”. “Bio-based products” that are able to replace fossil-based substitute goods, because they have similar properties to them, are called “bio-based substitute goods”. Most consumer goods are both fossil- and bio-based, and we consider a product bio-based if there is a biogenic share, no matter how high it is. “Biogenic resources” are unharvested and unprocessed living organisms in the environment, also sometimes called biotic resources, bioresources, resources from biological origin or biomass.

The Bioeconomy Transition Framework (BTF) focuses on bio-based substitute goods that are likely to reduce dependence on fossil resources (see red lines in Fig. 1). Due to its focus on bio-based substitute goods, the framework does not include food and feed, because these do not substitute products made from fossil resources. Food and feed production may constrain bioeconomy transition, if priority is given to it instead of bio-based substitute goods. Another peculiarity of the framework is that it only includes those biomaterials that can substitute fossil resources. To illustrate the specific focus of the BTF, “food/feed” and “bio-based non-

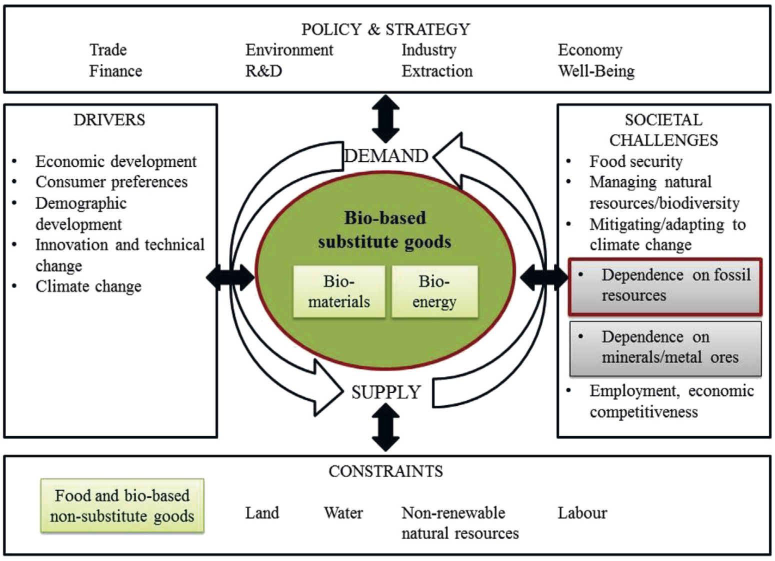

Fig. 1. Bioeconomy Transition Framework for analysing transition from a fossil-based to a bio-based economy (adapted from van Leeuwen et al., 2015).

Table 1
Key concepts for the Substitution Share Indicator (SSI).

System affiliation	Availability	
	Non-renewable	Renewable
Natural environment	Fossil resources (e.g. crude oil)	Biogenic resources (e.g. rapeseed plant)
Economy	Fossil-based products (e.g. diesel)	Bio-based products (e.g. biodiesel)

substitute goods” have been included in the “constraints” block, and different non-renewable resources (fossil fuels, minerals, metal ores) have been distinguished in the “societal challenges” block in Fig. 1.

The conceptual BTF (Fig. 1) can be used as a basis for answering questions concerning what to measure and how to measure bioeconomy transition processes. It not only can guide the design of new indicators, as in the present research, but also the development of a coherent bioeconomy transition monitoring scheme. A new indicator, two alternatives for its calculation, and data sources used for the case studies analysed here are presented in the following subsections.

2.2. Substitution Share Indicator (SSI)

The Substitution Share Indicator (SSI) is designed to be part of a bioeconomy transition monitoring scheme and as an aid for research on transition drivers, barriers, and impacts. As already mentioned in the introduction, such an indicator should be able to represent the transition of an entire economy, with all relevant sectors included (requirement D). The SSI in Equation (1) does this by adding up sectoral indicators (SSI_i), which are weighted (w_i):

$$SSI = \sum_{i=1}^{n} SSI_i * w_i \tag{1}$$

The SSI_i is the ratio of Fossil Resource Savings (FRS_i) due to substitution of bio-based products for fossil-based products within fossil resource consumption that would be required if no substitution took place, which is Fossil Resource Consumption (FRC_i) added to FRS_i (Equation (2), red line in Fig. 2).

$$SSI_i = \frac{FRS_i}{FRC_i + FRS_i} \tag{2}$$

A weight, $w_{i,}$is the ratio of the fossil resource consumption of a sector without substitution within the fossil resource consumption of all sectors without substitution, as described in Equation (3):

$$w_i = \frac{FRC_i + FRS_i}{\sum_{i=1}^{n} FRC_i + FRS_i} \tag{3}$$

The SSI is suited for country comparisons and can be simplified so that it is not necessary to calculate sectoral Fossil Resource Consumption (FRC_i) but only economy-wide consumption of fossil resources, which is available from most national statistics and is known as Raw Material Input of fossil energy carriers (RMI_f). A country-wide SSI is stated in a simple form in Equation (4).

$$SSI = \sum_{i=1}^{n} \left(\frac{FRS_i}{FRC_i + FRS_i} * \frac{FRC_i + FRS_i}{\sum_{i=1}^{n} FRC_i + FRS_i} \right) = \frac{\sum_{i=1}^{n} FRS_i}{\sum_{i=1}^{n} FRC_i + FRS_i} = \frac{\sum_{i=1}^{n} FRS_i}{RMI_f} \tag{4}$$

However, as it should be possible to compare sectors, the SSI_i and its components are presented in depth. A sector, i, is defined as the sum of fossil-based products (with and without substitution

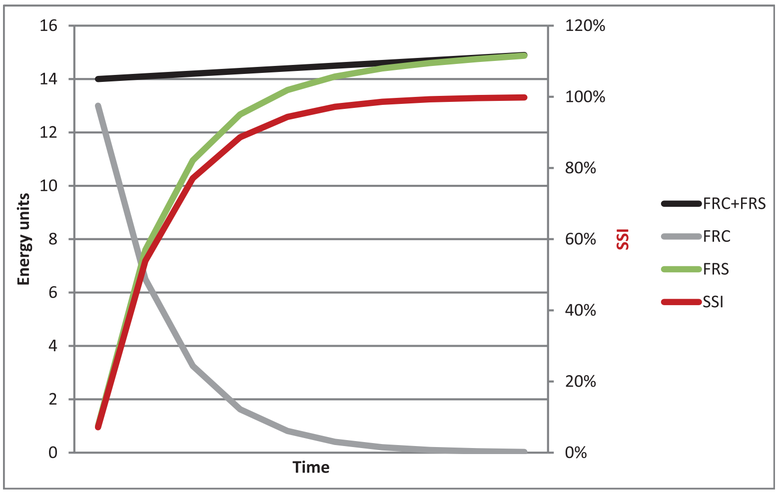

Fig. 2. Hypothetical example of the Substitution Share Indicator (SSI_i, red) for a sector, which is the ratio of Fossil Resource Savings (FRS_i, green) within fossil resource consumption without substitution ($FRC_i + FRS_i$, black). FRC_i (grey) is Fossil Resource Consumption with substitution. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

possibilities) and bio-based substitute products. Other products that are not based on fossil or biogenic resources, such as metal products, and bio-based products that do not substitute, such as food, wooden furniture or paper products, are presently beyond the scope of the monitoring system. The FRS_i represents the amount of fossil resources saved, in energy units, due to the production of bio-based substitute products (Equation (5), green line in Fig. 2). It is the quantity of bio-based substitute products (X_{bi}, a functional unit, i.e. mass or value), multiplied by a factor for cumulative (i.e. life cycle) per unit fossil resource consumption, which is called the Fossil Resource Equivalent of fossil-based products (FRE_{fi}, in energy units per functional unit; see Equation (5)). The FRE_{fi} is reduced by the Fossil Resource Equivalent of bio-based substitute products (FRE_{bi}, in energy units per functional unit), in order to account for fossil process energy use in the production of bio-based products and/or for fossil-based shares in bio-based products. A Substitution Factor (SF_i, dimensionless) − equal to 1 if substitute goods have the same functional unit − may be necessary to correct for different substitution ratios of substitute pairs. For example, the energy contents of a ton of natural gas and a ton of biomethane are the same, whereas a ton of biodiesel and a ton of diesel have different energy contents. The FRE_f needs to be corrected for such differences.

$$FRS_i = X_{bi} * \left(FRE_{fi} * SF_i - FRE_{bi}\right) \tag{5}$$

The denominator in Equation (2), $FRC_i + FRS_i$, is a reference scenario showing sectoral fossil resource use without substitution (black line in Fig. 2). The FRC_i is actual Fossil Resource Consumption of all products in a sector, no matter whether they are fossil- or bio-based (grey line in Fig. 2). It is a variable conceptually close to Raw Material Consumption (RMC) or material footprint, as used in material flow accounting (Lutter et al., 2016). The quantity of fossil-based products (X_{fi}, a functional unit, i.e. mass or value) and bio-based products (X_{bi}) are multiplied by their respective Fossil Resource Equivalents (FRE_{fi}, FRE_{bi}; see Equation (6)). Fossil Resource Equivalents are called Raw Material Equivalents (RME) in other, more general contexts (Lutter et al., 2016) and signify that a change in per-unit fossil resource use in upstream activities can influence the SSI_i. Posen et al. (2017), for example, find that fossil resource consumption of plastic products can be reduced more by using renewable energies as process energy than by substituting bio-based plastics.

$$FRC_i = X_{fi} * FRE_{fi} + X_{bi} * FRE_{bi} \tag{6}$$

The behaviour of SSI_i, FRS_i, and FRC_i depends on

1. production of bio-based substitute goods (X_b),
2. production of fossil-based goods (X_f),
3. direct and indirect use of fossil resources in the production of fossil-based goods (FRE_f),
4. indirect use of fossil resources in the production of bio-based substitute goods (FRE_b), and
5. substitution ratio (SF).

The SSI_i will increase if FRS_i is increasing and FRC_i is constant, which implies that there are no changes in production (X_{bi}, X_{fi}) or fossil resource equivalents (FRE_{bi}, FRE_{fi}). Change can be caused by improving the functional properties of bio-based products compared to those of fossil-based products, meaning here changing the Substitution Factor (SF). The SSI_i will also increase if FRC_i is declining and FRS_i is constant, implying that bio-based production (X_{bi}), fossil resource equivalents (FRE_{bi}, FRE_{fi}), and the Substitution Factor (SF) have not changed. It follows that reduced fossil-based production leads to an increase in SSI_i. It is most likely that production output will change in the short term, and SSI_i will only grow if bio-based production increases more than fossil-based production. The indicator can even rise if absolute fossil resource consumption increases, but only if a larger share of additional production is bio-based than fossil-based.

SSI_i is equal to zero before a transition begins, implying that FRS_i is zero (see Equation (2)). This means that there is no production of bio-based substitute goods ($X_{bi} = 0$) or that bio-based substitute goods require the same amount of fossil resources as fossil-based products ($FRE_{fi} = FRE_{bi}$), according to Equation (5). Once bio-based production starts and bio-based products consume less fossil resources than fossil-based products, the transition can begin gaining momentum. Production of a bio-based substitute good always leads to a reduction in the production of its fossil-based alternative. FRE_{fi} is larger than zero and larger than or equal to FRE_{bi}. The FRE_{fi} is larger than zero by definition; otherwise it would not refer to a fossil-based product. An FRE_{fi} that is smaller than FRE_{bi} results in a negative FRS_i and a negative SSI_i. As a share can only be between zero and one, bio-based products with a higher FRE_b than fossil-based products should be excluded from the indicator.

Transition is complete when SSI_i reaches a value of one. This is the case when the numerator in Equation (2), FRS_i, is equal to the denominator, FRC_i+FRS_i (see Fig. 2). This situation occurs if either X_{fi} or FRE_{fi} and either X_{bi} or FRE_{bi} are equal to zero. As FRE_{fi} cannot be equal to zero by definition, and there is no transition if X_{bi} is equal to zero, X_{fi} and FRE_{bi} need to be equal to zero for a transition to be complete. This is a state with no further production of fossil-based goods, and bio-based products will not require any fossil resources as inputs to production processes.

The SSI measures consistency, efficiency, and sufficiency effects (Allievi et al., 2015). An increase in X_{bi} signals a development consistent with substitution, decreasing FRE_{fi} and FRE_{bi} values show improved efficiency, and declining X_{bi} and X_{fi} indicate a sufficient level of production has been reached.

Two approaches for quantifying Fossil Resource Equivalents (*FRE*) are common in the field of industrial ecology (Suh and Huppes, 2009): 1) a bottom-up or coefficient approach, based on Material Flow Analysis and Life Cycle Assessment, and 2) a top-down or input–output approach, based on Environmentally Extended Input–Output Analysis (EEIOA) (Lutter et al., 2016). Bottom-up and top-down approaches have also been recently discussed for modelling interactions between bioeconomy and environment (O'Brien et al., 2017).

2.3. Methods for calculating fossil resource equivalents (FRE)

2.3.1. Bottom-up indicator

The bottom-up approach for the present analysis uses information from process analysis and scales it up to sector level (Lutter et al., 2016). *FRE* are based on a partial life cycle assessment (cradle to factory gate), including fossil resource consumption by upstream processes. Cumulative Energy Demand (CED; VDI, 1997) is used as an impact-assessment method for providing information on the life cycle fossil resource use of products. An attributional rather than a consequential model is used here for the SSI_i, to exclude feedback effects of by-products and avoid the uncertainty associated with consequential life cycle assessments (Martin et al., 2015).

With the bottom-up approach, FRS_i is the sum of the product-specific *FRS* of bio-based substitute products *b* (Equation (7)), with X_{bi}, FRE_{fi}, and FRE_{bi} referring to mass units; *SF* expresses how much of a bio-based product is necessary in order to provide the same benefit as the fossil-based alternative.

$$FRS_i = \sum_{b,f=1}^{n} X_{bi} * \left(FRE_{fi} * SF_i - FRE_{bi} \right) \tag{7}$$

FRC_i includes all bio-based (*b*) and fossil-based (*f*) substitute products (Equation (8)). As the bottom-up indicator begins from the product level, the FRC of other, non-substitutable fossil-based products (FRC_o) can be differentiated from the FRC of fossil-based substitute goods (FRC_f):

$$\begin{aligned} FRC_i &= \sum_{b=1}^{n} FRC_b + \sum_{f=1}^{n} FRC_f + \sum_{o=1}^{n} FRC_o \\ &= \sum_{b=1}^{n} X_{bi} * FRE_{bi} + \sum_{f=1}^{n} X_{fi} * FRE_{fi} + \sum_{o=1}^{n} X_{oi} * FRE_{oi} \end{aligned} \tag{8}$$

2.3.2. Top-down indicator

The top-down approach uses national input–output tables that show transactions between economic sectors in monetary terms and extend them by integrating information on the direct environmental effects of sectors (Lutter et al., 2016). From this perspective, *FRE* are termed total Fossil Resource Intensities (tFRI), which is a concept similar to *FRE*, as it includes direct and indirect fossil resource use. Yet it also differs from *FRE*, because it refers to a group of products (a sector) rather than individual products and links resource use to output values rather than mass. A link to values is necessary because physical input-output tables are generally not available in government statistics. Fig. 3, below, illustrates how *tFRI* are derived. At the top of Fig. 3 are a schematic input–output table (left) and a vector of direct Fossil Resource Consumption (*dFRC*, right). This data is typically provided by government statistical offices. Direct Fossil Resource Intensities (*dFRI*) are calculated by dividing *dFRC* values by output values (at the bottom of the input–output table) to obtain FRC per value unit produced in a sector. The input–output table is also used to calculate an input coefficient matrix, the A matrix, which shows in each column the share of required inputs from all sectors (in rows) in relation to the output value of a sector. By subtracting the A matrix from an identity matrix (I matrix) and inverting it, a Leontief inverse matrix (L matrix) can be calculated. Leontief inverse coefficients show how much more input by row sectors is needed to produce one more unit of column sectors. The aim of this method – *tFRI* (at the bottom of Fig. 4) – is achieved when the L matrix is multiplied by the *dFRI* vector (Kitzes, 2013).

Based on the top-down approach, FRS_i is the value of bio-based substitute products (X_{bi}, in €) multiplied by net Total Fossil Resource Intensity (*tFRI*, in energy units per value unit), meaning the difference of the $tFRI_{fi}$ of a fossil-based sector and the $tFRI_{bi}$ of a bio-based sector (Equation (9)). SF_i is not product-specific but corrects for different average prices of bio-based and fossil-based products in one sector. Prices have to be related to relevant functional units, for example MJ or cm^3 instead of kg, because different substitution ratios need to be considered. Higher bio-based prices than average fossil-based prices mean that FRS_i is actually lower than without SF_i, whereas lower prices mean that FRS_i is higher. If there is only one product in a sector, SF_i for the top-down approach is the same as SF_i for the bottom-up approach.

$$FRS_i = X_{bi} * \left(tFRI_{fi} * SF_i - tFRI_{bi} \right) \tag{9}$$

With the top-down approach, FRC_i is calculated by adding the values of two product groups, represented by different industries: bio-based substitute products (*b*) and fossil-based products (*f*). As shown in Equation (10), FRC_i can be obtained by multiplying output values (X_{bi}, X_{fi}, in value unit €) by the respective sectoral $tFRI_{bi}$, $tFRI_{fi}$ (in MJ/€):

$$FRC_i = X_{bi} * tFRI_{bi} + X_{fi} * tFRI_{fi} \tag{10}$$

2.4. Material used in the case studies

2.4.1. Process data for the bottom-up indicator

To calculate the SSI_i using the bottom-up approach, data on Fossil Resource Equivalents at the product level (*FRE* in MJ/t), production output (X_{fi} and X_{bi}, in t), and Substitution Factors for each substitution pair (*SF*, dimensionless) are required.

The *FRE* used in this analysis are based on Life Cycle Impact Assessment (LCIA) data, mainly from the ecoinvent database (2018) (Appendices 1 and 2). If values for representative European

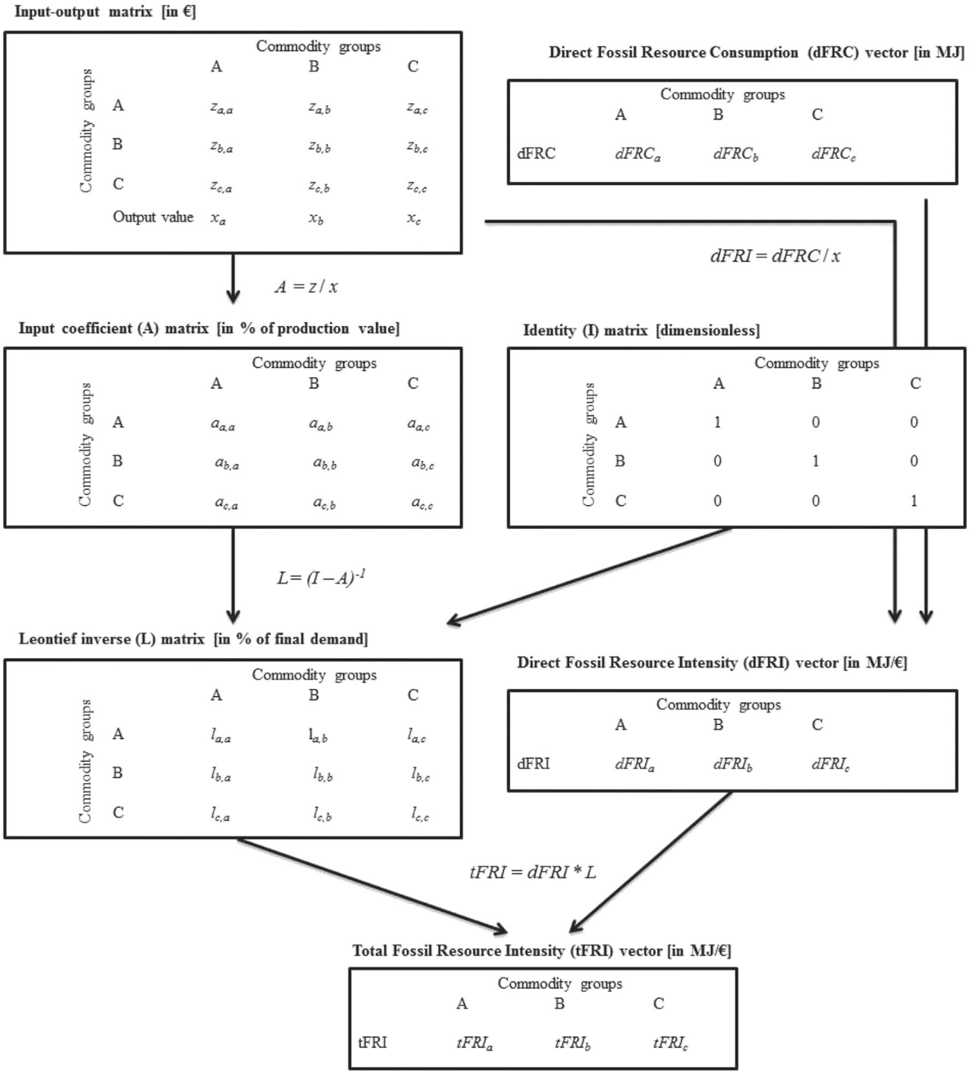

Fig. 3. Procedure for calculating Total Fossil Resource Intensities (*tFRI*).

production processes (RER) were available, they were included in the analysis; otherwise rest-of-world (ROW) or global (GLO) values were used. We follow ecoinvent's attributional model (Allocation at the Point of Substitution: APOS) and use the Cumulative Energy Demand (CED) method, which includes direct and indirect energy use of hard coal, lignite, crude oil, natural gas, coal mining off-gas, and peat, taking the upper heating value of fossil resources as a characterization parameter (Hischier et al., 2010). As many bioplastics processes are not yet represented in ecoinvent, additional LCA literature was also consulted.

Systematically collected and regularly updated quarterly and annual data on production outputs is available from production statistics for the period 2002–2016 (Destatis, 2017d). There was a change in product classification in 2009 but the 2002–2008 data can be and has been converted. Fossil-based plastics are grouped in the Classification of Products by Activity (CPA 2009) under "plastics in primary forms" (code 20.16), which also include resins, polymers for glues, silicones, cellulose derivatives, natural polymers, and ion exchangers. Through detailed product classification it was possible to exclude the latter group of fossil-based plastics from our case study. Neither specific product codes nor surveys regarding bioplastics production exist. Only one survey on bioplastics *capacities* in Germany exists, undertaken in 2011 but not yet repeated (Meo Carbon Solutions, 2014). Available production statistics for transport fuels include fossil- and bio-based. Although each fossil-based product has its own nine-digit product code, biodiesel and bioethanol are summarized under one product code. Biofuels output data by fuel type is available in a different survey (Destatis, 2017a). Biodiesel and bioethanol are not further disaggregated by feedstock in official statistics, but data from industry-specific associations can be used in addition.

Substitution Factors refer to densities for plastics and heating

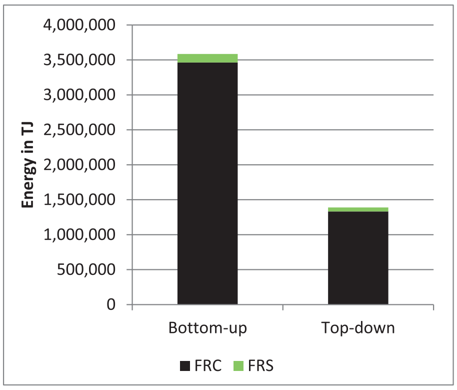

Fig. 4. Fossil Resource Consumption (FRC_i) and Fossil Resource Savings (FRS_i), calculated for the transport-fuels sector in Germany in 2011, using bottom-up and top-down approaches.

values for transport fuels. Bioplastics are often compared to petroleum-based plastics in terms of their densities (Endres and Siebert-Raths, 2011), with low densities of primary plastics meaning that less material is required for further processing into plastics goods. For example, in order to produce one clamshell container, 24.6 g of polystyrene (PS) are used compared to 29.6 g of polylactic acid (PLA) (Madival et al., 2009), with PS having a density of 1050 kg/m^3 and PLA of 1250 kg/m^3 (Endres and Siebert-Raths, 2011). Substitution Factors for biofuels are derived from the lower heating values (in MJ/kg) of fossil fuels and biofuels (FNR, 2017), with lower heating values meaning that more production output is required in order to provide the same benefit.

2.4.2. Input–output data for the top-down indicator

Calculating the SSI_i using the top-down approach requires data on output values (X_{fi} and X_{bi}, in €), Direct Fossil Resource Consumption ($dFRC_i$, in MJ), an economic input–output table, and information for Substitution Factors (SF_i, dimensionless). Output values from production statistics can be used for fossil-based products and biofuels (Destatis, 2017d), but for bioplastics data we had to rely on the only available study for Germany (Meo Carbon Solutions, 2014).

Annual, monetary input–output tables as well as data on the fossil resource consumption of individual production sectors are provided by official German statistics (Destatis, 2017c, 2017e). An input–output table from 2011, including domestic production and imports, was used. As the L matrix is only available without imports, inverse coefficients were calculated from the A matrix, which does include imports. The statistics for direct resource consumption by sectors and energy carriers was adapted to include only fossil energy carriers (coal, lignite, crude oil, natural gas). As energy consumption data is available for fewer sectors than the total compiled input–output data, energy consumption data was disaggregated, assuming linearity between a sector's economic output and energy consumption. This was necessary for most service sectors, which are for the most part less energy-intensive than manufacturing industries. Previous studies indicate that disaggregation is preferable to aggregation here (Lenzen, 2011).

The input–output table from 2011 had data for 72 sectors. We calculated *tFRI* for all of these sectors and then used only those factors that are directly related to our case study sectors. Diesel, gasoline, and liquefied petroleum gas have been classified in the “coke and refined petroleum products” sector (CPA C 19), natural gas in the “crude petroleum and natural gas” sector (CPA B 06), and biofuels in the “chemicals and chemical products” sub-sector (CPA C 20). Plastics and bioplastics were also classified as being in CPA C 20. Hence, two *tFRI* were generated for fossil-based transport fuels, whereas the same *tFRI* is available for biofuels, bioplastics, and plastics.

The Substitution Factor (SF_i) requires information on per-unit output values in addition to information on densities and heating values, which are also required for the bottom-up indicator. Average production values for the German transport fuels analysis were derived from production statistics as well as production values of fossil-based plastics. The survey by Meo Carbon Solutions (2014) provided information on the market values of German bioplastics. Densities and heating values were averaged with product shares in output quantities.

Based on the methods and material described in this section, the sectoral Substitution Share Indicator (SSI_i) was applied to two sectors of the German economy: transport fuels and plastics. In the pursuit of our main goal of suggesting a good transition indicator, these case studies have made visible shortcomings in terms of information and data availability and quality.

3. Results and discussion

3.1. Transition in the transport fuels sector

The transport fuels sector in this analysis includes liquid and gaseous energy carriers used in the internal combustion engines of moving vehicles. Diesel and gasoline have the highest shares in fuel consumption in Germany, at 64% and 30%, respectively (FNR, 2017). Liquefied petroleum gas and compressed natural gas play a minor role, at 1% each. Viable alternatives are biodiesel, hydrated vegetable oil, bioethanol, and biomethane, which together had a share of almost 5% in 2016 (FNR, 2017). Biodiesel production was based on rapeseed oil (70%), used cooking oil (22%), palm oil (4%), and soybean oil (2%; FNR, 2016), and bioethanol production was based on wheat/rye/maize (71%) and sugar beets (29%; BDBe, 2014).

The Substitution Share Indicator for the transport fuels sector (SSI_i) was low, at 3.4% according to the top-down approach and 3.1% according to the bottom-up approach (Fig. 4). The bioeconomy transition in the transport fuels sector had not led to substantial savings in fossil resources in Germany by 2011, and Fig. 4 shows that Fossil Resource Consumption (FRC_i) was much higher than Fossil Resource Savings (FRS_i) at that time. Values calculated with the top-down approach are substantially lower for FRC_i (62%) and somewhat lower for FRS_i (58%; Fig. 4), which explains the higher SSI_i value found when using the top-down approach.

The calculated FRS_i of 112,447 TJ (bottom-up) and 46,996 TJ (top-down) seems to reflect the contribution of biodiesel and bioethanol to the transport-fuel sector transition. It is higher for those biofuels that have low fossil energy input requirements, that is a lower FRE_{bi} according to the bottom-up approach. Biodiesel from used cooking and palm oils and bioethanol from sugar beets have relatively low requirements (Appendix 1). Biodiesel in Germany is mainly produced from rapeseed and bioethanol from rye, both having relatively high FRE_{bi} values. FRS_i is also influenced by the Substitution Factor (*SF*). For example, it is higher for biodiesel, with an *SF* of 0.86, compared to bioethanol, with an *SF* of 0.61 – a result of the higher heating value of biodiesel.

According to calculations made using the top-down approach, the production of biofuels saved 62.69 MJ/€. It is the difference between the fossil resource intensity of 80.84 MJ/€ of sector C19 (fossil fuels) and the intensity of 18.15 MJ/€ of sector C20 (biofuels). The difference between the direct (*dFRI*) and the total Fossil Resource Intensity (*tFRI)* reveals indirect fossil resource use for

Table 2
Direct and total Fossil Resource Intensities (*dFRI* and *tFRI*) of relevant energy-transition sectors in Germany in 2011.

Sector	CPA	dFRI (in MJ/€)	tFRI (in MJ/€)
Chemicals and chemical products	C 20	2.03	18.15
Coke and refined petroleum products	C 19	60.99	80.84
Crude petroleum and natural gas	B 06	3.13	6.39

Source: Own calculation based on (Destatis, 2017b, 2017c).

every Euro of output value. This is largest in CPA C20, representing biofuels, where *dFRI* was less than 10% of *tFRI* (Table 2). There is much uncertainty concerning the *tFRI* of CPA C20 because currently biofuels represent only a relatively small share of this sector, beside many other bio- and non-bio-based products, such as fertilisers, plastics, paints, and detergents. Fossil fuels represent a large share of their respective sector.

FRC_i of 3.46 M TJ (bottom-up) and 1.33 M TJ (top-down) was mainly due to production of fossil fuels with high FRE_{fi} values (i.e. diesel and gasoline). Transport fuels with lower FRE_{fi} values (e.g. natural gas and biofuels) had low shares in production (Table 3). The FRC_i value of natural gas differs substantially, depending on the calculation method used, with the value arrived at according to the top-down approach being much lower than from the bottom-up approach: 0.5% and 11.2%, respectively.

3.2. Transition in the plastics sector

The plastics sector in this analysis includes plastics in primary forms. Plastics are materials based on macromolecules, known as polymers, that can be processed into all kinds of goods (Türk, 2014). The most important petroleum-based plastics produced in Germany in 2013 were polypropylene (PP), polyvinyl chloride (PVC), low-density and linear low-density polyethylene (PELD/LLD), high-density and medium-density polyethylene (PEHD/MD), (expandable) polystyrene (PS/PSE), and polyamide (PA) (Consultic, 2016). Biopolymers are alternatives to such fossil-based polymers. “New” biopolymers are characterised as biodegradable/petroleum-based, biodegradable/bio-based, and non-biodegradable/bio-based (Albrecht et al., 2016). Bio-based polymers (biodegradable and non-biodegradable) are the focus of this study because they have been specifically designed to replace petroleum-based plastics while fulfilling the same principal functions (Endres and Siebert-Raths, 2011). In 2011, bioplastic production capacity was 78,700 t, of which 52% was for starch blends, 25% for polylactic acid (PLA) blends, 14% for bio-polyamide (PA), 7% for cellulose acetate, and 1% for bio-polyurethane (PUR) (Meo Carbon Solutions, 2014), and the main feedstocks used were castor oil (29%), corn starch (24%), wheat starch (19%), potato starch (18%), and wood (10%) (Meo Carbon Solutions, 2014).

The calculated Substitution Share Indicator (SSI_i) in the plastics sector are 0.6% for the top-down approach and 0.09% for the bottom-up (Fig. 5), indicating that the German plastics-sector transition was hardly recognizable in 2011.

The main reason for the low FRS_i calculated here appears to be the low level of bio-based plastics production in 2011. For example, polylactic acid (PLA) blends production capacity was only 20,000 t, which is low compared to production of 740,000 t of polystyrene (PS) in the same year. As it is assumed that PLA is blended with 55% fossil-based polybutylene adipate terephthalate (PBAT) or polybutylene succinate, pure bioplastics production must have been even lower, and only about 9000 t of PLA (i.e. 45%) was actually used to substitute for fossil resources. FRS_i appears to have been low because bioplastics production requires large amounts of fossil resources (Appendix 2). For example, PLA production requires more than 50% of the fossil resources that are normally used for the production of high-density polyethylene (PEHD). FRE_{fi} is even further reduced by the Substitution Factor (*SF*), which is based on material densities. Except for bio PA and bio PUR, for which densities are equal to densities of fossil-based PA and PUR, bioplastic densities are generally higher than fossil-based, requiring more material to fulfil the same functions.

When using the top-down approach, the SSI_i value is much higher than with the bottom-up approach, because the FRC_i of the former is much lower (76%) whereas its FRS_i is 65% higher. A significant factor influencing FRC_i value is the *tFRI* of sector C 20 (chemicals), which was 18.15 MJ/€ in 2011. This value has been used in the present analysis for all plastics, because they are classified as being in the same sector. FRS_i does not include differences between the *tFRI* of bio-based and fossil-based products, because the available data only provides one value. This shortcoming means that either the same *tFRI* must be assumed, which would result in an FRS_i of zero and 0% substitution, or no *tFRI* can be assumed for the bio-based sector. Although the latter assumption is not realistic – bioplastics also require fossil energy, as can be seen via the bottom-up approach – and likely overstates results, data constraints did not leave another option.

3.3. Discussion

3.3.1. Transition beginning and end

Transition in a sector starts when X_{bi} and *SF* are greater than zero and FRE_{bi} is smaller than FRE_{fi} (see 2.2). Choice of bio-based products included in transition analysis is important, as only some bio-based products are able to substitute fossil-based ones. In a transition monitoring scheme, a clear reference point in time needs to be determined, depending on the goals of monitoring. Existing indicators include bio-based products that we do not consider substitute products, such as food and wood products, or they include a selection of bio-based substitutes but without explaining selection criteria. “Innovative” bio-based substitute products are characterised by their technical ability to substitute the essential functions of fossil-based goods. They began to be invented, developed, and commercially produced after awareness of the finite nature of fossil resources and the environmental problems linked to fossil resource use grew among many societal actors. The *Limits to Growth* report from 1972 (Meadows et al., 1972) marks such a change in thinking as well as the UN Framework Convention on Climate Change in 1992. The German-based cases included in this study are within both baselines suggested here: 1972 and 1992. A

Table 3
Comparison of *FRC* values by product group and approach. *FRC* values are smaller for the top-down approach than for the bottom-up approach, which can be read from the last column, giving the share of the top-down value in the bottom-up value. Shares of fuel groups also differed and are given in brackets behind *FRC* values.

Product group	Bottom-up	Top-down	Share of top-down value in bottom-up value
FRC of diesel, gasoline, and petroleum gas (TJ)	3.026.228 (87.4%)	1.298.371 (97.4%)	42%
FRC of natural gas (TJ)	387.549 (11.2%)	6.743 (0.5%)	2%
FRC of biofuels (TJ)	50.422 (1.4%)	27.450 (2.1%)	54%
Total *FRC*	3.464.199 (100%)	1.332.566 (100%)	39%

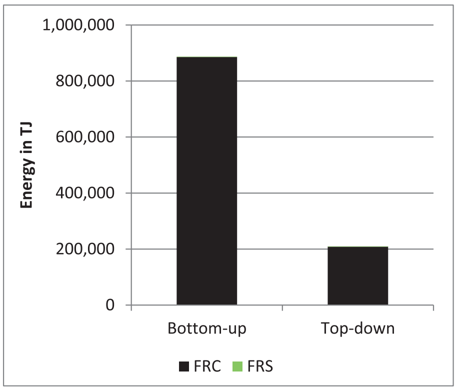

Fig. 5. Fossil Resource Consumption (FRC_i) and Fossil Resource Savings (FRS_i), calculated for the German plastics sector in 2011, using bottom-up and top-down approaches.

challenge for including more recent products is that systematic and regular data collection regarding them has been rare thus far. Although biofuels production has been statistically recorded since 2009, values for bioplastics production rely on a one-time market study set from 2011 (Meo Carbon Solutions, 2014). Due to such data-availability issues, the focus of the SSI as presented here is on the production of goods rather than their consumption. It is assumed that producer decisions are based on real as well as expected demand for bio-based products and that producers are important agents in determining environmental damage or improvement (Lifset, 2009). Adjustments could be made in the future to represent substitution in consumption by adding imports to production outputs of fossil- and bio-based products and by subtracting exports as well as stored goods, so bio-based imports that replace domestic fossil-based production can be included as well as bio-based imports that replace imported fossil-based products.

Conventional bio-based products, such as the biopolymers linoleum and rubber, or products based on other renewable and non-renewable resources, such as electric mobility, have been excluded here, although they might also replace fossil-based products. These other means of substitution may be reflected by a decreasing output of fossil-based products (i.e. X_{fi}), resulting in an increasing substitution share if FRS_i is constant. If fossil resources are used in the process of producing products based on other renewable and non-renewable resources, this will not be reflected by the indicator, as such processes lie outside of the selected system boundary. Rebound effects tend to result from increased fossil-based supply, caused by a combination of lower prices and higher demand, triggered by an increased supply of bio-based products that have similar properties as their fossil-based counterparts (Smeets et al., 2014). All other things being equal, a rebound effect is indicated if both X_{bi} and X_{fi} increase.

Transition is complete when there is no more fossil-based production ($X_{fi} = 0$) in the whole economy and bio-based products do not rely on fossil resources anywhere in the supply chain ($FRE_{bi} = 0$; see 2.2). If a closed economy with no trade is assumed, FRE_{bi} will be zero if no fossil-based products are available. As economies are generally involved in trade, FRE_{bi} will be positive so long as there is fossil resource use globally, and SSI will not reach a value of one.

3.3.2. Methods for upstream fossil resource consumption

A very important feature of the SSI is the connection between bio-based production and fossil-based alternatives through multiplication of X_{bi} by FRE_{fi}, which seeks to ensure that developments in fossil resource use are directly attributed to substitution. The accuracy of the indicator strongly depends on FRE parameters, but uncertainty can arise from the methods applied. Case study results presented here indicate that FRE parameters may differ substantially. Similar to Feng et al. (2011), who analyse water footprints on a sectoral level and ended up calculating a water footprint for China that is 25% higher when using a bottom-up rather than a top-down approach, the present study finds that each method has its shortcomings. A more detailed methodological comparison can be found in Lutter et al. (2016).

With the bottom-up approach, it is possible to include product-level information on substitute pairs and individual FRE values. For some sectors, such as transport fuels, substitute pairs are clear, due to their technical properties, whereas for other sectors, such as plastics, a multitude of matches are possible. Based on bioplastics properties and market observations, it is assumed that starch and PLA blends can replace PEHD and cellulose derivatives can replace PS. PLA blends could also substitute low-density polyethylene (PELD), polypropylene (PP) or polyamide (PA), and starch blends could substitute either PELD, PP or polystyrene (PS; Wolf et al., 2005). Cellulose acetate (CA) could substitute PA and PP rather than PS, which was assumed as the fossil-based substitute good. Substitution of starch and PLA blends for PA would significantly increase FRS_i, as the FRE_{bi} of PA is 55,000 MJ/t higher than that of PEHD. Substitute pairs can be matched with more certainty if substitution of final products is considered instead of intermediate products, such as biopolymers.

A methodological shortcoming of the bottom-up approach is truncation error, meaning here that FRE values might be underestimated if relevant processes lie outside of the chosen system boundaries. Reports from the literature estimate that a process-based method may, for example, capture only one third of energy demand for US laptop computers (Deng et al., 2011), only two thirds of greenhouse gas emissions in Australia (Yu and Wiedmann, 2018), and only half of greenhouse gas emissions in the Australian construction industry (Teh et al., 2018) compared to a method using input–output data.

The top-down approach has the advantage of considering all inputs, without having to draw a cut-off threshold, and also requires less effort for collecting data, as it primarily relies on official statistics. High aggregation of products into sectors means that matching of substitute pairs is not necessary, but this assumed homogeneity of sector outputs in combination with low sector resolution can be problematic. Each sector produces a single good that has representative input shares and direct fossil raw material demand. The SSI requires that there be a difference in $tFRI$ between fossil-based and bio-based products, but such a difference cannot be included if all substitute products are classified within the same sector, as in the plastics case study, or if bio-based substitute products are classified in the same sector as fossil-based chemicals, as in the transport fuels case study. The top-down approach “can at best be used as a first proxy”, according to Suh and Huppes (2009, p. 279), as it might misrepresent FRE values of relevant sectors such that it would be difficult to say whether values are over- or underestimated.

3.3.3. Outlook for further research

One advantage of the SSI is its inclusion of all economic sectors, seeking to make visible spillover effects between them. How these sectors are defined could be specified further, meaning the system boundary of the index, i, in SSI_i. Especially the plastics case study illustrates that choosing appropriate substitute pairs is not an easy and unambiguous task. Better knowledge of what bio-based products are, or can be, substituted for fossil-based ones is also necessary. As substitution is triggered at the final-demand level, end products might constitute a more feasible alternative system boundary than intermediate products, which were subject of this study. A consumption-based indicator may prove to be more adequate, but its applicability with the bottom-up and top-down approaches needs further investigation.

The SSI is not at present able to show spillover effects between countries, as it may rise in one economy due to substitution, but fossil-based production may shift to another so that global fossil resource use remains constant. Development of accompanying indicators for changing trade and resource use patterns is strongly recommended. Spillover effects on environmental impacts other than fossil resource use might be demonstrated through combination with environmental indicators. The main focus of the SSI as presented here is to show the transition from a fossil-based to a bio-based economy. Case study results do not appear well suited for comprehensively analysing progress towards, for example, climate change mitigation targets. Further analysis revealing the implications of substitution for greenhouse gas emissions will hopefully show how much bioeconomies can contribute towards climate change mitigation. By analysing absolute Fossil Resource Consumption (FRC) values in addition to relative SSI values, it may be possible to obtain a first indication of implications for climate change.

The proposed BTF is a potential basis for connecting the SSI to sustainability indicators so that multi-criteria assessment of the transition can be facilitated. It could be developed further by taking into account circular economy (CE) frameworks (Iacovidou et al., 2017; Parchomenko et al., 2019) to assess the implications of a bioeconomy transition for the circular economy of a country.

Due to possible truncation errors, the bottom-up indicator is less suited for systemic, economy-wide analysis but rather for comparisons of a few, small sectors, as in Rogers et al. (2016). Improvements in life-cycle data are necessary for using the bottom-up approach. Only a few processes have thus far been analysed, among them PLA (Vink and Davies, 2015), PHA, and starch-based polymers (Yates and Barlow, 2013), and results are often only available for a global average, or the region is not specified. A promising solution is the development of Life Cycle Inventories for bioplastics, including extension of the GaBi LCA tool to bioplastics (Thinkstep, 2018) and continuing current research on updating LCIA data for fossil-based plastics. Applicability of the SSI with the bottom-up approach depends on the availability of data in the country under study, which could result in high data-collection costs.

The top-down indicator could become more reliable if sectors were separated into fossil-based, bio-based, and other products, as was done recently for chemicals (Escobar et al., 2018). Direct fossil resource demand of fossil-based and bio-based sectors can then be more accurately represented. Hybrid approaches could integrate process-based information into input—output tables by disaggregating sectors, thereby trying to reduce the effect of the homogeneity assumption. One challenge is to develop a cost-effective hybrid method. A data collection procedure will be required that can include data on new bio-based substitute products and information on their fossil-based counterparts. Exploring data collection and aggregation strategies in collaboration with, for example, statistical offices, developers of certification schemes, and business representatives could be useful. Using multi-regional input—output (MRIO) tables in addition to disaggregation procedures could adequately address the domestic technology assumption, which holds that imported goods have the same input shares and fossil resource requirements as domestically produced goods. With such improvements, a multi-regional hybrid model could significantly enhance the accuracy of the SSI.

4. Conclusions

Fossil resource use generates many negative externalities, especially for the environment. Using biogenic instead of fossil resources may mitigate some of these externalities but may also end up causing others. Careful consideration of policy options is necessary in order to avoid “jumping out of the frying pan into the fire”. Bioeconomy transition indicators can support such decision making by making substitution of renewable for fossil resources and its implications for sustainable development more visible. Having advanced the Bioeconomy Transition Framework (BTF) and developed the Substitution Share Indicator (SSI), it is hoped that these concepts can become a basis for further discussion around developing bioeconomy monitoring schemes with appropriate and practical measurement instruments.

The case studies analysed here regarding the transport fuels and plastics sectors in Germany demonstrate to our satisfaction that the SSI is applicable. It shows that the transition in the selected sectors is still incipient and is slightly more advanced in transport fuels than in plastics. These results are in line with recent findings on avoided fossil energy consumption in the US, where biofuels and bioplastics currently avoid about 2.4% of fossil fuels (Rogers et al., 2016).

Such currently low levels can only be strongly increased if transition is pushed through appropriate policies. The main reason for a higher SSI in German transport fuels than in plastics is likely to be renewable energy obligations set by the German government. Similar incentives for substitution may advance the transition in other sectors as well and could build on lessons learned from previous biofuel policy. A major insight derived from the work presented here is that substitution should be linked to sustainability requirements such as life-cycle greenhouse gas emissions savings and non-food resource uses. The case studies underline these findings as follows: 1) merely substituting a bio-based product for a fossil-based one is not sufficient and 2) choice of substitute pairs is important for accelerating transition. Pairs with a higher difference in per-unit fossil resource use will contribute more productively to bioeconomy transitions. The European Commission's updated bioeconomy strategy (EC, 2018b) announces greater investment into research and innovation regarding bio-based plastics products.

Efficiency and sufficiency strategies should be considered as additional strategies for promoting bioeconomy transitions, apart from merely focusing on the production of bio-based substitute goods. Higher fossil resource use efficiency and a decrease in overall consumption of both bio- and fossil-based products will lower overall fossil resource use. The European plastics strategy (EC, 2018a) already emphasizes achieving greater efficiency in plastic production through recycling.

In the near future, it will be important to carefully design further policy instruments that can advance a sustainable transition from a fossil-based to a bio-based economy in more and more sectors. Relevant questions concerning the SSI have to be addressed before it can be applied on a regular basis and serve as an adequate tool for policy analysis and appropriate decision making.

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Declarations of interest: none.

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Appendix A. Supplementary data

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Chapter 4. Analyzing the sustainability of plastics substitution with an input-output model

The contribution of Chapter 4 to this thesis' objectives is emphasized by changing the title to "Analyzing the sustainability of plastics substitution with an input-output model" from the original title in Jander (2022).

The published research paper has been added to this thesis in the next pages.

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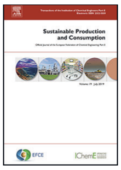

Advancing bioeconomy monitorings: A case for considering bioplastics

Wiebke Jander[1]

Department of Technology Assessment and Substance Cycles, Leibniz Institute for Agricultural Engineering and Bioeconomy e.V. (ATB), Potsdam, Germany

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ABSTRACT

Substituting fossil-based with bio-based products is a promising approach for addressing environmental problems, but assessing potential trade-offs is challenging. Bioplastics, for example, are considered both a potential solution as well as a new source of harmful environmental impacts, mainly arising from their use of agricultural biomass. Yet, bioeconomy monitoring systems do not currently capture such net effects of substitution at the sub-sectoral level. This paper explores how such monitoring could be enhanced to support sustainable transition by analysing plastics substitution and related economic and environmental effects using an extended input-output model that includes environmental data and disaggregates the plastics and bioplastics sectors. The ongoing transition in the German plastics sector – measured by combining information from expert interviews with secondary sources – is characterized by low domestic demand, high dependence on imported inputs, and relatively low fossil-resource savings. Results for selected indicators reveal few trade-offs regarding fossil resource use, water use, value added, and employer compensation. Process greenhouse gas emissions are significantly higher when substituting bioplastics for plastics, if credits for bio-based carbon are neglected. This study proposes that sustainable transition in the German plastics sector would benefit from more specific monitoring and clearly justified policy targets, based upon reconsideration of stated objectives in bioeconomy strategies. Methodological recommendations include accounting for carbon cycles in greenhouse gas emissions modelling, using further indicators related to possibly harmful impacts on the environment, and distinguishing between domestic and foreign effects by applying the proposed input-output model to the most relevant countries in bioplastics value chains.

1. Introduction

Bioplastics are considered a classic example of how bioeconomy can contribute toward sustainable development, as they can be as durable, lightweight, protective, and versatile as conventional plastics while being produced from renewable, biogenic resources rather than crude oil and, thus, can reduce dependence on fossil resources, CO_2 emissions, and plastic pollution (Hottle et al., 2013; Spierling et al., 2018; Oliveira et al., 2021). Bio-based and compostable bags, for example, have similar properties to conventional plastic bags but can promote separation of organic from residual waste while not introducing microplastics into compost (Kern et al., 2020; UBA, 2020b). Incinerating residual waste is much more energy-intensive if moist organic waste is included. Substitution of conventional plastics through bioplastics is seen as one of several strategies for coping with worldwide plastics pollution, in addition to overall reduction of plastics production, substitution with paper, and mechanical and chemical recycling (Lau et al., 2020). On the downside, there are concerns about unsustainable production of biogenic resources in the production of bioplastics. Compared to fossil-based plastics, bioplastics can for example increase eutrophication and acidification potentials due to the current input of agricultural biomass, cultivated with fertilizers, in their production (Detzel et al., 2012; Broeren et al., 2017; Venkatachalam et al., 2020). Turning again to the example of bio-based bags, most of them are currently made from starch-based materials (Meo Carbon Solutions, 2014; European Bioplastics, 2016) such as wheat and maize, which have some of the highest fertilizer-application rates compared to many other crops. A considerable risk of higher greenhouse gas (GHG) emissions from land use change prompted by bioplastics production has also been recently computed (Escobar et al., 2018; Escobar and Britz, 2021).

Capturing and understanding such trade-offs via bioeconomy monitoring systems can contribute toward decision-making that is more consistent with sustainable development principles. As part of the 'reflexive strategies' (Köhler et al., 2019) used for transition management, monitoring and evaluation can perform important functions, such as delivering feedback, guiding action, improv-

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E-mail address: wjander@atb-potsdam.de

[1] Max-Eyth-Allee 100, Potsdam 14469, Germany.

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Nomenclature

A	technology coefficients matrix
B	technology coefficients matrix
D	market shares matrix
$dFRC_s$	direct fossil resource consumption of sector s (in MJ/€)
$dFRI_s$	direct fossil resource intensity of sector s (in MJ/€)
I	unity matrix
L	Leontief coefficients matrix
SSI_s	substitution share indicator of sector s (dimensionless)
q_{sb}	total output of bio-based commodities by domestic sector s (in €)
q_{sf}	total output of fossil-based commodities by domestic sector s (in €)
$tFRI_{sb}$	total fossil resource intensity of the bio-based part of s (in MJ/€)
$tFRI_{sf}$	total fossil resource intensity of the fossil-based part of s (in MJ/€)

ing accountability, defining actor roles, creating mutual learning, and improving communication between industry, government, and the population (Georgeson and Maslin, 2018; Alaerts et al., 2019; Behnsen et al., 2020; Schoenefeld, 2021). The growing literature on monitoring circular economies emphasizes the importance of comprehensive monitoring that can provide feedback on all relevant sustainability dimensions and governance levels (Alaerts et al., 2019; Llorente-González and Vence, 2019; Harris et al., 2021; Papageorgiou et al., 2021).

Bioeconomy monitoring systems are under development by the Joint Research center for the EU (Robert et al., 2020), individual European countries (Diakosavvas and Frezal, 2019), the FAO (Bracco et al., 2019), and the US (Golden et al., 2015; Frisvold et al., 2021). Currently they are being built on aggregate information from economic sectors and on selected indicators. Although many indicators have been suggested (Robert et al., 2020; Kardung et al., 2021), few have been quantified (Asada et al., 2020; Ronzon et al., 2020; Bringezu et al., 2021) and net effects of substitution have rarely been addressed (with the exception of Asada et al., 2020). Sectoral resolution of bioeconomy monitoring is rather low at the moment and not always suited to the level of analysis needed for political decision-making. Databases for current bioeconomy monitorings are input-output tables with 65–200 sectors that each include a large variety of products. Asada et al. (2020) roughly estimate impacts of reducing vehicle weight by substituting wood for steel by assuming that inputs from the metals sector to the vehicle manufacturing sector are replaced with inputs from the wood sector. In current bioeconomy monitoring, the chemical and other selected sectors are often split, based on their bio-based shares (Ronzon et al., 2017; Bringezu et al., 2021). Different “input-based” methods for calculating shares of mixed industries have been proposed (for an overview, see Kuosmanen et al., 2020) which have in common that they do not account for downstream bio-based products but only for those that use inputs from typical agri-food industries. For example, 13% of the German chemicals industry’s resources are biogenic, and these approaches acknowledge this bio-based component (FNR, 2021). However, the industry’s bio-based output, such as bio-based surfactants and lubricants, is not accounted for in calculating bio-based shares of downstream sectors, such as the pharmaceutical, textiles, and construction industries. Meanwhile, “output-based” methods rely on the bio-based content of outputs but “ignore the use of bio-based inputs in the production process” (Kuosmanen et al., 2020) that do not show up in final products, such as the use of bio-based surfactants in industrial cleaning. They are also relatively imprecise when bio-based content is difficult to identify, such as with some biopolymers in plastic packaging. Thus, information on bio-based inputs is not passed on in supply chains, making it difficult to estimate bio-based shares within final goods production or even consumption. Another problem is that non-competitive imports do not count towards the input-based share, as it is normally assumed that such imports have the same input structure as those from domestic production (Eisenmenger et al., 2016). If significant amounts of biopolymers are imported, for example, they are assumed to have the same input structure as all other relevant domestic chemical inputs, thereby underestimating their actual bio-based composition. In sum, a significant challenge of bioeconomy monitoring today is that “industries with conceptually similar products but different production processes, input requirements, and emission intensities are often combined in a single sector” (Vendries Algarin et al., 2015). Consequently, current bioeconomy monitoring systems hardly measure developments at the meso-level, which is particularly relevant for tailoring action to societal needs (Alaerts et al., 2019).

Starting from these oversimplifying assumptions, this present paper seeks to contribute toward improving the precision and relevance of bioeconomy monitoring by elaborating indicators at the sub-sectoral level, taking the German plastics industry as an example. The analysis presented here is guided by the overall question “What enhancements of bioeconomy monitoring systems are necessary to support sustainable transition in the plastics sector?” and by the following sub-questions:

1) What factors need to be considered when monitoring substitution in the German plastics sector and its economic and environmental effects?
2) What are the methodological and data requirements for integrating the bioplastics industry into existing bioeconomy monitoring systems?

The present analysis builds on previous research that developed the Substitution Share Indicator (SSI) for assessing transition from fossil-based to bio-based economies from a theoretical point of view and that calls for methodological improvements (Jander and Grundmann, 2019). The SSI can help to more precisely chart sustainable transition via an extended understanding of the term ‘substitution’. Other studies and most bioeconomy strategies refer to resource, that is input, substitution or assume that output substitution is automatically linked to input substitution. With the SSI, output substitution is linked to input substitution. Thus, substitution refers to a replacement of outputs, that is substitution of intermediate or final bio-based goods for fossil-based ones, and its implications for the use of inputs, that is fossil resources.

Here, plastics substitution will be defined rather narrowly to include only substitute goods that are produced within the same industry, namely bioplastics, as substitution by paper or wood products is beyond the scope of this paper. Plastics are considered to be “materials that contain as an essential ingredient a high polymer and which at some stage in their processing into finished products can be shaped by flow” (Kabasci, 2014, p. 2). In the Commodity Classification for Foreign Trade Statistics, plastics are described as materials that acquire their final shape through compounding of polymers, additives, and solvents, using heat and pressure without reference to a specific resource, which is why in the present analysis bioplastics are assumed to be classified under this category. Note that the focus here is on plastics that are ready for conversion into a plastic product rather than polymers which have not been compounded. Plastics are broadly classified into thermoplastics, thermosets, and elastomers. Elastomers, or more colloquially rubbers, are infusible, have traditionally been bio-based, still have a relatively high bio-based share, and are therefore called “old economy” bioplastics (Albrecht et al., 2016). However, substitution of elastomers is neither as dynamic nor relevant in terms of overall volume compared to thermoplastics and, hence, is excluded from this analysis. By contrast, thermoplastics can be reshaped any number of times and have a high production share (Kabasci, 2014), and fossil-based thermoplastics can be replaced with bio-based plastics, which are sourced at least partly from biomass and either have the same (“drop-in”) or a different chemical structure. Bio-based share may be verified with the Carbon-14 method, which gauges bio-based carbon content, or through disclosure of bio-based mass content, which contains further chemical elements. Bio-based polymers can be synthesized using living organisms (“natural polymers”) or through chemical processes (Kabasci, 2014) and can be biodegradable or not (Albrecht et al., 2016). In the absence of an official definition of bio-based plastics in German legal documents – the current biowaste regulation only requires plastic waste to be “predominantly” from renewable resources (BMU, 2013), refers to few concrete products, and leaves room for interpretation – the present analysis includes all thermoplastics that use bio-based polymers rather than fossil-based ones, regardless of their synthetic pathway, chemical structure, or biodegradability. This rather broad definition of bioplastics enables a more nuanced discussion of their place in sustainable transition strategies.

2. Methods and materials

2.1. Hybrid input-output modelling

A bioplastics model was designed to compare several upstream supply chain effects of bioplastics to those of fossil-based plastics. Its basic structure is explained in this section and details are provided in Jander (2021). The bioplastics model was built to derive values for a sectoral Substitution Share Indicator (SSI_s), which can be used to estimate how far a sector has made a transition from a fossil-based to a bio-based economy (Jander and Grundmann, 2019). The indicator relies on quantification of total fossil resource intensities ($tFRI_{sb}$ and $tFRI_{sf}$) and output (q_{sb} and q_{sf}) of the bio- and fossil-based sectors:

$$SSI_s = \frac{q_{sb}\left(tFRI_{sf} - tFRI_{sb}\right)}{tFRI_{sf}\left(q_{sf} + q_{sb}\right)} \tag{1}$$

Total fossil resource intensity ($tFRI$) expresses how much fossil energy is used along upstream supply chains and involves matrix multiplication of all sectors’ direct fossil resource intensities ($dFRI$) by Leontief coefficients (L), which express how much more input from all sectors is required for producing one more unit of one sector:

$$tFRI = dFRI * L \tag{2}$$

The $dFRI_s$ is direct fossil resource consumption ($dFRC_s$) divided by sectoral production values (q_s, total output of a commodity by a domestic industry, not including imports):

$$dFRI_s = dFRC_s / q_s \tag{3}$$

Net intensity is total intensity of fossil-based products ($tFRI_{sf}$) reduced by total intensity of bio-based products ($tFRI_{sb}$). In the same way, sustainability indicators can be calculated with low additional effort using the bioplastics model, if sectoral data on direct intensities is available.

In this case study, s refers to plastics in primary forms. According to the Statistical Classification of Economic Activities in the European Community (NACE Rev. 2, 2008), manufacturing sectors were given the code C. Plastics in primary forms belong to the sector “manufacture of chemicals and chemical products” (C20) and have the code C20.16. For this study, the plastics sector was further divided into a fossil-based plastics sector (C20.16f) and a bioplastics sector (C20.16b). Thus, $SSI_{20.16}$ refers to substitution in the plastics sector and $tFRI_{20.16b}$ and $q_{20.16b}$ to intensity and output of the bioplastics sector, respectively. The model year is 2016, for which the most complete data sets are presently available.

The $tFRI_{sb}$ and $tFRI_{s,f}$ are modelled through an extended hybrid input-output (IO) model (Eq. (2)) the main components of which are explained step-by-step in the following paragraphs (Fig. 1). The basic model in step 1 is used for all sustainability indicators. The extensions in step 2 refer to specific intensities, and Fig. 1 shows an example for the indicator fossil resource use. Step 3 further develops the extended IO model to represent the fossil-based and bioplastics sectors.

The bioplastics model starts from supply and use tables (SUT) for calculating technology matrix A. Compared to symmetric input-output tables (IOT), SUT allow for greater flexibility regarding the way multiproduct processes are represented by multiplying matrix B, based on a use table, and matrix D, based on a supply table, to obtain matrix A (Eurostat, 2008; Miller and Blair, 2009, 184ff.; Wiedmann et al., 2011; Vendries Algarin et al., 2015). Matrix A is in a product-by-product rather than industry-by-industry form, because substitution of products is the focus of the present analysis, and data for derived environmental indicators refer to production sectors rather than industries (Rueda-Cantuche, 2011). The model is based on an industry-technology assumption, which better represents by-production than a product-technology assumption, because input coefficients are not affected by changes in output mix (Eurostat, 2008, pp. 311–313). In future bioeconomy analysis, by-products and residues will become increasingly important in order to avoid pressure on (land) resources.

Calculation of intensities follows the established method of extending the basic IO model via economic and environmental information to obtain relevant multipliers (Miller and Blair, 2009, pp. 446–452). With reference to bioeconomic objectives as stated in bioeconomy strategies (EC, 2018b; BMEL, 2020) and to achieve a reliable data base, *value added, employer compensation, greenhouse gas (GHG) emissions* and *water use* were selected as multipliers to investigate possible trade-offs with fossil-resource substitution.

Extended IO models have been applied many times since the late 1960s (Miller and Blair, 2009), and recently the body of literature on input-output-based analysis of bioeconomies has been growing rapidly (Brizga et al., 2019; Loizou et al., 2019; Asada et al., 2020; Bringezu et al., 2021).

A challenge arises, however, when integrating more specific industry information into existing bioeconomy monitoring systems. Hybrid input-output models have been suggested as a solution (Castellani et al., 2019) and successfully applied for specific bioeconomy sectors and technologies, such as the wood industry (Budzinski et al., 2017), biotechnology industry (Wydra, 2011), biofuels (Acquaye et al., 2012; Watanabe et al., 2016), and (ligno)cellulosic products (Malik et al., 2016; Lamers et al., 2021). ‘Hybrid’ in the present paper refers to the integration of process and input-output data rather than to mixed unit input-output tables (Kjaer et al., 2015). Out of several hybrid methods, all which have distinct aims (Crawford et al., 2018), ‘matrix augmentation’ was chosen for the present analysis. Assuming that the sector of interest is already included within the aggregate sector, here chemicals and chemical products, the latter can then be disaggregated into several sectors, such as plastics, bioplastics, and other chemicals (Joshi, 1999). Matrix augmentation is intended as a way to relax the assumption of sectoral homogeneity inherent in IO analysis and can be less time-consuming compared to alternative methods. For example, unknown inputs to a bio-based industry can be kept proportional to the original data of the sector, and only inputs where process data is available are then changed, and sales struc-

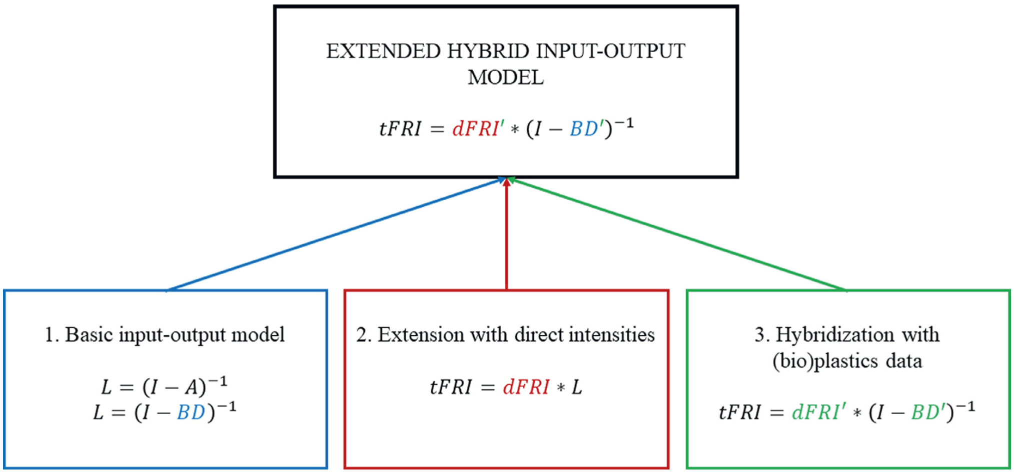

Fig. 1. Approach to building a bioplastics model in three steps, using the example indicator of total fossil resource intensity.

tures can be maintained if more detailed information is missing. General steps in matrix augmentation involve matching of process data with IO classifications, conversion of physical values to monetary values using price information, and estimation of total input values by multiplying per unit inputs by production capacities (Malik et al., 2016).

The matrix augmentation method has been adapted here to the case of plastics substitution in two ways. First, a procedure was developed to integrate information on non-competitive biopolymer imports. Standard IO models are built upon a domestic technology assumption (DTA) that imports are produced with the same technology, that is input shares, as domestic products. The error resulting from this assumption is small for industries with competitive imports from countries with similar technologies and energy sources but can be significant for non-competitive imports (Peters and Hertwich, 2004). Approaches have been developed to relax the DTA, mainly by including the IOTs of exporting countries (Tukker et al., 2018). Here, assumptions regarding bioplastics input structures are changed rather than adding fossil-based plastics and bioplastics industries to other countries' SUTs, in order to not unduly complicate the *SSIs*. Second, similarly to Vendries Algarin et al. (2015), information on inputs to the bioplastics sector from sectors that were not covered by process data were used proportionately to a fossil-based plastics sector. As the latter is also not represented in the original SUT either, differences between the chemical sector included in SUTs and the plastics sector are modelled with results from the German *Material- und Wareneingangserhebung* (MWE; Record of Industrial Materials and Goods Received) from 2014 (Destatis, 2017), a survey of input costs that are used in manufacturing. This was possible for 20 out of 85 sectors. All other inputs are distributed proportionally to the chemical sector. Having a separate fossil-based plastics sector in the IO model improves the level of detail and, ultimately, the accuracy of the *SSIs* as total intensity for fossil-based plastics can be included instead of aggregate intensity for the chemical sector.

2.2. Data sources

Fig. 2 illustrates what and how data and information sources were used in each of the three steps of the model, which will be explained in more detail below.

For the basic model (Fig. 2, in blue), SUTs for 2016 were used from the German Federal Statistical Office, which are available consistently on an annual basis back to 2008 (Destatis, 2020d). In a digression, the basic model was disaggregated to better represent potentially important upstream agri-food sectors. More detailed data on plant and animal production, belonging to the agricultural sector, and on vegetable oil, sugar, and starch production, classified in the broader food sector, were available in multi-regional IO databases. A SUT for Germany (2011) from EXIOBASE Version 3.7 has been used here (Stadler et al., 2018, 2019), as other available data does not seem to sufficiently link agri-food sectors to all other sectors (Schmidt and Osterburg, 2009), provides physical SUTs (Bruckner et al., 2019), or was not yet available (Mainar-Causapé et al., 2021). Countries' agricultural sectors have been disaggregated using FAOSTAT data, trade data, and coefficients from the AgroSAM model (Wood et al., 2015). Data on products in EXIOBASE was aggregated to the desired sectors for the IO model. For example, meat and dairy products were combined to the production sector "other food products" (C10*) and meat, dairy, fish, tobacco, and beverage industries were subsumed under the economic sector "manufacturing of other food products" (C10*-12). The starch industry is not as well represented in EXIOBASE as the oil and sugar industries because it is combined with many other products, including fruit and vegetable products, milled grain products, bakery and farinaceous products, cocoa, tea, coffee, and animal feed. Detailed supply and technical coefficients from the EXIOBASE data were multiplied with aggregate data from the 2016 SUT.

Data for model extensions (Fig. 2, in red) has also mostly been based on German Federal Statistical Office publications. Economic data for calculating value added and employment is included in use tables (Destatis, 2020d). Environmental data for calculating fossil resource use (coal, lignite, crude oil, natural gas), water use (from natural sources and from water utilities), and GHG emissions (CO_2, CH_4, N_2O) by sector are included under Environmental Accounting (Destatis, 2020b, 2020c). As data was only available for fewer sectors than are included in the bioplastics IO model, the extant data was split, based on the output value of each aggregate sector, except for fossil resource consumption of coke products/petroleum products and electricity/gases and GHG emissions of plastics, for which more specific data was obtainable (AGEB, 2018; Eurostat, 2021).

Matrix augmentation for representing (bio)plastics in the model (Fig. 2, in green) relied on specific biopolymer process data and information from market studies, technical literature, and expert in-

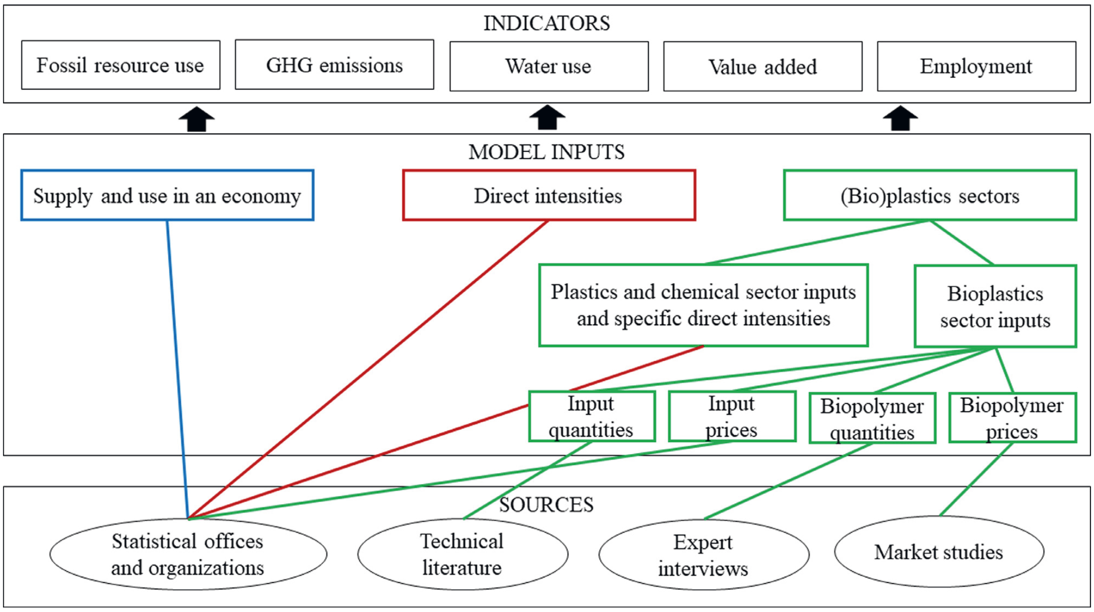

Fig. 2. Relationship between data sources, model components, and indicators.

terviews as well as to some extent on official statistical data. Specific data and information on biopolymers was collected from different sources, because there are currently no statistical codes that specifically allow for structured data collection over time except for polylactide acid and cellulose acetate. Polylactide acid is listed in EU trade statistics under code WA39077000, but production data is not collected for it. Cellulose acetate is included in code 201659400 of the CPA (Statistical Classification of Products by Activity, Version 2.1), but other cellulose ethers and esters are also subsumed under this code. This empirical gap has been filled by the nova-Institute, based on expert interviews, and by the Institute for Bioplastics and Biocomposites (IfBB), based on news research. Both of these German-based institutes regularly publish bioplastics market data by type and region; however, country-level data was not available on request. Thus, I conducted semi-structured interviews with 13 German bioplastics producers and distributors in 2020 (see Supporting Information) in order to estimate biopolymers production quantities, imports, and the kind of biomass used. Due to confidentiality concerns, prices were not discussed in the interviews and were, instead, estimated through market studies, most notably van den Oever et al. (2017). Input quantities from other sectors into biopolymer production were sourced from the life-cycle assessment database ecoinvent (Ecoinvent, 2018), the IfBB (2019) and the literature (Steinmeier, 2004; Hummel, 2004; Righi et al., 2017). Related input prices for food products, refined petroleum products, chemicals, and energy were estimated from unit values found in production and trade statistics. All inputs not detailed in specific biopolymer sources, inputs to fossil-based plastics, and direct intensities of bioplastics and fossil-based plastics were estimated, either based on the aggregate chemicals sector's input shares and intensities or on data informing German IOTs (Destatis, 2017), as described in 2.1.

The different sources used for the model were largely compatible, though some work was required to translate EXIOBASE data, which uses an older classification system from 2002, to the 2008 classification used in the bioplastics model. Input data from ecoinvent was provided with information about statistical codes from the Central Product Classification (CPC) and a correspondence table was used to translate these codes to the International Standard Industrial Classification of All Economic Activities (ISIC). Data from the MWE (Destatis, 2017) helped to more precisely specify differences in input shares between the aggregate chemical sector (C20) and the plastics sector (C20.16), because it provides more detailed data on costs of intermediate products that are inputs to these sectors. These inputs are also structured by NACE Rev. 2 classification and, hence, were unambiguously assignable to input sectors in the bioplastics model.

3. Results

3.1. Current bioplastics production in Germany and related material flows

Estimating based on the expert interviews (see Supporting Information), bioplastics production was about 170,000 tons and €503 million in Germany in 2016, which was 1.0% (weight-based) and 2.3% (value-based) of the output of the primary plastics industry. Because this refers to the amount of ready-to-process material, including fossil-based polymers and imported biopolymers, comparison with other estimates is only possible for domestic polymer production, excluding the amount of imported biopolymers. This newly calculated share of 0.6% is above the average share for European countries, which was 0.02–0.03% of primary plastics production in the EU, corresponding to 309,000 tons (IfBB, 2019) and 527,500 tons (European Bioplastics, 2020). German biopolymer production is, however, lower than the global average of 1.0% (European Bioplastics, 2020).

Bioplastics production includes the most important polymers, domestically produced and imported as well as bio and fossil-based, that are necessary to produce bioplastics materials to be processed into bioplastics products. The use of thermoplastic starch (TPS), starch, polyhydroxyalkanoates (PHA), polylactide acid (PLA), bio-polyethylene (Bio-PE), bio-polyamide (Bio-PA), and cellulose acetate (CA) led to an overall bio-based mass share of 60% (Fig. 3).

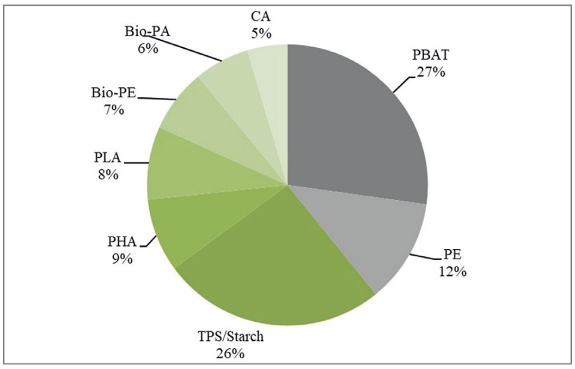

Fig. 3. Polymer inputs used by the German bioplastics industry in 2016; shares based on production value (green = biopolymers, grey = fossil-based polymers). Quantities based on own data collection (expert interviews, SI 1) and prices based on van den Oever et al. (2017).

Fossil-based blending components (polybutylene adipate terephthalate, PBAT, and polyethylene, PE) are currently necessary for yielding similar functions in bioplastics as those of conventional plastics.

German and international bioplastics markets were highly interdependent, with two-thirds of biopolymers for German bioplastics production being imported in 2016 (see Fig. 4). Of the 177,000 tons of biomass required, 14% was sourced from Germany or neighbouring countries, mainly starch and cellulose, while the bulk of the starch, cellulose, sugar, and vegetable oil used was sourced from other regions. Polyamide production, even though located in Germany, relied exclusively on imported castor oil. The export share was also high, at about 58%, whereby 76% of exports were biodegradable materials and 24% non-biodegradable. As illustrated in the diagram, non-biodegradable material for the production of packaging exhibited greater demand on the domestic market than biodegradable material.

3.2. The economic and environmental effects of substitution

Using results from the expert interviews conducted to create the bioplastics IO model, the $SSI_{20.16}$ measuring the rate at which the bioeconomy transition in German primary plastics production occurred in 2016, was found to be 0.37%. Bioplastics had a total fossil resource intensity (*tFRI*) of 12.39 MJ/€ and fossil-based plastics 14.83 MJ/€, resulting in a net fossil resource saving of 2.44 MJ/€. In comparison to earlier results using a non-hybrid input-output model, which estimated values for the $SSI_{20.16}$ of 0.6% (Jander and Grundmann 2019), it can be concluded that the older study overestimated the $SSI_{20.16}$ and that the indicator can be calculated more accurately by integrating input-output- and process-based approaches. In the non-hybrid model, the upstream fossil resource intensity of bioplastics could not be estimated, whereas the hybrid model shows that these have a considerable effect. Both bio- and fossil-based plastics have a somewhat lower *tFRI* than the chemicals sector as a whole (15.59 MJ/€). Additional information on agri-food industries in the extended hybrid input-output model changes the $\mathrm{SSI}_{20.16}$ to 0.25%, indicating slight overestimation by the basic model and implying that input-output tables with higher resolution may yield more accurate results.

The implications of German plastics substitution in 2016 for the environment and the economy do not seem to be uniform. Although increased bioplastics production saved about 16% of fossil-based energy per Euro of substitution and about 9% of water resources, cradle-to-gate GHG emissions increased by 34% (Fig. 5, black bars). Substitution triggered a higher output throughout the economy (11%), and this can be attributed overall to higher employer compensation rather than net operating surplus. Employing the extended model, similar effects across all indicators are observable (see Fig. 5, grey bars). First, fossil resource saving was lower by 5%, whereas GHG emissions increased by 13%. Value added was 3% higher and employer compensation was 5% higher while output was 1% lower, in large part due to the different direct intensities of animal and plant products.

Substitution effects arise from the bioplastics industry having a different input structure compared to the plastics industry, the ripple effects of plastics substitution on all other sectors of the economy, and different direct intensities of the most relevant input industries (effect per Euro of bioplastics production). The most important differences between the input structures of bioplastics and plastics industries are, of course, their different resource bases. Whereas bioplastics production is based on products from food industries, plastics production relies on refined petroleum products and chemicals. Direct inputs from agriculture are low because biomass products already processed by the food industry are assumed as inputs. For example, maize is not directly used as an input for PLA production but rather maize starch. Electricity and direct water consumption is higher in bioplastics production, which is likely due to the small-scale production methods of a young industry where potentials for energy efficiency improvements have hardly been exhausted (Fig. 6). Similarly, increased use of services by the bioplastics industry may indicate an initially higher demand for marketing, legal consulting, and transportation.

Ripple effects can be determined by comparing the Leontief coefficients of the fossil-based plastics industry to those of the bioplastics industry. Fig. 7 indicates how much more or less output from each sector is necessary to supply one Euro more of bioplastics and one Euro less of plastics. The model shows that substitution of bioplastics for fossil-based plastics results in higher bioplastics production and lower fossil-based plastics production, which is reduced by more than one Euro (1.09 €) because it is assumed that some primary plastics are input to other plastics in the model. Lower demand for refined petroleum products, chemicals, and plastics is partly offset by higher demand for food products, services, and electricity, in particular, as well as for almost all other sectors.

Direct intensities, meaning here the economic or environmental effect per Euro of a sector's output, varied strongly with regard to the most important input sectors. The green-shaded cells in Table 1 indicate the intensities of sectors that supplied more output due to substitution, while the grey-shaded cells specify the intensities of sectors that had lower output. Substitution decreases fossil resource use because sectors with higher output, such as the food sector, had a much lower direct fossil resource intensity than sectors with less output, such as chemicals (0.72 vs. 3.07 MJ/€, respectively). This also holds for water use intensity. By contrast, GHG emissions were higher because the direct intensities of the energy and agricultural sectors were much higher than the chemical sector's GHG intensity. Economic effects were small because differences in direct intensities were not very pronounced.

These results refer to supply chain effects not differentiated by region. A closer look at changes in trading patterns, however, reveals that substitution effects have been distributed unequally between Germany and the rest of the world. Still today, a large part of the fossil-based plastic supply chain is located in Germany. Substitution of bioplastics has been shifting production of major inputs and bioplastic products to other regions. Hence, in the 2016 data, fossil resource and water use saving in Germany were higher than indicated, due to lower output from the chemical sector, while fossil resource saving was lower and water use higher in biopolymer producing regions due to higher demand for crop production and

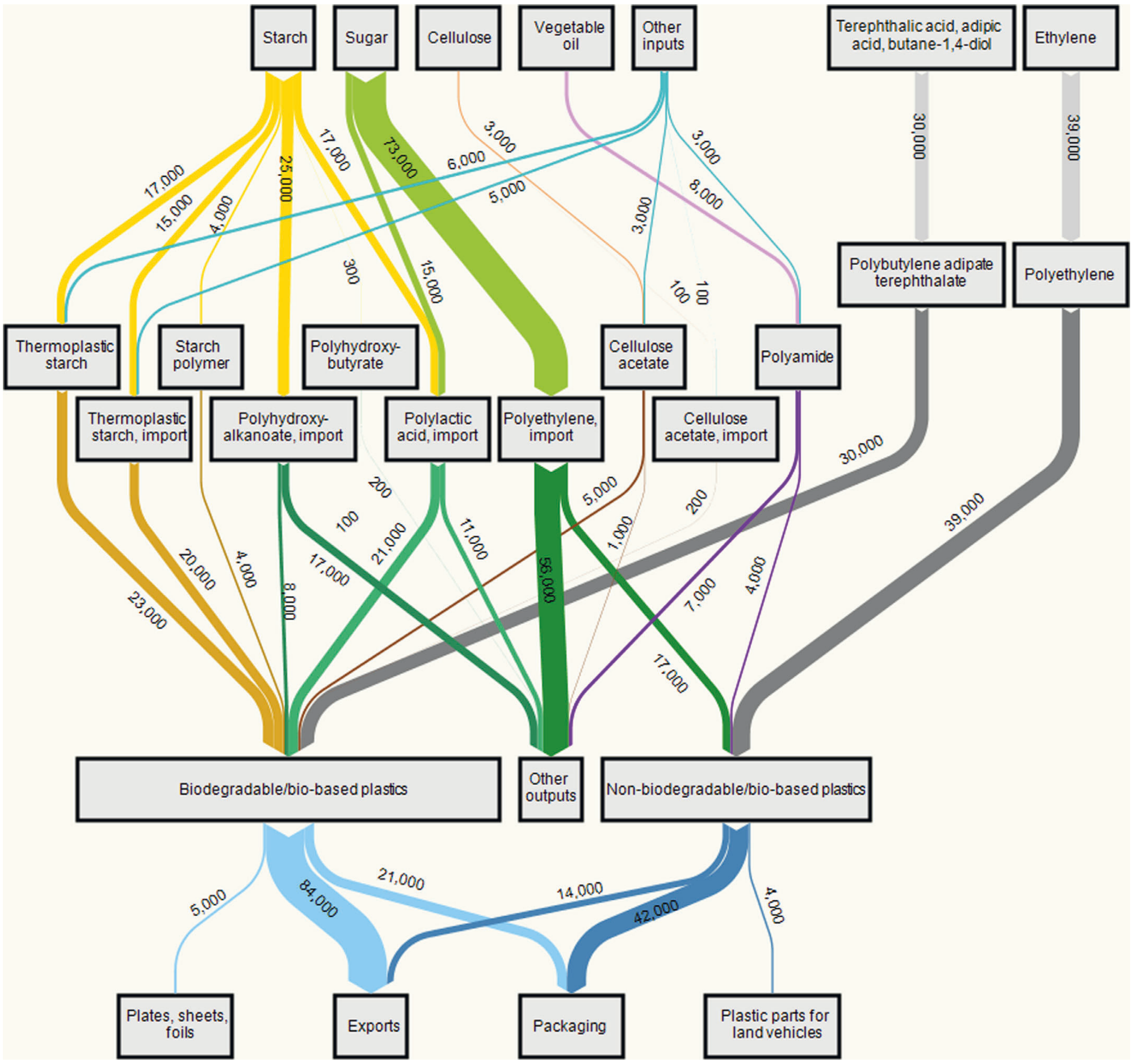

Fig. 4. Resource and material flows related to bioplastics production in Germany in 2016, in tons. Based on own data collection (expert interviews, SI 1), and Ecoinvent (2018), IfBB (2019).

Table 1
Direct input and output intensities of selected economic sectors in Germany, 2016. Based on Destatis (2020b, 2020c, 2020d).

Sector	Fossil resources (MJ/€)	Greenhouse gas emissions (kg CO2-Eq/€)	Water use (m³/€)	Value added (€/€)	Employer compensation (€/€)
Food	0.72	0.05	0.0023	0.26	0.18
Services	0.11	0.04	0.0002	0.56	0.32
Electricity, gas	33.71	3.61	0.1205	0.41	0.17
Other manufacturing	0.85	0.09	0.0010	0.40	0.25
Agriculture	0.18	1.54	0.0112	0.43	0.16
Petroleum products	92.29	0.57	0.0028	0.12	0.03
Chemicals	3.07	0.24	0.1169	0.41	0.20
Plastics	3.27	0.23	0.1169	0.36	0.20

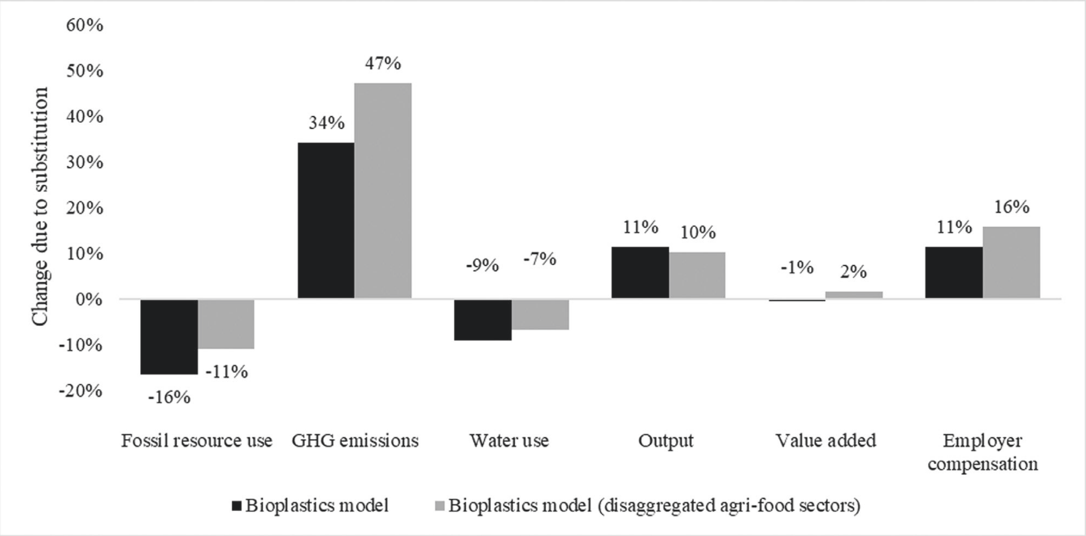

Fig. 5. Net substitution effects from bioplastics production in Germany in 2016. Based on the bioplastics model developed for this study (all sources described in 2.2).

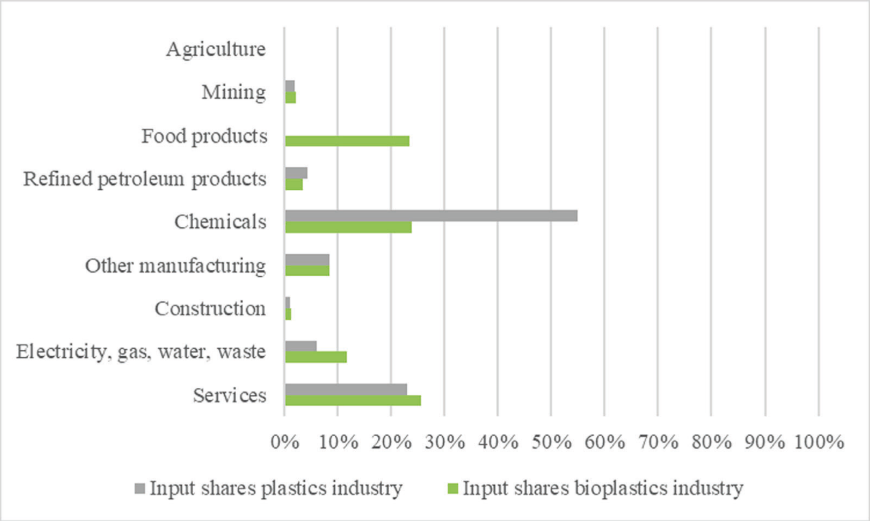

Fig. 6. Differences in the input structures of bioplastics and plastics industries in Germany in 2016. Based on the bioplastics model developed for this study (all sources described in 2.2).

processing. Much of the cradle-to-gate increase in GHG emissions in the 2016 data can be directly attributed to higher energy demand of biopolymer production compared to plastics production, meaning that the burden of GHG emissions was exported as well. Economic effects in Germany are likely to have been more negative than indicated by the model, because value added was lost in the German chemical sector and gained in the food sector elsewhere. In short, the shift of production of inputs from German petroleum products and chemical sectors to other countries' agricultural, food, and chemicals sectors due to the substitution of bioplastics for plastics is likely to have improved environmental indicators in Germany while slowing down economic indicators, and vice versa in biopolymer-exporting countries. However, this particular version of the model does not allow for estimation of domestic and international effects.

4. Discussion

4.1. Insights gained from monitoring bioplastics

The results examined from the German plastics sector in 2016 demonstrate that sectoral and regional disaggregation is possible. Through the method developed here, German production and import of the main bioplastics product groups were approximated and successfully integrated into an existing input-output table. Monitoring at lower regional levels is quite relevant to policymak-

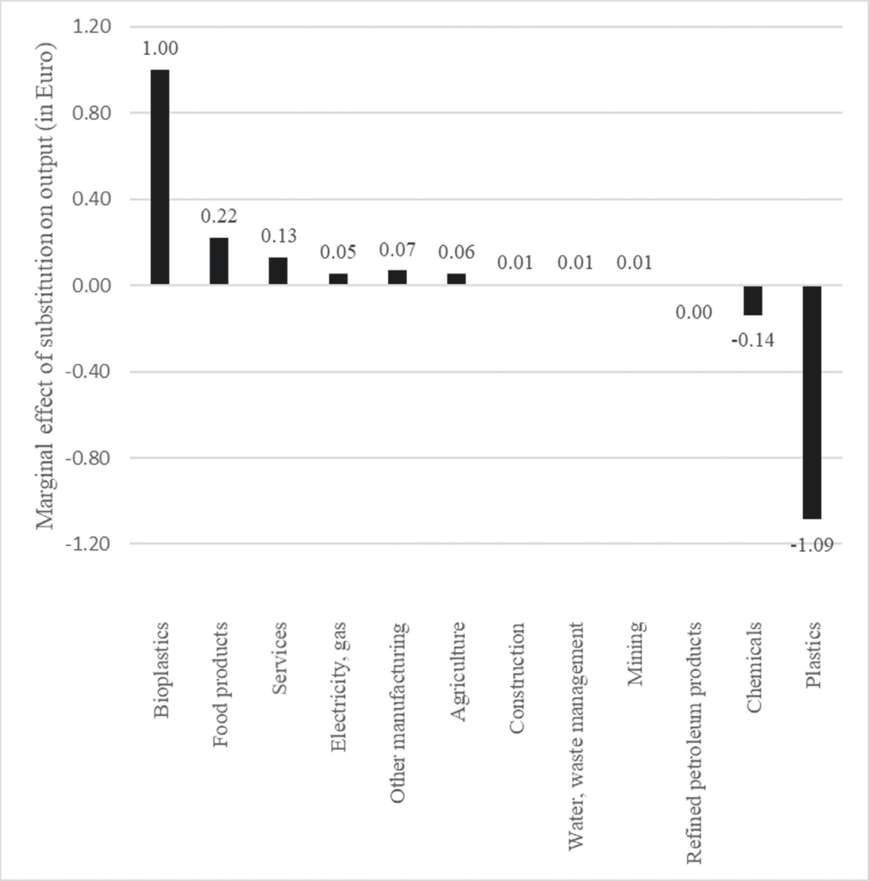

Fig. 7. Change in output due to plastics substitution in Germany in 2016. Based on the bioplastics model developed for this study (all sources described in 2.2).

ing purposes, because potential support would be implemented at the national level, or even lower, and not at the European or international levels. Likewise, monitoring at sub-sectoral levels has many advantages that can enhance the accuracy of monitoring and, ultimately, the success of policymaking measures. Relevant improvements from monitoring at the sectoral and regional levels include information gained about production structures and linkages between sectors, the significance of consumers, the role of imports, and the assessment of trade-offs. Necessary technical improvements in modelling and data collection that would be required to achieve reliable monitoring of this sort are discussed in the next section (4.2).

4.1.1. Production

The proposed monitoring approach can provide insights into the behaviour of bioplastics producers, indicate important input ('upstream') sectors, and improve estimation of bio-based shares in processing ('downstream') sectors. Results show that bioplastics producers used fossil-based components to guarantee certain desired capacities (Fig. 3) and fossil-resource-intensive energy (Fig. 6 and Table 1), which is why fossil-resource saving was lower for bioplastics than might be expected, with the intensity of bioplastics only being 16% lower than that of fossil-based plastics (Fig. 5). Some research has already been devoted to substituting fossil-based blending components with bio-based ones. For example, adipic acid, a copolymer in polybutylene adipate terephthalate (PBAT), has been successfully replaced with a sebacic acid group based on vegetable oil to yield polybutylene sebacate-co-terephthalate (PBSeT; Kim et al., 2020). A focus on higher process energy efficiency in bioplastics production could also positively contribute towards transition as measured by the SSI_s.

As energy has been identified as an important upstream sector, lower fossil-resource intensity and a higher renewables share might have a significant positive effect on bioeconomy transition in all sectors, not just the energy sector itself. Using less fossil resources in the energy sector can even have a greater effect on fossil-resource and GHG emissions savings than substituting resources in the plastics industry (Posen et al., 2017). Of course, differences in energy use for bioplastics and fossil-based plastics production would have to be represented in the model, which is currently not the case, in order to assess the relevance for substitution effects. This has, however, been done here for other upstream sectors, namely agriculture and food. As shown in Fig. 5, disaggregation changes the magnitude of effects, albeit not their direction.

With the sub-sectoral approach, it is possible to estimate bio-based shares in downstream production and consumption sectors. It could, for example, inform an input-output approach that has been suggested for EU bioeconomy monitoring (Cingiz et al., 2021). By including the bio-based shares of partly bio-based sectors when modelling downstream, partly bio-based, sectors through a hybrid modelling approach, complex value chains such as for the production of chemical products can be sufficiently represented. Cingiz et al. (2021) include direct inputs of, for the most part, natural rubber and cellulose that are processed into rubber products and fibre composites in order to calculate the bio-based value added of the rubber and plastics sector. Yet they do not include the processing of bioplastics into bioplastics products and, thus, underestimate the true value added. By monitoring at the sub-sectoral level, the bio-based value added of the rubber and plastics sector would very likely be higher.

4.1.2. Consumption

Another advantage of the approach is its ability to gather information about the role of consumers. Results indicate low demand for bioplastics in Germany, because much of this material was exported, and a strong preference of German consumers for non-biodegradable plastic packaging (Fig. 4). Consumer intention to purchase bioplastic products depends, above all, on their attitudes towards bioplastics according to a representative survey of the German population (Klein et al., 2019), which found that attitudes have not been entirely positive because high initial expectations for bioplastics were not fulfilled by products on the market leading to disappointment and fear of greenwashing. Bioplastics were expected to have a very high bio-based composition; degrade in natural, especially marine, environments or under home composting conditions; be produced from locally and organically grown biogenic resources; reduce GHG emissions significantly; have certain functional properties such as heat resistance; and be cheaper overall (Blesin et al., 2017; Scherer et al., 2018). Such observations in Germany have been confirmed for other regions as well: “Current terminology and associated technical definitions of bio-based and biodegradable plastics are incongruent with how the public understands them” (SAPEA, 2020, p.154).

Preference for non-biodegradable materials that can be recycled in the same way as their fossil-based counterparts may be due to confusion about correct separation and disposal of bioplastics waste (Neves et al., 2020), especially in countries with well-developed recycling systems where consumers rate recyclability higher than biodegradability (Korhonen et al., 2015). Current regulations in Germany encourage use of products of bio-based origin, whereas the use and disposal of biodegradable products is restricted or unclear. For example, the German *Verpackungsgesetz* (packaging law) calls on producers to use packaging based on renewable resources (BMU, 2017 Art. 21 (1), sentence 2). Yet the *Bioabfallverordnung* (regulation on biowaste) explicitly excludes biodegradable packaging (BMU, 2013 Appendix 1) and only includes biodegradable mulch films and organic waste bags certified for industrial composting according to EN 13432 or EN 14995. Boisourced waste bags are rejected by some composting facilities due to reservations concerning biodegradability and other technical issues (Kern et al., 2017). Confusion may have been further exacerbated by the discussion surrounding the exemption of biodegradable plastics in recently adopted regulations on disposable plastics (BMU, 2017 §5 (2); BMU, 2021). Only products based on natural polymers are exempt, while all chemically modified polymers do not qualify, although some biodegradable plastics, notably PHA and TPS, degrade in a number of natural environments within less than one year (Burgstaller et al., 2018).

In order to overcome these barriers to bioplastics consumption, policies could focus on reducing GHG emissions and pollution created by plastics consumption and disposal. Bioplastics targets could be tied to the bio-based carbon content of plastics, for reducing fossil-based carbon release during waste incineration, or to the biodegradability of plastics products that are neither recycled nor incinerated but end up in terrestrial or marine ecosystems, for reducing pollution in the open environment. Supporting selected bioplastics products with more specific aims, not just reduction of fossil resource use, could be more consistent with public expectations and perception of bioplastics. The GHG emissions reduction potential due to plastics substitution is 0.3% of total GHG emissions in Germany. Plastic waste constitutes about 13% (3.3 million t; Lindner, 2014) of total waste that is incinerated, and total waste incineration contributed 2% of total GHG emissions in Germany in 2018, not considering bio-based carbon emissions (UBA, 2020a). Of course, this requires balancing with net-process GHG emissions (cradle-to-gate), which was positive for bioplastics in the IO model developed here. Emissions-reduction potential is higher in sectors with low recycling rates, as incineration is the most frequent option. Recycling rates are above 10% in packaging, construction, and agricultural sectors but below 5% for furniture, electronics, household goods and toys, and medical products (Lindner et al., 2020). In the future, the reduction potential of packaging will become less significant, however, because waste incineration is projected to decrease by 9% until 2035, due to recycling requirements in current packaging laws (BMU, 2019). A bioplastics target in sectors with low recycling rates should be chosen with care. If novel bioplastics material contaminates conventional plastic waste streams and prevents sorting, less fossil-based plastic will be recycled and more incinerated. For example, PLA did not inhibit recycling of polypropylene and polystyrene (up to a share of 3% and 10%, respectively) in waste streams but was incompatible with other polyolefins and polyesters (Alaerts et al., 2018; Hiebel et al., 2018). Thus, in the short term and without changes to waste-sorting systems, the focus should be on chemically identical materials, whereas chemically different bioplastics materials might be promoted in the long-term when appropriate waste systems are in place. At present, the benefits of biodegradable plastics that can neither be recycled nor incinerated are limited to a few products in countries with established waste management systems like Germany. Some products, such as mulch films and microbeads in cosmetics, enter the environment after use because removal or collection is difficult (SAPEA, 2020). Targets for biodegradable plastics may be derived from consideration of useful applications and respective production data. In any case, a clear regulatory framework should accompany biodegradability targets, as demanded in the European Plastics Strategy (EC, 2018a).

These examples show that, on the one hand, more detailed monitoring can support the formulation of policies while, on the other hand, such policies require even better monitoring methods and strategies. It is necessary to assess cradle-to-cradle energy use and GHG emissions of bioplastics that includes different post-consumption pathways and monitor developments in the recycling rates of fossil-based plastics products.

4.1.3. Imports

The results presented here reveal that German bioplastics producers have been highly dependant on biopolymer imports (Fig. 4) and, thus, implicitly on embodied biomass imports. Compared to an import share of about 66% for bioplastics production, the import share of fossil-based primary plastics is much lower, at 40% (Destatis, 2020a). The experts interviewed for this study do not expect many new biopolymer plants in Germany in the future, which will likely have implications for monitoring as well as for policymaking because the ways that different biomass and biopolymers are produced in different regions influences the sustainability assessment of plastics substitution. The modelling of German bioplastics use undertaken for this study indicates that the domestic technology assumption (DTA) for bioplastics is not realistic, as the most significant biopolymers (PLA, PHA, Bio-PE) are imported *and* not produced domestically. Employing the DTA would overemphasize the technology of starch-based (TPS), cellulose-based (CA), and oil-based (Bio-PA) biopolymers and underrepresent sugar-based

(PLA, Bio-PE) ones, mainly affecting the shares of biomass inputs (22% with DTA, 34% relaxed DTA). This is why the technology of non-competitive biopolymer imports was considered in the model. However, the same production structure was assumed for every biopolymer, not differentiating by region of origin.

Although more modelling is still required, it is obvious that economic and environmental effects relocate as a result of substitution. It appears as if intermediate production might further shift abroad, while final goods will be produced and consumed nationally. Thus, environmental impacts in Germany may be lower, but jobs and value added may also decline. This implies that international cooperation is necessary to improve the environmental performance of production in other countries. One possible way to do this is to extend the recent German legislation on corporate due diligence in supply chains that addresses human rights. Another way is to establish standards regarding what products can be sold on the German market. In the same vein, new job opportunities are necessary if conventional, domestic production declines and jobs are transferred to biomass- and biopolymer-producing regions. Such new jobs could be related to establishing a circular bioeconomy, that is products and services that keep bio-based products within an economy.

4.1.4. Trade-offs

According to the model presented here, bioplastics production scores better than fossil-based plastics production in terms of fossil resource and water use as well as employer compensation (Fig. 5). The model does not, however, provide robust conclusions regarding the climate change effects of substitution, because important dimensions of carbon cycles have not been considered. By showing cradle-to-factory gate GHG emissions, the model does not account for carbon storage in plants. Nevertheless, comparative product life-cycle assessments having a broader cradle-to-grave system boundary usually indicate GHG emissions savings due to bioplastics substitution (Brizga et al., 2020; Oliveira et al., 2021). Thus, improving the model in this regard is necessary to better estimate such savings. Furthermore, indicators used for this model neither represent all dimensions of sustainability sufficiently nor relate environmental impacts relevant for policymaking. The present analysis, in line with other recent work (Escobar et al., 2018; Asada et al., 2020; Bringezu et al., 2021), has relied on available data sets for extended input-output modelling of pressure or so-called footprint indicators but how well these indicators can estimate damage to human health or ecosystems is contested (Heijungs, 2017), and there are other approaches for building impact indicators by linking IO models to life cycle impact assessments (e.g. Verones et al., 2017). More indicators for all dimensions are necessary, but their integration within bioeconomy monitoring systems is at present strongly restricted, because data that is required for the input-output model is not yet available. Consequently, policymakers are currently forced to rely on scarce information about the actual effects of substitution and can generally only justify support for bioplastics with some degree of certainty by pointing toward reduced fossil resource and water use and possibly the creation of more jobs in upstream supply chains.

4.2. Further modelling requirements

As explained in Methods and Materials, integration of information and data on bioplastics production into the main database of current bioeconomy monitorings, input-output tables, with matrix augmentation method was successful in providing a more detailed picture of bioplastics. However, as the previous section has identified, there are some challenges requiring methodological and data improvements to increase the model's capacities and precision.

Concerning methods, modelling biogenic carbon storage is recommended, because it is significant for drawing conclusions regarding the sustainability of bioplastics substitution (Pawelzik et al., 2013). Different methods have been proposed for this, either for “cradle-to-gate” or “cradle-to-grave” systems (Pawelzik et al., 2013). Factors related to carbon storage are not easily determined because they depend on many variables (Sun and Liu, 2020) and, thus, might contribute to model uncertainty. Nonetheless, effects of bioplastics substitution on GHG emissions could be further modelled using different end-of-life pathways. Biodegradable polymers, for example, neither release fossil-based carbon during incineration nor require energy for physical or chemical recycling if they are treated by composting facilities. Post-consumption pathways have been considered in waste input-output models (Nakamura and Kondo, 2009), but few studies are available for bio-based goods, with the exception of food products (Reynolds et al., 2015). Apart from improving methods for indicators already included in the model, choices about further indicators should be made by analysing the literature and connecting relevant available databases.

Better data collection can improve modelling, but it is important to keep costs of monitoring at a reasonable level. The bioplastics data for this study was collected with great effort and was still rather unreliable. Production data for Germany was not available, so expert interviews were conducted. Information from the interviews was at times vague, due to confidentiality concerns. Meanwhile, input data used from life-cycle inventories and the literature was often not traceable at all (e.g. for PA), not freely accessible (e.g. sugar cane-based PE) or outdated (e.g. PLA). More systematic, reliable, and regular data collection of bioplastics production quantities, prices, imports, exports, and input structures would improve modelling significantly. To facilitate better data collection, first, indicators should be observed over time, which is absolutely necessary for monitoring to be relevant for decision-making. Here, developments in the prices of bio- and fossil-based plastics could be modelled, though a potentially major drawback of using monetary IOT, in the absence of physical ones, is the influence of prices. If bioplastics were to become cheaper while fossil-based plastics remained the same price, the bioplastics model would indicate decreased fossil-resource saving even though it did not actually change. This is because fossil-resource use is related to production values in calculating fossil-resource intensity (Eq. (3) and Section 2.1). Thus, high relative variation in prices requires a correction factor that relates production values to production quantities – a modification that comes at a much lower cost than creating physical IOTs (Wieland et al., 2020). Second, greater confidence regarding the accuracy of import data would make results for currently used indicators more robust. To achieve this, regions could be more adequately represented by using methods suggested in Tukker et al. (2018), if bioplastics data is also available for the most important biopolymer-producing countries. Third, improved production and export data can positively influence the validity of conclusions about producer and consumer behaviour and determine bio-based shares in downstream sectors. Fourth, improved data on inputs to bioplastics production would better indicate what upstream sectors are worth disaggregating in the IO model. A challenge for disaggregating the agricultural and food sectors for the present study was the available database, because EXIOBASE 3 is based on a balancing procedure, which is required in creating multi-regional databases; the data is from 2011 and, thus, older than the model year of 2016; and a different classification was used than in 2016. Hence, even though data was available, it had to be treated before integration into the model, meaning greater effort and possibly increased uncertainty. With better bioeconomy databases, such as those now being developed for the EU (Mainar-Causapé et al., 2021), these data-related uncertainties might be reduced in the future. This will also enable inclusion of carbon credits specific to biomass, thereby improving GHG emissions modelling.

5. Conclusions and recommendations

By analysing the plastics sector in Germany at the sub-sectoral and country-level, valuable insights for designing improved bioeconomy transition monitoring systems has been gained. The results of the present analysis indicate that more specific information about bioplastics production, consumption, trade relations, and trade-offs integrated into existing bioeconomy monitoring systems through hybrid modelling can enable monitoring results that are more useful for political decision- and policymaking in this sector. The indicators proposed here were used to compare the net effects of output substitution with regard to fossil-resource use, GHG emissions, water use, value added, and employer compensation, thereby relating bioeconomy strategy objectives to more specific production and consumption patterns and providing guidance in, for the first time, setting targets for bioplastics that are specific, measurable, achievable, reasonable, and time-bound (SMART; EC, 2017).

At present, bioplastics production relies strongly on fossil-based process energy and materials and on imported biomass and biopolymers. Bioplastics processing and consumption in Germany is much more significant than material production, and there is much uncertainty about the sustainability and recycling options associated with bioplastics amongst consumers. Thus, effective policies, geared towards a lower dependence on fossil resources through substitution, could more strongly support the sourcing of sustainable biomass and bio-based materials in international value chains and increase focus on post-consumption waste treatment. Bioplastics consumption targets might be a possible means for motivating consumers and producers alike, because they could increase acceptance by consumers, if designed with consumers' understanding of bioplastics in mind, and guarantee a long planning horizon for firms, which is necessary for encouraging investment into research.

Reflection upon setting targets has, in turn, implications for improving monitoring and modelling. First of all, and to be more certain about modelling results before integrating bioplastics in a continuous bioeconomy monitoring, priorities in collecting better data could be explored with a sensitivity and uncertainty analysis of the bioplastics model. Second, for consumption-related targets, indicators should inform regarding substitution in these sectors by, for example, presenting the bioplastics shares in household goods rather than in primary plastics. Associated with this, significant efforts need to be made towards systematically collecting data on the production of bioplastics goods, trade relations, and current waste-treatment practices, which can be mandated via appropriate policies. Third, increased monitoring efforts are also worth undertaking regarding bio-based industries and upstream and downstream sectors that are considered to be important for the success of a future bioeconomy transition, of which many belong to the chemicals sector. Generalizing from the case of bioplastics, these include the agriculture, food, energy, and chemicals sectors as well as waste treatment. Finally, monitoring efforts could be further strengthened by revisiting bioeconomy strategies, better detailing what bio-based industries are considered most important and what specific objectives are to be pursued. For example, rather than focusing on reduced dependence on fossil resources, the ultimate objective of supporting bioplastics should be to mitigate climate change and reduce pollution in the open environment.

Improved monitoring combined with the concerted action of various stakeholders can bring society one step closer to a sustainable bioeconomy transition, as shown here for the case of bioplastics. Of course, these first steps need to be followed by targeted actions, their evaluation, and adaptation or updating of monitoring systems when feasible or necessary.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.spc.2021.11.033.

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Chapter 5. The robustness of bioplastics sustainability indicators

The contribution of Chapter 5 to this thesis' objectives is emphasized by changing the title to "The robustness of bioplastics sustainability indicators" from the original title in a manuscript with the preprint DOI 10.13140/RG.2.2.22772.63368.

The research paper has been added to this thesis in the next pages.

Title: A robustness check for bioplastics sustainability indicators that are based on a hybrid IO-LCA model

Authors: Wiebke Jander

Keywords: uncertainty, sensitivity, data quality, bioeconomy, monitoring, industrial ecology

Abstract:

Bioplastics are one strategy for tackling environmental problems related to plastics production and consumption but may nevertheless result in different challenges to sustainable development. Showing trade-offs of plastics substitution, models at different sectoral and regional levels of analysis have been developed. Hybrid input-output models seem to be particularly suited to analyze subsectoral levels because the modelling assumption that sectors produce homogenous goods is relaxed by augmenting aggregate sector data with more specific process data. This is essential in the wider context of monitoring bioeconomies that requires differentiation between bio- and fossil-based sectors. However, by reducing one source of uncertainty, other potential sources may arise, such as use of process-based data. Checking the robustness of results derived with a deterministic hybrid input-output life cycle assessment (IO-LCA) model is particularly relevant if indicators are part of a continuous bioeconomy monitoring. Consequently, this article presents an assessment of bioplastics sustainability indicators' robustness derived with such a model and recommends how uncertainties can be reduced. This is achieved by combining quantitative step-wise Monte Carlo (MC) simulations with qualitative data analysis. All indicators can be considered robust because probabilities that previous conclusions have to be corrected are low, even though uncertainty ranges can be considerable and data quality is mixed. Improving data on chemicals prices, production values of bio-based goods, and direct environmental intensities of chemicals subsectors should be high on the agenda if indicators on new bio-based sectors, such as bioplastics, are to be integrated into monitoring bioeconomies.

1. INTRODUCTION

In pursuit of sustainable development, societies are advancing their bioeconomies through increasing production and consumption of bio-based products. Governments are supporting such endeavors via bioeconomy strategies (EC, 2018; BMEL, 2020) and bioeconomy monitoring systems that are being developed to draw attention to trade-offs between conflicting sustainable development goals (Robert et al., 2020; Bringezu et al., 2021; Kardung et al., 2021). Suggested monitoring systems have been built upon input-output (IO) data because it is available for most countries on a regular basis and enables modelling of indirect impacts of bioeconomy developments on other sectors and economies. A challenge in monitoring bioeconomies with IO data is that sectors are not distinguished between bioeconomic and non-bioeconomic activities (Cingiz et al., 2021). This long-recognized problem of the homogeneity of sectors in standard IO models has been identified as a significant source of uncertainty (Lenzen, 2000). Hybrid input-output life cycle assessment (IO-LCA) models that integrate specific process-based data into IO data have been proposed as a solution (Suh and Huppes, 2009; Crawford et al., 2018), and efforts have been made to build hybrid models for analyzing the bioeconomy by integrating process-based data for specific bio-based products into IO data (Wydra, 2011; Acquaye et al., 2012; Malik et al., 2016; Watanabe et al., 2016; Budzinski et al., 2017; Lamers et al., 2021). In a new hybrid IO-LCA model, I assess bioplastics production in Germany, showing that, compared to fossil-based plastics production, with bioplastics fossil resource and water use decrease, cradle-to-gate GHG emissions and employer compensation increase, and net value added does not change (Jander, 2022). This bioplastics model reduces the uncertainty found in another bioplastics assessment based on a pure IO model, where the whole chemicals sector was used as a proxy for the bioplastics industry (Jander and Grundmann, 2019). By integrating more specific process data on bioplastics into IO data with the matrix augmentation method (summarized in Crawford et al., 2018), the total fossil resource intensity (tFRI) indicator has been corrected to be 12.39 MJ/€ (Jander, 2022) from 18.15 MJ/€ (Jander and Grundmann, 2019).

However, augmenting IO tables with process-based data may introduce a new source of uncertainty compared to non-hybridized IO models if, for example, given process-based data is outdated or vague (Eisenmenger et al., 2016; Font Vivanco et al., 2016; Islam et al., 2016). Process-based data in the bioplastics model refers to input quantities and prices required for biopolymer production as well as biopolymer production quantities and prices. This data has been used to represent bioplastics in German IO tables, which do not provide high levels of sectoral resolution. The process-based data is based on a number of sources, including ecoinvent database (Ecoinvent, 2018), a market study (van den Oever et al., 2017), technical literature (Hummel, 2004; Steinmeier, 2004; Righi et al., 2017; Ecoinvent, 2018; IfBB, 2019), and interviews with German bioplastics experts conducted in 2020 (Jander, 2022). These sources provide data that was unavailable before but may now be subject to change. For example, ecoinvent data on input quantities for some biopolymers is from 2011, and assessments of the technologies used should likely be updated. Similarly, the market study could be improved in the future if information on specific biopolymer prices becomes available. Biopolymer production quantities are vague because interviewed experts could not provide exact numbers, due to issues of confidentiality. In contrast, the IO data used in the model is considered more reliable because it has been collected from official sources, which can provide more consistent and precise values. For the bioplastics model, I rely on German monetary supply and use tables from 2016, including 85 commodity groups and 63 industries (Destatis, 2020e). They form the basis for modelling industry inputs and outputs in the German economy, based on the industry-technology assumption (Miller and Blair, 2009: 184-201), and for disaggregating the chemicals sector into “bioplastics”, “fossil-based plastics”, and “other chemicals” sectors. The model has been extended with economic, fossil resource use, GHG emissions, and water use data, also available from the German Federal Statistical Office, to build several sustainability indicators (Destatis, 2020b, 2020c; for a more detailed description of the model, see Jander, 2021, 2022).

Using such hybrid models in bioeconomy monitoring systems would appear to be worthwhile, as they make bio-based sectors more visible, but little is known about the robustness of indicators derived in this way. An indicator is considered robust if it cannot be easily manipulated so that results are to a great extent objective (EC, 2017). Manipulation of indicator values is possible if there are many significant sources of uncertainty in underlying models, such as uncertainty in source data or modelling choices (Lenzen, 2000; Loucks and van Beek, 2017). Uncertainty arising from process-based data in hybrid IO-LCA models is largely unexplored and methods for its determination should be developed (Islam et al., 2016). Therefore, I assess robustness of bioplastics sustainability indicators against changes in process-based data with a stochastic model in this article. If changes in indicator values are likely to be large, affect conclusions about the sustainability of plastics substitution, and can be attributable to influential inputs that have low-quality databases, the indicators affected can be considered less robust. Large changes to indicator values are expressed by wide probability distributions, but this alone would not necessarily mean that an indicator can be easily manipulated. Only if conclusions are affected, measured by the probability that the direction of net effects changes, would an indicator possibly be considered less robust. For example, a narrow distribution can affect conclusions if deterministic values for bioplastics and fossil-based plastics are close. Wide distributions, in turn, may not affect conclusions if the deterministic value for fossil-based plastics lies outside of the range of possible bioplastics values. Even if conclusions are affected, this may be due to variables that are based on high-quality data and, hence, the likelihood of changes in input data would be rather low and the indicators considered more robust.

Below I present a novel method combining uncertainty, sensitivity, and data quality analysis that is specifically designed to assess the robustness of hybrid IO-LCA models using matrix augmentation (section 2). The results from the bioplastics hybrid IO-LCA model are then presented in section 3. To conclude, I heighten the transparency of the indicator results derived from this particular bioplastics model by discussing their robustness in section 4.1 and point toward model inputs that should receive more attention for data collection in section 4.2.

2. METHODS

2.1 Basic procedure

Robustness was assessed via quantitative sensitivity and uncertainty analyses using MC simulation, supplemented by qualitative data analysis. In MC simulations, a model is repeated many times for different combinations of input values, sampled using probability distributions. This enables uncertainty analysis by generating probability distributions of model outputs and, at the same time, supports sensitivity analysis by quantifying the influence of several inputs on model outputs through regression analysis. Standardized regression coefficients are a simple measure of sensitivity. MC simulation has previously been used to assess the uncertainty and sensitivity of IO models (Wiedmann, 2009; Jiang et al., 2014; Asada et al., 2020) and is an advanced and popular method because several inputs are varied simultaneously and randomly. In the present analysis, each simulation with the Excel add-in @*Risk* had 10,000 iterations. A two-step simulation procedure was suggested and tried here, as the software does not support running simulations with target functions that use matrix inversion. With this limitation in mind, a first group of auxiliary simulations was used to estimate maximum and minimum values of some technical coefficients by varying process-based input data. These upper and lower boundaries informed possible maximum and minimum Leontief coefficients, which are the simulation inputs in the second, main group of simulations. The outputs of the auxiliary simulations became inputs for the main simulations, depicted as light green cells with a question mark in Figure 1. The following subsections describe the three main steps of the MC simulations, which were repeated for every simulation, and the linkage of the MC simulation results to my qualitative analysis.

2.2 Defining simulation outputs and target functions

For the first step, model outputs were specified for uncertainty ranges of interest. In the main simulations, simulation outputs were outputs of the deterministic extended hybrid IO-LCA model described in Jander (2021), namely the indicators *total intensities of fossil resource use* (tFRI), *value added* (VA), *employer compensation* (Empl), *GHG emissions* (GHG), and *water use* (Water) of bioplastics throughout production processes. Total intensities of a sector show how much more of a resource is necessary from all sectors of an economy to produce one more Euro of output in that sector. In order to compare uncertainty ranges between bioplastics and fossil-based plastics, indicator results for the latter were also defined as simulation outputs. Figure 1 shows simulation outputs on the right-hand side for bioplastics (in green) and for fossil-based plastics (in grey). The deterministic model involves multiplication of the intensities of all production sectors by their Leontief coefficients. For example, the green indicator in the top row on the right of Figure 1, total fossil resource intensity of bioplastics production ($tFRI_b$), is found by multiplying a vector of all sectors' direct fossil resource intensities ($dFRI$, top row on the left side of Figure 1) by a vector of Leontief coefficients (L_b, green column) from the bioplastics sector, b, using matrix multiplication (Equation 1). The L coefficients are direct and indirect input requirements from all sectors in the economy necessary to produce one more Euro of bioplastics. The direct intensity of a sector j ($dFRI_j$) are based on the sectoral data of the respective indicator dimension relative to a sector's output. Forcases of direct fossil resource intensity, direct fossil resource consumption ($dFRC$) in energy units is divided by the total domestic output (q^{do}) of sector j (Equation 2).

Equation 1

$$tFRI_b = dFRI * L_b$$

Equation 2

$$dFRI_j = dFRC_j / x_j$$

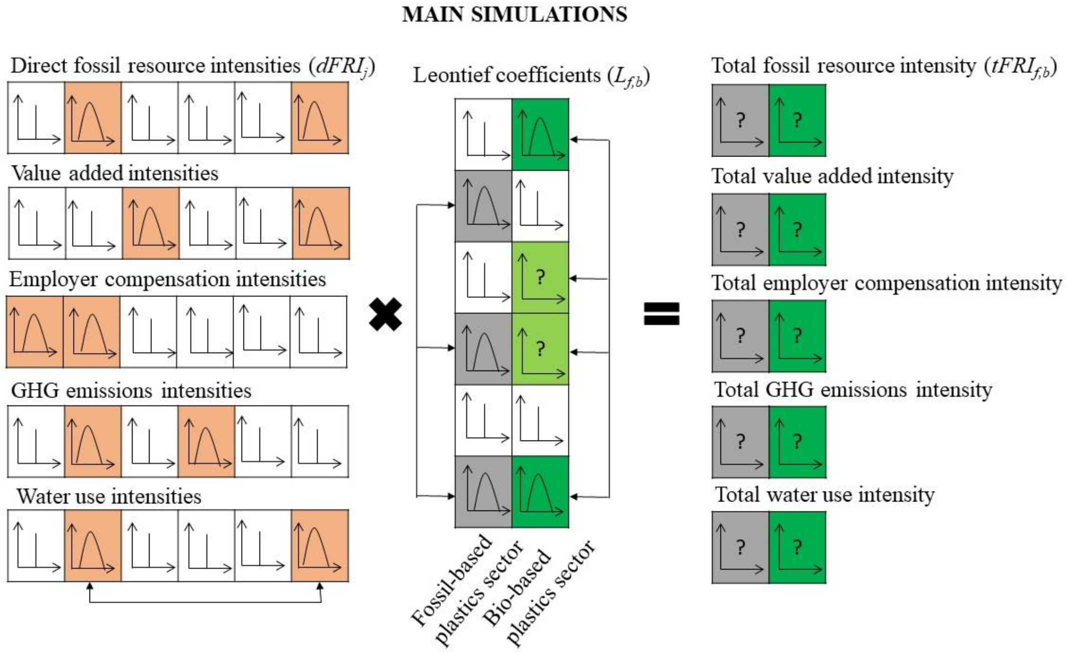


Figure 1. Basic model structure and relation to inputs and outputs of the main simulations for this study. Model inputs and outputs selected for simulation are color-coded (orange = direct intensities, grey inputs = Leontief coefficients for the fossil-based plastics sector, grey outputs = total intensities of the fossil-based plastics sector, dark green inputs = Leontief coefficients for the bio-based plastics sector, light green inputs = Leontief coefficients based on process and market data, dark green outputs = total intensities of the bio-based plastics sector).

For the auxiliary simulations, outputs were chosen that were used as inputs to distributions of the following process-based L coefficients of the bioplastics sector: food, refined petroleum, chemicals, and energy inputs. The L coefficients for all sectors were calculated through matrix inversion of a technology matrix, A, which represents shares of all inputs to all sectors (Equation 3). In the bioplastics model, matrix A was augmented with a bioplastics sector and a fossil-based plastics sector. An element of A (e.g. a_{jb}) is the input of sector j, expressed in value terms, used for the production of biopolymers b (Equation 4), calculated by multiplying a share for each input sector s_{jb} by total input value required for bioplastics production. Input share, s_{jb}, across individual biopolymers is a weighted input share calculated from each biopolymer's input share (s_{jbb}, j = input commodity, bb = biopolymer; Equation 5). Individual biopolymer input shares, s_{jbb}, are derived from process-based data – physical inputs to biopolymer production (q_{jbb}) – and market data regarding prices of inputs (p_{jbb}), production quantities of biopolymers (q_{bb}), biopolymer prices (p_{bb}), and value added (va_{bb}; Equation 6).

Equation 3

$$L = (I - A)^{-1}$$

Equation 4

$$a_{jb} = s_{jb} * \sum_{j=1}^{n} a_{jb}$$

Equation 5

$$s_{jb} = \sum_{bb=1}^{n} (s_{jbb} * (q_{bb} * p_{bb} / \sum_{bb=1}^{n} (q_{bb} * p_{bb})))$$

Equation 6

$$s_{jbb} = (p_{jbb} * q_{jbb}) / p_{bb} * (p_{bb} * q_{bb}) / (p_{bb} - va_{bb})$$

2.3 Defining inputs and distributions

The second step involved selection of the most relevant simulation input parameters, which were then assigned probability distributions. Inputs in the auxiliary simulations came from the parameters in Equation 6. Distributions were assigned to all of these inputs, except for value added (va_{bb}). The deterministic model assumes 25% value added for all biopolymers, and this was replicated in the simulation due to lack of information on static values and their possible distribution. Consequently, the number of uncertainty parameters was smaller, which might have resulted in a smaller uncertainty range. However, as this assumption is effective for all bioplastics and indicators, it is unlikely to influence conclusions about the relative robustness of particular indicators. Distributions of bioplastics production quantities (q_{bb}) were estimated using information from interviews with bioplastics producers and distributors (Jander 2022), which generated uncertainties in calculating actual production from capacities. Minimum, maximum, and mode values were specified in triangular distributions, where the mode corresponded to the value used in the deterministic model. Bioplastics price (p_{bb}) ranges were based on available estimations in the literature (van den Oever et al., 2017) and translated into Pert distributions which, by specifying minima and maxima, exclude very unlikely values. In contrast to triangular distributions, values around the most likely value (mode) and values far away from the mode are considered more likely in Pert distributions. Input quantity (q_{jbb}) distributions have their minima and maxima at +/-10% of the mode and have a continuous form (Pert distribution). Values were chosen with rather small deviations from the mean, assuming that 1) per-unit input requirements may vary somewhat in physical terms, depending on the quality of given inputs andespecially when using biomass, and that 2) some firms may be more or less efficient but that very large deviations are unlikely. Input price (p_{jbb}) distributions were discrete and randomly selected from recent historical data. Uncertainty ranges related to market data of biopolymers are summarized in Table S1, and an overview of relevant inputs and sources for historical data is available in Table S2.

The main simulations contained some inputs that were assigned distributions and some inputs that used static values, depicted as colored and blank cells in Figure 1. Distributions were defined for model inputs that exhibited both high intensity and a high input share at the same time, with the 10% most important inputs being selected (Table S3). Distributions were assigned to corresponding *L* coefficients and direct intensities. The *L* coefficients had Pert distributions, with their basic value as the mode, -20% of the mode as minimum and +20% of the mode as maximum. Four *L* coefficients had different maxima and minima as a result of the auxiliary simulations. The distributions of all relevant direct intensities were based on time series data for sectoral inputs (fossil resource, water, employer compensation) and output (GHG emissions, value added) quantities relative to production values for 2008–2018 (Destatis, 2020b, 2020c, 2020e).

2.4 Defining correlations between inputs

In the third and final step of setting up the simulation model, correlations between simulation input variables were specified to avoid the assumption that all variables are independent. This is important because adding correlations provides a more realistic simulation with wider uncertainty ranges. Possible correlations between the main simulations' inputs, direct intensities and *L* coefficients, are indicated with arrows in Figure 1. Correlations between direct intensities of selected sectors were derived from time-series sectoral consumption data relative to production values for 2008–2018 (Destatis, 2020b, 2020c, 2020e), which could indicate correlations due to similar developments in price levels or efficiencies. Sufficient historical data on water consumption during this time period was not available, so mutual developments in water use intensity of selected sectors could not be empirically observed, and a uniform correlation coefficient of 0.2 was assumed. Simulations for all other indicators often had higher coefficients, meaning that uncertainty related to the water use indicator might be underestimated compared to the other indicators. The implications of this are discussed in 4.1. Correlations between *L* coefficients can be the result of input price developments or changes in production technology. Here, focus is on correlations between price levels, which were derived from German producer price indices for 2001–2020 (Destatis, 2021a, 2021b). Due to missing information and disproportionate effort required for estimating correlations between production inputs, it was assumed that changes in the quantity of one input used would not have an effect on other inputs' shares. It seems reasonable to assume that prices have a much larger influence on correlations between a sector's inputs than input quantities because technologies change at a much slower rate than prices, and it is in many instances less likely that an increasing share of one input is directly associated with an increasing or decreasing share of another input. However, this remains to be validated empirically for the fossil-based plastics and bioplastics industries.

Correlations among input prices and between input prices and biopolymer prices in the auxiliary simulations varied. Castor oil, maize starch, and sugar prices were loosely associated ($-0.2 < r < 0.4$) and potato starch and castor oil had a high correlation ($r = 0.8$). The mineral oil products considered – naphtha and paraffin – were also highly correlated ($r = 0.8$), as would be expected because their prices rely on crude oil prices to some extent. Among the chemicals, ammonia, hexamethylene diamine, natural gas stood out as having a high positive correlation ($0.6 < r <$

0.9) along with dimethyl carbonate and sodium hydroxide (r = 0.6), both of which were negatively correlated with hexamethylene diamine (r = -0.4). Electricity and heat prices were negatively correlated to some degree (r = -0.4). Finding coefficients expressing correlations between input prices and biopolymer prices and between biopolymer prices was more challenging, as no suitable database was available. Rather than assuming no correlation, which would result in a lower uncertainty range, it was estimated that relevant biogenic and energy inputs would be associated with respective biopolymer prices with r = 0.5 and all other inputs with r = 0.2. These assumptions were then effective for all indicators and, thus, it is unlikely to influence conclusions about their relative robustness. Since TPS (thermoplastic starch) / PLA (polylactide acid), TPS/PHA (polyhydroxyalkanoate), and PLA/PHA are biodegradable biopolymers occasionally used for similar applications, they were assumed to be loosely correlated with r = 0.2, whereas the non-biodegradable biopolymers bio-polyethylene (Bio-PE) and bio-polyamide (Bio-PA) were assumed to be uncorrelated because they have very different uses. Bio-PE is used more often in everyday products and Bio-PA in specialized applications (Brehmer, 2014).

2.5 Categorizing data quality

The foregoing three main steps were essential for performing quantitative sensitivity and uncertainty analyses. Results of the sensitivity analysis then informed my qualitative data analysis by relating the most influential inputs for simulation outputs to the sources used. Some sources informing the deterministic bioplastics model can be considered of relatively high and others of lower quality, depending on common data quality dimensions (Batini et al., 2009; Cai and Zhu, 2015). Category 1 data – associated here with national and environmental accounting data as well as production and trade data from national or international statistical institutions – is of rather high quality because it is easy to obtain (accessible) within a given time period and regularly updated (current); it is also precise, in the sense that exact values are provided rather than ranges, and consistent over time and across countries due to common accounting standards. Missing data and information in the bioplastics model was estimated with the support of market studies, technical literature, and expert interviews, all of which have some obvious limitations. The market study by van den Oever et al. (2017) provided otherwise scarce information on biopolymer prices, but it has not been updated and indicates estimated price ranges rather than exact values. The technical literature documenting the life cycle inventories of biopolymers provides exact values for production inputs and is largely compatible with the classifications used here, at least those provided by the LCA database ecoinvent, but access is partially restricted, updates are rarely available, and there was no stock-taking of all relevant biopolymers at the time of building the model. Semi-structured interviews with experts in 2020 (Jander 2022) generated important insights into the German bioplastics market, challenges, and potential future developments; yet, exact values for bioplastics production and imports were not obtainable due to confidentiality concerns. Hence, in this study lower data quality is associated with stronger reliance on values from market studies (category 2), technical literature (category 3), and expert interviews (category 4).

3. RESULTS

3.1 Uncertainty

While preparing the main simulations, uncertainty ranges for four selected bioplastics-production input values were generated via the auxiliary simulations. These were found to be wider than for other inputs, for which minima and maxima were assumed to be +/-20% of the mode. The actual simulated minima were well below 80% of the respective static values, from 70% of the static value for energy inputs to 28% of the refined petroleum input value. Maxima turned out higher for energy inputs (+21%), food products (+39%), and refined petroleum products (+91%) and somewhat lower for chemicals (-6%). The results are summarized in Table S4.

Uncertainties determined in the main simulations are highest for the fossil resource use intensity indicator and lowest for the water use intensity indicator. The fossil resource use intensity indicator has the widest distribution, expressing more uncertainty than the other indicators. Values range from a minimum that is 50% lower than the mean (6.6 MJ/€) to a maximum that is 60% higher (20.6 MJ/€). Roughly 68% of values lie within -18% and +18% compared to the mean, according to a calculated standard deviation of 2.3 MJ/€. By contrast, all other indicators have a narrower distribution, with GHG emissions intensity having a standard deviation of 7% of the mean, economic indicators 3% and water use intensity 2%.

The risk of the bioplastics industry performing worse than suggested by the results of the original bioplastics model described in Jander (2022) varies by indicator. For the economic indicators, the chances of worse performance, meaning lower values, are highest, with 87% for the employment indicator and 88% for the value added indicator. This means that the deterministic model very likely overestimates economic indicators. Similarly, with a probability of 57%, fossil resource use of bioplastics is underestimated by the model (Figure 2). By contrast, GHG emissions and water use intensity are more likely to be lower (60% and 78%) than higher in the new model, compared to the original. Figures S1-4 illustrate these results, revealing that the magnitude of positive effects of substitution may be lower for economic and fossil resource use indicators and higher for GHG emissions and water use indicators, but they do not provide information about changes in the direction of net effects that could lead to different conclusions.

Comparison with static values for fossil-based plastics is even more informative for assessing robustness. There is a considerable risk that the production of bioplastics, and hence their substitution for fossil-based plastics, does not result in reduced consumption of fossil resources, which was concluded in Jander (2022). The probability that fossil resource use of bioplastics is higher than the fossil resource use of fossil-based plastics is 21% (Figure 3). It is much less likely that conclusions about value added will change if process-based data is corrected. The probability of a higher value added per Euro of bioplastics production compared to fossil-based plastics production is 10%. A change in the direction of net results is not expected for the three other indicators, which points to a higher level of robustness. Employer compensation per Euro is always higher in the bioplastics industry, water use intensity is always lower, and GHG emission intensity is never lower than in the fossil-based industry. Figures S1–8 illustrate these results.

In sum, conclusions derived from the deterministic model without uncertainties are largely supported by this analysis. Some substitution has occurred in the past in the German plastics sector. As with the original model, fossil resource savings is unlikely to be very large, but negative substitution is also unlikely. Using fossil resource savings as an indicator for the transition from a fossil- to a bio-based economy, as suggested in Jander and Grundmann (2019), bioplastics production can contribute to this transition with a high degree of certainty. This supports the argument that bioplastics production should be increased to reduce dependence on fossil resources, though reduction potential is not large. Meanwhile, another important argument in favor of bioplastics growth – climate change mitigation – continues to be invalidated even after analyzing the indicator's uncertainty. However, as this uncertainty analysis has not included modelling choices, further research and improved modelling is urgently needed in this regard. Moreover, employer compensation throughout the value chain is very likely to be higher due to substitution, water use is likely to be lower, and value added is probably not significantly influenced. Thus, economic arguments for substitution continue to weigh more strongly than environmental ones, if only the selected indicators discussed here are considered in decision-making.

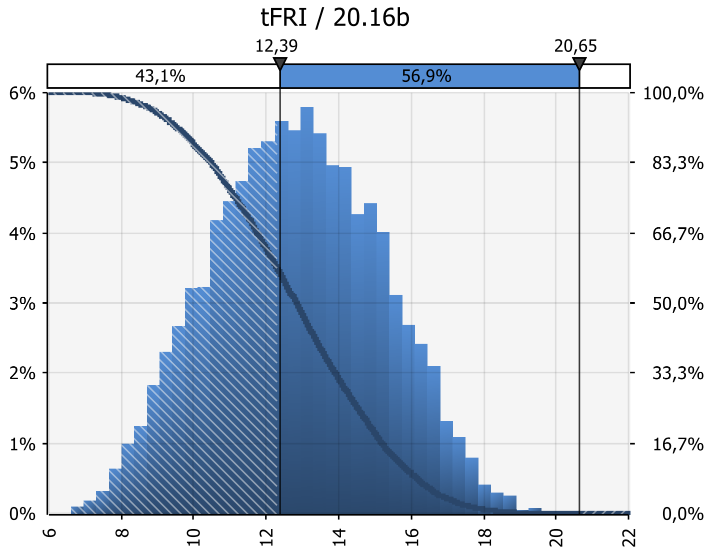


Figure 2. Uncertainty range for the fossil resource use intensity indicator for the bioplastics sector. The probability of a higher value compared to the static model's value for the bioplastics sector is shown in blue (top of figure). Based on data from Jander (2022).

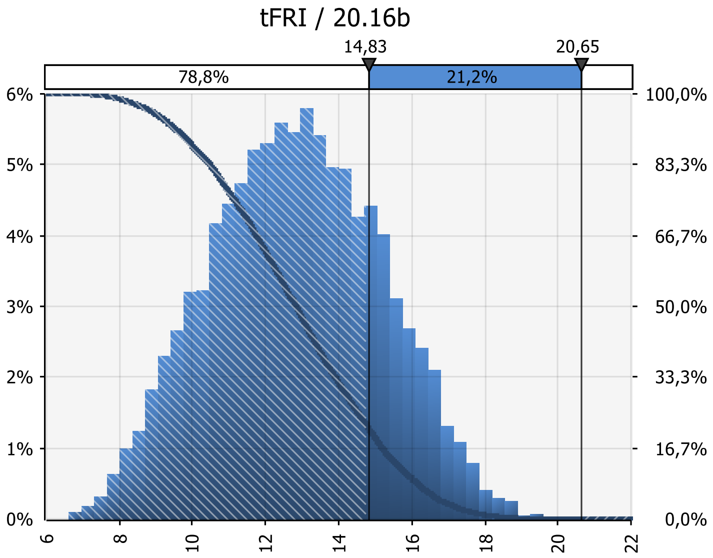
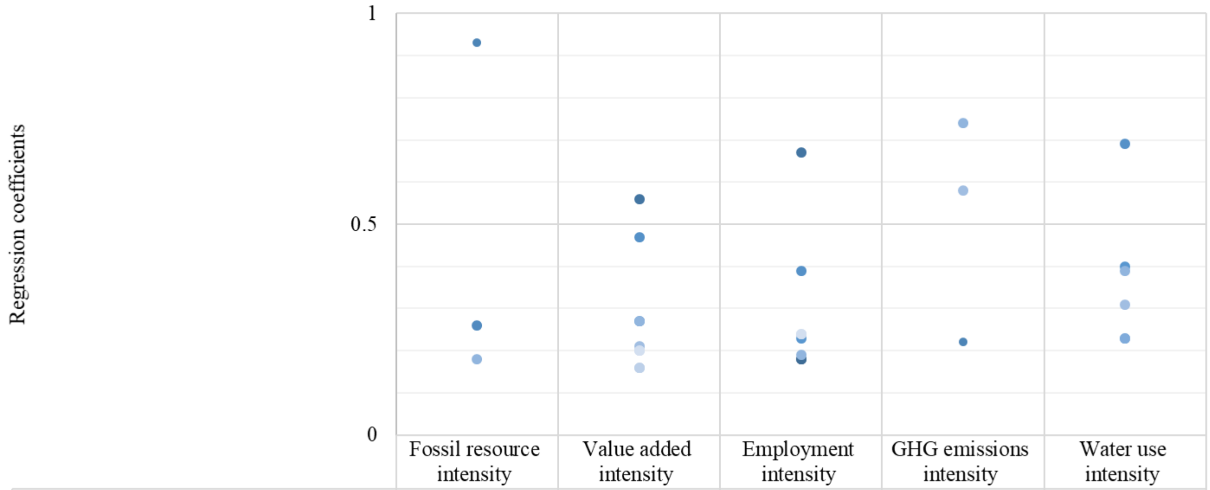


Figure 3. Uncertainty range for the fossil resource use intensity indicator for the bioplastics sector. The probability of a higher value compared to the static model's value for the fossil-based plastics sector is shown in blue (top of figure). Based on data from Jander (2022).

3.2 Sensitivity

All of the selected indicators rely strongly on only a few input variables. This finding is in line with Mattila et al. (2018), who have concluded that very few components in IO tables have a significant effect on GHG emissions. Economic indicators are sensitive to more input variables and have a weaker relationship to them, whereas uncertainty in environmental indicators can be attributed to fewer, more strongly associated input variables. Figure 4 summarizes the sensitivity of bioplastics industry indicators to sectoral input shares (Leontief coefficients) and direct intensities. Each indicator is particularly sensitive to one model input, illustrated by regression coefficients above 0.5. Total GHG intensity of bioplastics is very sensitive to two inputs (energy input share and intensity). Biomass inputs produced by the food sector influence economic but not environmental indicators. Uncertainties in the environmental impacts of bioplastics production are due to assumptions regarding the input shares of the mineral-oil products, chemicals, and energy sectors. The value for the total GHG emissions intensity of bioplastics production further depends on the energy sector's direct GHG intensity. Variables related to the crude oil and natural gas, fossil-based plastics, and two service sectors have a consistent relationship with economic and water use intensity indicators, though not a strong one.



	Fossil resource intensity	Value added intensity	Employment intensity	GHG emissions intensity	Water use intensity
● Crude oil / natural gas (input share)			0.18		
● Crude oil / natural gas (intensity)			0.18		
● Food products (input share)		0.56	0.67		
● Refined petroleum products (input share)	0.93			0.22	
● Refined petroleum products (intensity)	0.26				
● Other chemicals (input share)		0.47	0.39		0.69
● Other chemicals (intensity)		0.27	0.23		0.40
● Fossil-based plastics (input share)					0.23
● Fossil-based plastics (intensity)					0.23
● Energy (input share)	0.18	0.27	0.19	0.74	0.39
● Energy (intensity)		0.21		0.58	0.31
● Real estate activities (input share)		0.16			
● Real estate activities (intensity)		0.16			
● Legal/accounting activities (input share)		0.20	0.24		
● Legal/accounting activities (intensity)		0.20	0.24		

Figure 4. Sensitivities of indicators (simulation outputs) to direct intensities and Leontief coefficients of selected sectors (simulation inputs). The table includes regression coefficients of variables that have a consistent influence (correlation coefficient > 0.15). Based on data from Jander (2022).

The relationships between model inputs and outputs by indicator are illustrated in Figures S9–12 with Tornado diagrams, which rank input variables according to their effect on the output variable's mean. For example, Figure 6 shows that the fossil resource intensity indicator is sensitive to values for mineral oil product inputs for bioplastics production, as changing the Leontief coefficient of that sector in a predefined range causes the indicator's base value to vary between 9.8 and 15.8 MJ/€ (+/-23%) while holding all other inputs at their base values. The top three variables listed in Figure 5 have a consistent relationship with the fossil resource intensity indicator because they have a correlation coefficient above 0.15. A perfectly consistent relationship, where input always increases or decreases output, would be expressed with a Spearman rank correlation coefficient of +/-1. A lower coefficient means that the relationship is less consistent, and a coefficient of 0 means that the chance of increasing output is just as high as the chance of decreasing it. The strength of a given relationship is expressed by regression coefficients. A regression coefficient of +/-1 means that reported sensitivities are stable, whereas coefficients between -0.5 and 0.5 indicate unstable ordering of input sensitivities. In the example, only the highest-ranked variable – input of mineral oil products for bioplastics production – can be considered a strong influence on indicator results. Here, an increase of one standard deviation in the input value for refined petroleum products would lead to an increase of 0.93 standard deviations of fossil resource intensity.

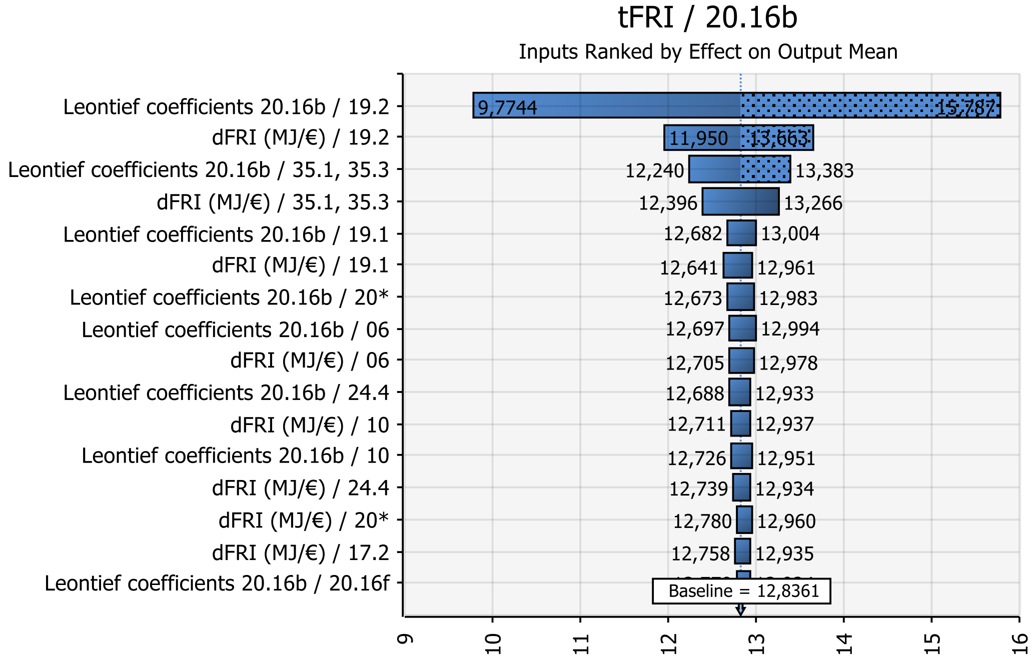
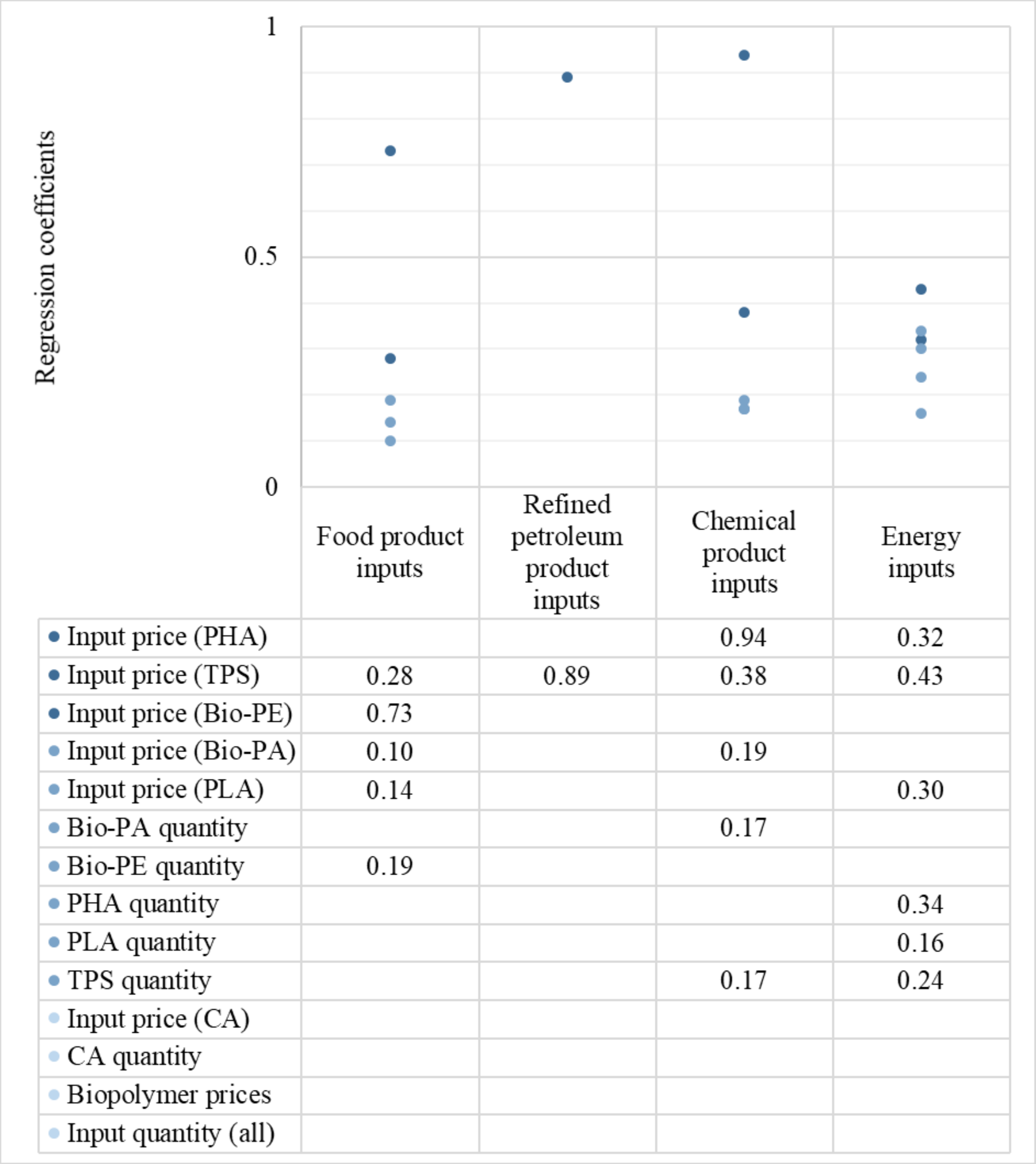


Figure 5. Tornado diagram showing ranking of simulation inputs that determine the uncertainty of total fossil resource use intensity of the bioplastics sector. Based on data from Jander (2022).

Most of the influential inputs for the deterministic model rely on process and market data used for hybridization. What, then, are the determinants of the most influential model inputs? This was assessed in the auxiliary simulations, the results of which are summarized in Figure 7. Sectoral inputs to bioplastics production are not very sensitive to input quantities and biopolymer prices but are, partly, very sensitive to input prices and biopolymer quantities. Data for cellulose acetate (CA) do not play a significant role, whereas data for thermoplastic starch (TPS) is crucially important because this biopolymer is the one most used in the German bioplastics industry, which is the focus of this study. For each sector's input value, one process variable always has a very strong influence on its uncertainty, indicated by a regression coefficient larger than 0.5, except for the energy sector, which has less strong associations with simulation inputs. The value for inputs of food products is mainly determined by uncertainties related to sugar prices, which is relevant in Bio-PE and PLA modelling, and somewhat determined by starch and castor oil prices as well as Bio-PE quantities. Mineral oil product inputs for the bioplastics industry are greatly and solely influenced by the input value of naphtha for TPS production. The price for dimethyl carbonate, used for modelling PHA inputs, determines the uncertainty of chemical product inputs. Meanwhile, natural gas prices, used for modelling TPS inputs, and data for PA and TPS production quantities have a weak influence. The value of energy inputs is influenced more evenly by more variables, which all have a weaker influence overall (regression coefficient < 0.5). Nevertheless, assumed heat prices are more important than electricity prices because heat consumption is much higher than electricity consumption across all biopolymers. The influence of TPS, PHA and PLA production quantity and imports is also relevant.



	Food product inputs	Refined petroleum product inputs	Chemical product inputs	Energy inputs
● Input price (PHA)			0.94	0.32
● Input price (TPS)	0.28	0.89	0.38	0.43
● Input price (Bio-PE)	0.73			
● Input price (Bio-PA)	0.10		0.19	
● Input price (PLA)	0.14			0.30
● Bio-PA quantity			0.17	
● Bio-PE quantity	0.19			
● PHA quantity				0.34
● PLA quantity				0.16
● TPS quantity			0.17	0.24
● Input price (CA)				
● CA quantity				
● Biopolymer prices				
● Input quantity (all)				

Figure 6. Sensitivities of sectoral inputs (simulation outputs) to process inputs (simulation inputs). The table includes regression coefficients of variables that have a consistent influence (correlation coefficient > 0.15). Based on data from Jander (2022).

3.3 Data quality

None of the sustainability indicators relies strongly on lower-quality data or solely on higher-quality data. They rather depend on different data sources to varying degrees and, thus, cannot be easily distinguished and ranked. Nevertheless, there are some minor differences. The main simulation inputs (second row in Figure 7) relying strongly on prices for their respective inputs (food, refined petroleum products, chemicals, energy) tend to have higher data quality associated with data from organizations and statistical offices, whereas inputs reliant on biopolymer production quantities have been based on expert interviews, considered a source of lower quality data. In Figure 7, variables with a more solid database are shaded with a darker blue. As input of refined petroleum products only relies on prices, it is considered a variable with a strong database. Input of chemicals relies much more strongly on prices than on biopolymer quantities and, thus, ranks second, while food inputs rank third, as they rely somewhat strongly on prices, and energy inputs rank fourth, as they depend equally on prices and quantities. Strength of influence is expressed by arrow thickness and was quantified using regression coefficients (Figure 4, Figure 6). The thickest arrow was chosen for a regression coefficient of 1 > 0.9, the second thickest for 0.9 > 0.5, and the thinnest for <0.5. For ranking the indicators (top row of Figure 7), this ranking of inputs was considered. The fossil resource intensity indicator ranks highest among the indicators because it relies very strongly on input share of refined petroleum products. Meanwhile, the water use intensity, value added and employment indicators rank next, in that order, because they are strongly influenced by food or chemical inputs and not much by energy inputs. Finally, the GHG emission intensity indicator ranks lowest among the indicators because its most significant input variable – energy input share – is equally influenced by input prices and biopolymer quantities. However, in assessing the robustness of these indicators it should be kept in mind that differences between them are small.

Some information is not relevant for differentiating between indicators in terms of data quality. First, input quantities and biopolymer prices have been based on lower-quality data (technical literature and market studies), but no influence on input shares was identified via the auxiliary simulations (see Figure 6). Second, as can be seen on the right-hand side of Figure 7, all indicators rely on input shares from “other sectors” and “direct intensities”, which are based on higher quality data, but not strongly (see Figure 4).

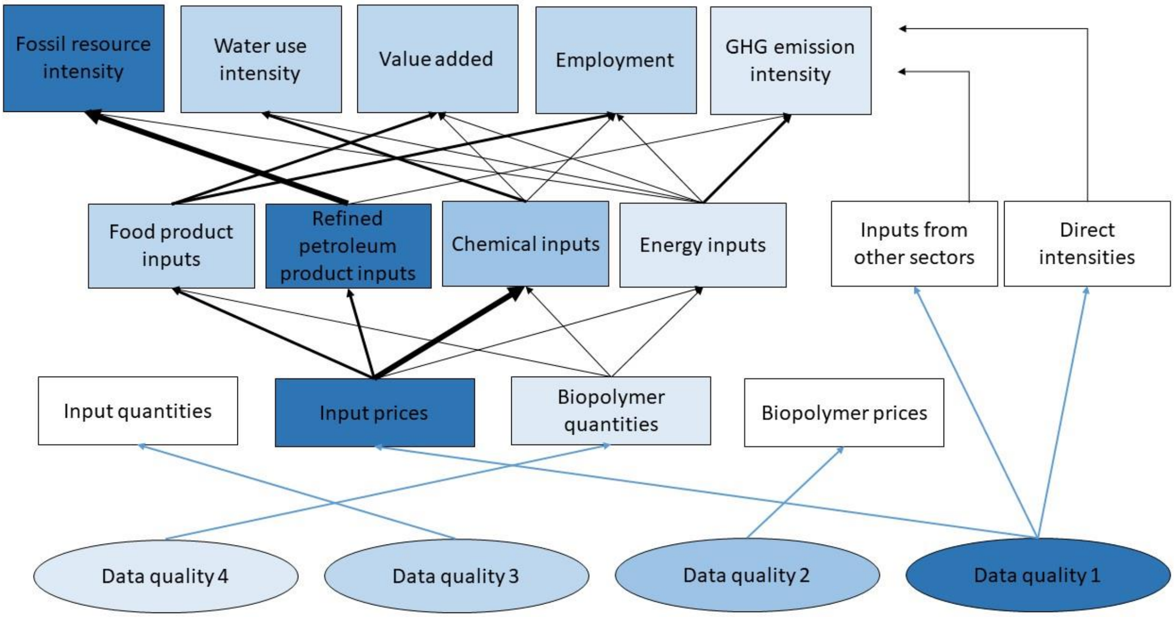


Figure 7. Relationships between main simulations outputs (top row), auxiliary simulations outputs / min simulations inputs (second row down), auxiliary simulations inputs (third row down), and data quality (bottom row). Black arrow width shows strength of relationships between inputs and outputs. Shades of blue indicate data source reliability, with dark blue representing the most reliable data sources.

4. DISCUSSION

4.1 Are the indicator results robust?

The results of the performed uncertainty, sensitivity, and data quality analyses are combined here to give an indication of the relative robustness of the studied bioplastics indicators. A central finding is that, although some indicators are more robust than others, none of the indicators exhibits a very low level of robustness. Robustness could be increased for all, as discussed in 4.2.

Based on the results presented above, the least robust indicator appears to be GHG emission intensity, as it scores lowest with regard to source data quality – based on the less solid data source of expert interviews – and due to a modelling input (energy share) that strongly influences its uncertainty (Figure 7). Yet, one of the most solid sources, data reported under the United Nations Framework Convention on Climate Change, is used for its second most-influential variable: the GHG emissions intensity of the energy sector. Although it has the second highest standard deviation of all indicators, it is very unlikely that conclusions from the deterministic model need to be adjusted because all bio-based values for the simulation are above the fossil-based original values (Figure S7). In sum, although some of the source data is of lower quality and might be subject to subsequent change, it is not very likely that this would alter the previous conclusion that bioplastics production increases process GHG emissions.

Fossil resource intensity also has drawbacks with respect to its robustness, as its standard deviation is the highest of all indicators and the conclusion from Jander (2022) that substitution in Germany is triggered through bioplastics production is supported with only 79% probability (Figure 4). There is, then, a 21% chance that the fossil resource intensity of bioplastics is higher than that of fossil-based plastics. In that case, the substitution share in the plastics sector would be negative, and an important argument for developing bioplastics and increasing their production would become insignificant. However, this uncertainty can almost exclusively be attributed to inputs that have a very solid database, that is, data regarding the fossil resource intensity of the refined petroleum products sector and naphtha prices (Figure 7). Naphtha prices, which determine the input value of refined petroleum products for TPS production (Figure 6), were assumed to fluctuate greatly based on their past development. The assumed minimum value is 85% lower and the maximum value 65% higher than the mean. Because the source, the stock market, is very reliable, it can be concluded that fossil resource intensity is very robust as an ex post indicator but less so as an ex ante one.

The economic indicators used are almost equally robust because they exhibit the same standard deviations and rely to the same degree on similar data sources. The value added indicator could be considered somewhat less robust than the employment indicator because there is a 10% chance that bioplastics production will lead to an increase in value added, while a change in net effects is not expected at all (Figure S5). Increasing bioplastics production would increase employer compensation throughout the upstream value chain with great certainty (Figure S6). According to the data quality ranking in Figure 7, it can be inferred that the selected economic indicators have a moderately solid database, one that is better than for GHG emission intensity but somewhat worse than for fossil resource use intensity. In addition, the data from statistical offices for direct value added and employer compensation is weaker than for direct environmental intensities because economic data is related to economic sectors rather than production sectors so that, in the product-by-product input-output model, values for production sectors were approximated with data for economic sectors (Jander 2022).

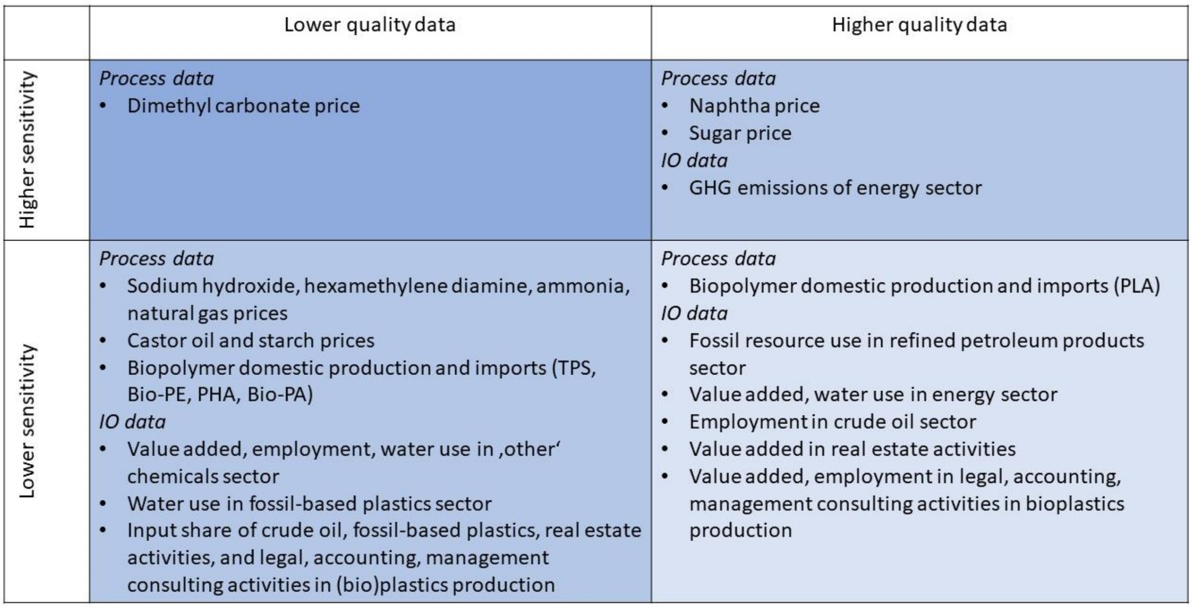
The water use intensity indicator can be considered the most robust of all. Having a standard deviation of 2% of the mean, it is very certain that less water is required in bio-based than in fossil-based plastics production. All values for water use in bioplastics production are below the fossil-based original value (Figure S8). This relatively low level of uncertainty is influenced by higher quality data to a larger extent than by lower quality data. A drawback is the quality of statistical data for direct water use by production sectors. As correlation coefficients could not be calculated from historical data as it was for the other indicators, the uncertainty range of water use might be underestimated and, thus, its relative robustness might have to be corrected. Improvements are suggested in the next section.

In this article, a method for assessing the robustness of bioplastics indicators, derived using a hybrid IO-LCA model, has been developed and tested for the first time. Combining well-established MC simulations with qualitative analysis, this novel method is intended to provide valuable insights into uncertainties related to process-based parameter values. Although such values for the bioplastics industry in Germany are often uncertain, resulting indicators are fairly robust, as the influence of process-based input values on indicator values is limited. This qualitative assessment enables relative ranking of indicators and can only be compared to quantitative results in the literature to a limited extent. Robustness in other IO models is often assessed using standard deviations. Wiedmann, Lenzen, and Wood (2008) consider the indicator CO2 emissions, derived with a multi-regional input-output model (MRIO) for the UK, robust because their results have a standard deviation of between 3.3% and 5.5%. In the present study, the standard deviations of the indicators water use, value added, employer compensation, and GHG emissions intensities are 2-7%. By contrast, the fossil resource use indicator, with a standard deviation of 18%, has scored worst. This is similar to a result by Asada et al. (2020), who conclude for their MRIO model analyzing the EU bioeconomy that distribution of results for fossil and mineral use are wider than for other indicators, especially for their chemical scenario. In particular, this indicator "appears to be exceptionally sensitive to variations in flows at the sub-sectoral level" (Asada et al. 2020, 9). Thus, uncertainty related to actual fossil resource substitution in the chemical sector may be large, possibly due to uncertainty in the plastics sub-sector. Future improvements of the method proposed here could aim at providing a quantitative measure of robustness, which would enable comparisons between hybrid models using matrix augmentation for different sectors as well as the robustness of bioplastics sustainability indicators.

4.2 How can source data uncertainty be reduced?

I have just argued that the bioplastics indicators derived using a hybrid IO-LCA model are robust but also that their robustness could be improved by reducing the uncertainties of specific input data. Here, I suggest to developers of bioeconomy monitoring systems and political decision-makers how future data collection can be prioritized, with the aim of improving its robustness, by analyzing relationships between the most influential input variables and data quality. Whenever variables contribute towards higher sensitivity in indicator values and are based on lower-quality data, additional data collection is strongly recommended for increasing the bioplastic model's robustness. It is also advisable if either sensitivity is high and data quality acceptable or both sensitivity and data quality are low. Meanwhile, less effort is required if variables do not have much influence on indicator results and already have an acceptable level of data quality. Variables with higher sensitivity in Figure 8 – input shares for the food, refined petroleum products, other chemicals, and energy sectors and the direct GHG intensity of the energy sector – have a regression coefficient above 0.5 (Figure 4). As input shares for these sectors are based on process data, sensitive input variables for them have also been included, meaning all variables related to specific input prices with a regression coefficient above 0.5 in Figure 6. On the other hand, variables with lower sensitivity have regression coefficients between 0 and 0.5 (Figure 4, Figure 6).

Data quality is determined by its origin, as specified in Figure 8, but analyzed in more depth here. Higher-quality data is mostly sourced from national or international statistical offices or other reliable organizations. However, some significant drawbacks of official statistical data are discussed below as well and, thus, it is here classified as a lower-level category. Other lower-quality data based on expert interviews, technical literature, and market studies that provide a one-time snapshot of relevant inputs is often outdated by the time it is applied.



	Lower quality data	Higher quality data
Higher sensitivity	*Process data* - Dimethyl carbonate price	*Process data* - Naphtha price - Sugar price *IO data* - GHG emissions of energy sector
Lower sensitivity	*Process data* - Sodium hydroxide, hexamethylene diamine, ammonia, natural gas prices - Castor oil and starch prices - Biopolymer domestic production and imports (TPS, Bio-PE, PHA, Bio-PA) *IO data* - Value added, employment, water use in ‚other' chemicals sector - Water use in fossil-based plastics sector - Input share of crude oil, fossil-based plastics, real estate activities, and legal, accounting, management consulting activities in (bio)plastics production	*Process data* - Biopolymer domestic production and imports (PLA) *IO data* - Fossil resource use in refined petroleum products sector - Value added, water use in energy sector - Employment in crude oil sector - Value added in real estate activities - Value added, employment in legal, accounting, management consulting activities in bioplastics production

Figure 8. Classification of model input variables by sensitivity and data quality for prioritizing data collection efforts (dark blue = higher priority, light blue = lower pritority).

In terms of prioritizing efforts in order to reduce uncertainties in the bioplastics model for Germany, it is foremost advisable to provide better price data for chemicals. Figure 8 shows on the upper left that prices for dimethyl carbonate, in particular, have been identified as highly influential and, yet, have a lower-quality database. Dimethyl carbonate prices very much determine the value of chemicals used in PHA production (r = 0.94) and, thereby, overall chemicals use in bioplastics production. Although price data for chemicals is sourced from statistical offices, they do not represent true prices but rather unit values, which are calculated by dividing sales value by production quantity. Sales value includes packaging but not sales or excise taxes, freight costs, or discounts (Destatis, 2021c).

A secondary priority is assigned to improving model inputs with lower impact on sensitivities and lower data quality (Figure 8, lower-left quadrant). The challenge of estimating prices with (import) unit values also applies to inputs of ammonia, sodium hydroxide, hexamethylene diamine, natural gas, castor oil, and starch for production of all biopolymers, and having price data would increase the model's correctness. Much improvement of data on biopolymer production in Germany and imports is necessary, as it is at present highly uncertain. Except for PLA, this data is not included in trade or production statistics and, hence, the proposed model only relies on the estimations of a few experts interviewed for this research. All biopolymers that are produced or imported in significant quantities should also be included in data collection and given their own classification codes. According to expert assessments, this is particularly important for TPS and Bio-PE because their produced and traded quantities are similar to or even higher than those of PLA. Quantities of PHA might not yet be significant, but world capacities are growing due to increasing demand for biodegradable plastics. Meanwhile, Bio-PA quantities are highly uncertain because this information was kept confidential by interviewees, but specialty biopolymers in general might become more significant economically, even if their relative volumes might be low. Share of CA in bioplastics production is less important and, according to one of the experts (Jander 2022), is not expected to grow much. More information on value added, employer compensation, and water use in the "other chemicals" sector (not including plastics) and the fossil-based plastics sector could also reduce uncertainties and yield more exact results.

Less effort is required for improving naphtha and sugar prices and GHG emissions data for the energy sector because available data is already of higher quality (Figure 8, upper-right quadrant). As already mentioned, GHG emissions data for the energy sector is particularly reliable because data is reported under the United Nations Framework Convention on Climate Change. Naphtha and sugar prices are international prices and, thus, data regarding them could be made more specific for regionally diverse biopolymer producers.

Direct intensities may increase uncertainty significantly in non-hybrid models (Chen et al., 2018), but the present hybrid-model analysis suggest that process data for estimating sectoral input shares is even more relevant. Thus, improving IO data concerning environmental and economic extensions can be considered least important for reducing the bioplastics model's uncertainty (Figure 8, lower-right quadrant). The main problem here is that data for model extensions, necessary to build sustainability indicators, is only available on the aggregate sector level. For example, the value for direct fossil resource use concerns the coke and refined petroleum products sector, but only a value for refined petroleum products is needed for the model. Thus, aggregate values were split by sub-sector output values, not accounting for differences. The problem pertains to water use in the energy sector as well.

Variables related to quantities of inputs for biopolymer production and biopolymer prices were not found to significantly influence indicator results (Figure 6) and, hence, do not appear in Figure 8. It could be concluded that it would be sufficient to approximate these values via technical literature and market studies, even if they are not up to date. However, this can only be supported if there is more certainty about the uncertainty ranges of simulation inputs. In the present analysis, uncertainty ranges for prices were estimated with historical price data, which could result in overestimation of their true uncertainty and lead to a stronger impact of price variables on the uncertainty of simulation outputs compared to input quantities. Consequently, acquiring better information on probability distributions for all inputs is particularly relevant for analyzing the sensitivity of ex post indicators. By contrast, historical data may be better suited for estimating the sensitivities and uncertainties of ex ante indicators. The rather small uncertainty ranges assumed for input quantities in the model should be double checked with producers to gain more confidence in generated results.

In sum, the robustness of the indicators considered here for assessing bioplastics via a hybrid IO model can be improved by

- reporting prices for chemicals, vegetables oils, and starches more transparently, similarly to other biomass and energy prices;
- assigning statistical codes to economically significant bio-based products, such as TPS, Bio-PE, PHA, and Bio-PA;
- disaggregating the chemicals sector in IO tables to show differences in input structures;
- providing more specific environmental information on the plastics sector;
- providing regionally differentiated prices in international databases; and
- increasing sectoral resolution for environmental accounting in line with economic accounting.

What does the foregoing analysis of bioplastics imply for modelling further bio-based sectors? Analysis is most likely to be quite robust for bio-based industries that are sufficiently large to be represented in national and environmental accounts and, therefore, do not require a hybrid model. This may vary by country, but in Germany examples of such industries would include leather, paper, and wood products. If newer bio-based industries were to become the focus of sustainability assessments in the future, hybrid IO models combining product, process, and national data – albeit associated with some uncertainties – would be well-suited to inform decisions about what bio-based sectors could be properly modelled. Such assessments could integrate data and information for bio-based industries with high potentials for market penetration and reduction of environmental impacts, previously determined in industry studies and comparative product analyses, into an overall model of the economy, thereby indicating priorities for more systematic data collection. More robust indicators based on national economic-environmental analyses with greater sectoral resolution could, in turn, hint at sectors and products that are worth being explored in sector studies and environmental assessments specific to particular products.

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SUPPORTING INFORMATION

Table S1. Input values for estimating distributions of biopolymer quantities and prices. This information is used in the main simulations. Source: Interviews described in Jander (2022).

Biopolymer	*Domestic production and imports*			*Prices*		
	Mode (t)	Min.	Max.	Mode (€/t)	Min.	Max.
Bio-polyamide (Bio-PA)	4,000	63%	125%	8,000	88%	125%
Bio-polyethylene (Bio-PE)	16,667	80%	140%	2,200	68%	105%
Cellulose acetate (CA)	5,157	90%	110%	4,500	89%	111%
Polyhydroxyalkanoate (PHA)	7,830	80%	120%	5,430	74%	110%
Polylactide acid (PLA)	20,683	90%	110%	2,043	88%	108%
Thermoplastic starch (TPS)	42,500	100%	124%	3,000	67%	133%

Table S2. Inputs by sector into the production of different biopolymers (Bio-PA – bio-based polyethylene, Bio-PA – bio-based polyamide, CA – cellulose acetate, PHA – polyhydroxyalkanoate, PLA – polylactide acid, TPS – thermoplastic starch) and sources of price data. This information is used in the main simulations.

	Bio-PA	Bio-PE	CA	PHA	PLA	TPS	*Source for prices*
Food sector							
Castor oil	x						Import unit values, Germany, 2006-2020 (Destatis, 2020a)
Maize starch				x	x		Import unit values, Germany, 2006-2020 (Destatis, 2020a)
Potato starch						x	Import unit values, Germany, 2006-2020 (Destatis, 2020a)
Sugar		x			x		International sugar price, 2007-2020 (The World Bank, 2021)
Refined petroleum products sector							
Naphtha			x		x	x	Daily international naphtha price, 2007-2021 (finanzen.net, 2021)
Paraffin		x					Unit value, Germany, 2009-2018 (Destatis, 2020d)
Chemicals sector							
Acetic acid			x				Import unit values, Germany, 2006-2020 (Destatis, 2020a)
Ammonia	x						Import unit values, Germany, 2006-2020 (Destatis, 2020a)

Dimethyl carbonate				x			Unit value, Germany, 2009-2018 (Destatis, 2020d)
Hexamethylene diamine	x						Import unit values, Germany, 2006-2020 (Destatis, 2020a)
Natural gas					x	x	Unit value, Germany, 2009-2018 (Destatis, 2020d)
Sodium hydroxide	x						Import unit values, Germany, 2006-2020 (Destatis, 2020a)
Energy sector							
Heat	x		x	x	x	x	Germany, 2004-2019 (Statista, 2020b)
Electricity	x		x	x	x	x	Germany, 2000-2020 (Statista, 2020a)

Table S3. Selection of sectors as simulation inputs by indicators for bioplastics sector (b) and fossil-based plastic sector (f). Direct intensities and Leontief coefficients of these sectors are assigned probability distributions.

Sector name	*Classification number*	$tFRI_b$	$tFRI_f$	VA_b	VA_f	$Empl_b$	$Empl_f$	GHG_b	GHG_f	$Water_b$	$Water_f$
Crop/ animal production	A01							x	x		
Hard coal	B5.1									x	x
Lignite	B5.2									x	x
Crude oil/ natural gas	B06	x	x		x	x	x	x	x		
Stone/ sand/ clay	08 - 09									x	x
Food products	C10	x		x		x					
Paper/ paperboard	C17.2	x	x					x	x		x
Coke oven products	C19.1	x	x								
Refined petroleum products	C19.2	x	x					x	x		
Other chemicals and chemical products	C20*	x	x	x	x	x	x	x	x	x	x
Primary plastics, fossil-based	$C20.16_f$	x	x	x	x	x	x	x	x	x	x
Non-metallic mineral products (except glass)	C23.2 – 23.9								x		

Basic iron/ steel/ ferro-alloys and products of first processing of steel	C24.1-3		x								
Basic precious and other non-ferrous metals	C24.4	x	x								
Electricity, steam/ air conditioning supply	D35.1, C35.3	x	x	x	x	x		x	x	x	x
Gas	D35.2							x	x		
Sewerage	E37									x	x
Waste collection, treatment, disposal	E38									x	x
Land transport	H49				x		x				
Computer programming/ consultancy	J62 - 63			x		x	x				
Real estate activities	L68			x	x						
Legal/ accounting/management consultancy activities	M69 – 70			x	x	x	x				
Architectural/ engineering activities, technical testing/ analysis	M71						x				
Security/ services to buildings/ landscape/ business support activities	N80 – 82			x	x	x	x				
Public administration	O84.1 – 84.2						x				

Table S4. Minimum and maximum values of inputs into biopolymer production used for estimating distributions in the main simulations as a result of the auxiliary simulations.

Key statistics	**Inputs into biopolymer production (in million Euro) in 2016**			
	Food products	Refined petroleum products	Chemical products	Electricity and heat
(1) Static value	73.3	6.1	6.1	29.2
(2) Mode	64.6	7.1	4.5	29.2
(2) relative to (1)	*88%*	*116%*	*73%*	*100%*
(3) Minimum	41.6	1.7	2.7	20.4
(3) relative to (1)	*57%*	*28%*	*44%*	*70%*
(4) Maximum	102.0	11.7	5.7	35.3
(4) relative to (1)	*139%*	*191%*	*94%*	*121%*

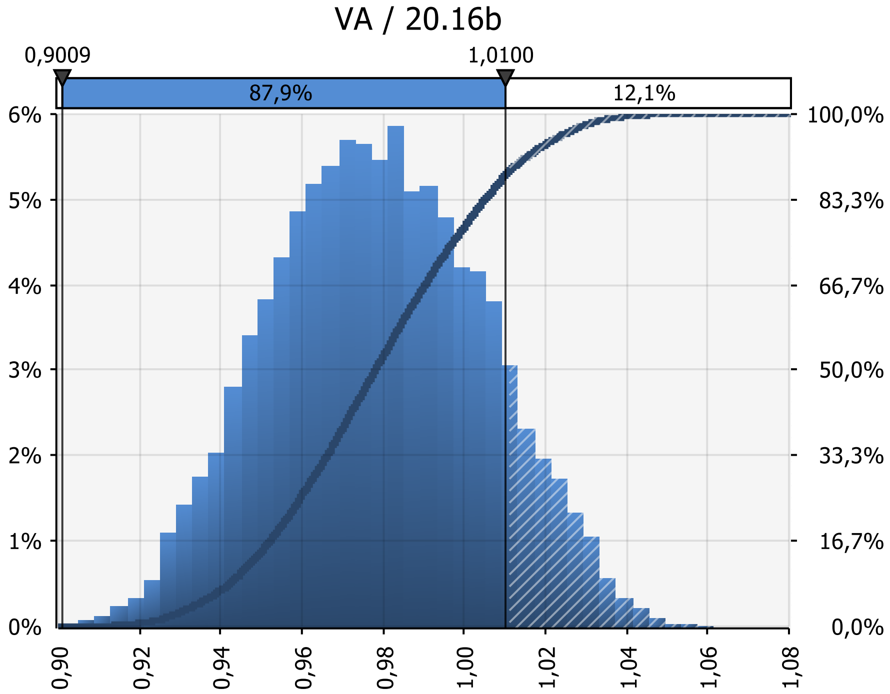


Figure S1. Probability distribution for the value added indicator and probability of lower value compared to the bioplastic model's static value.

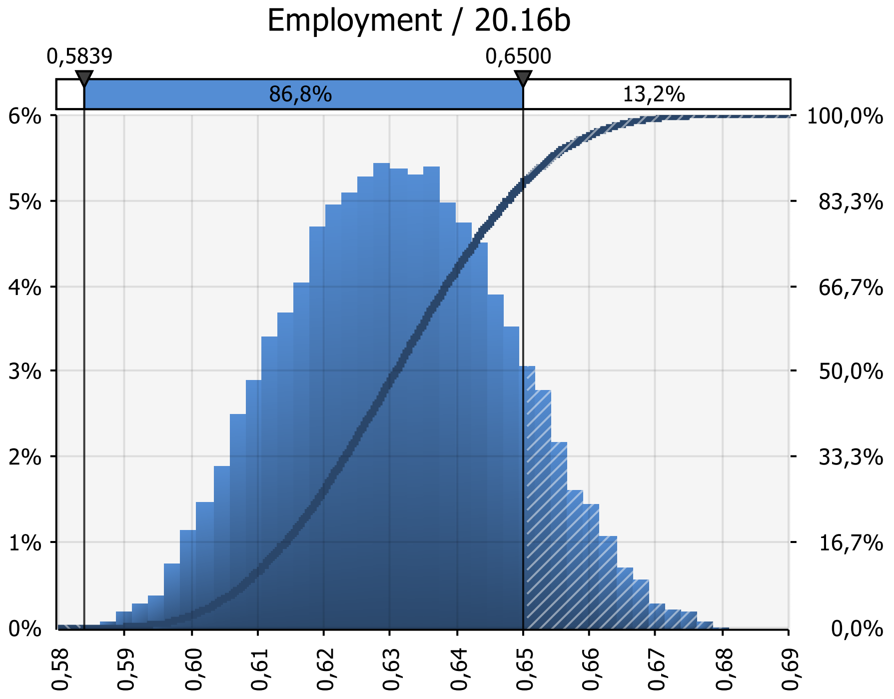


Figure S2. Probability distribution for the employer compensation indicator and probability of lower value compared to the bioplastic model's static value.

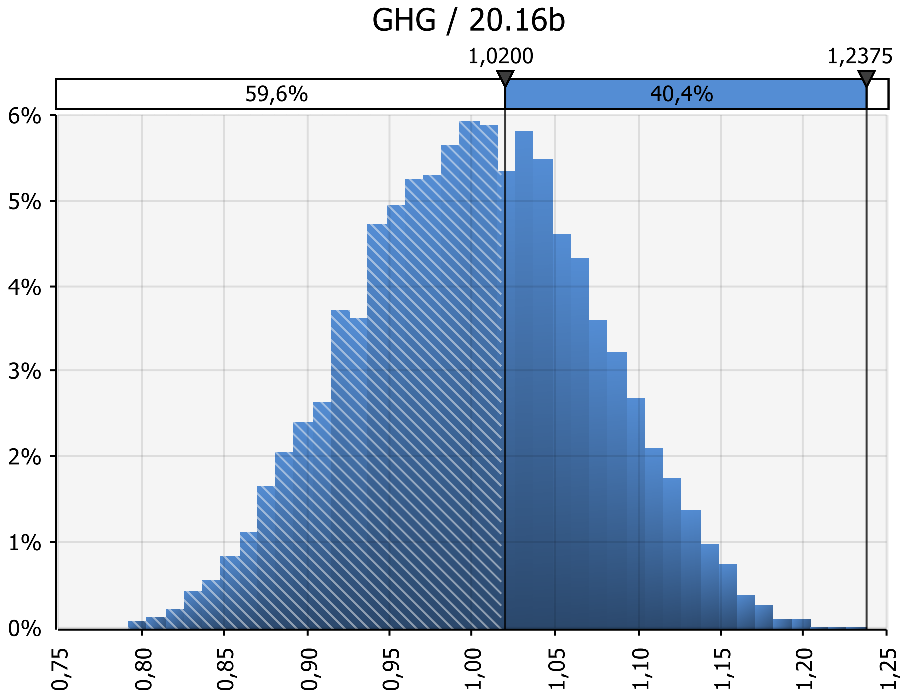


Figure S3. Probability distribution for the GHG emission intensity indicator and probability of higher value compared to the bioplastic model's static value.

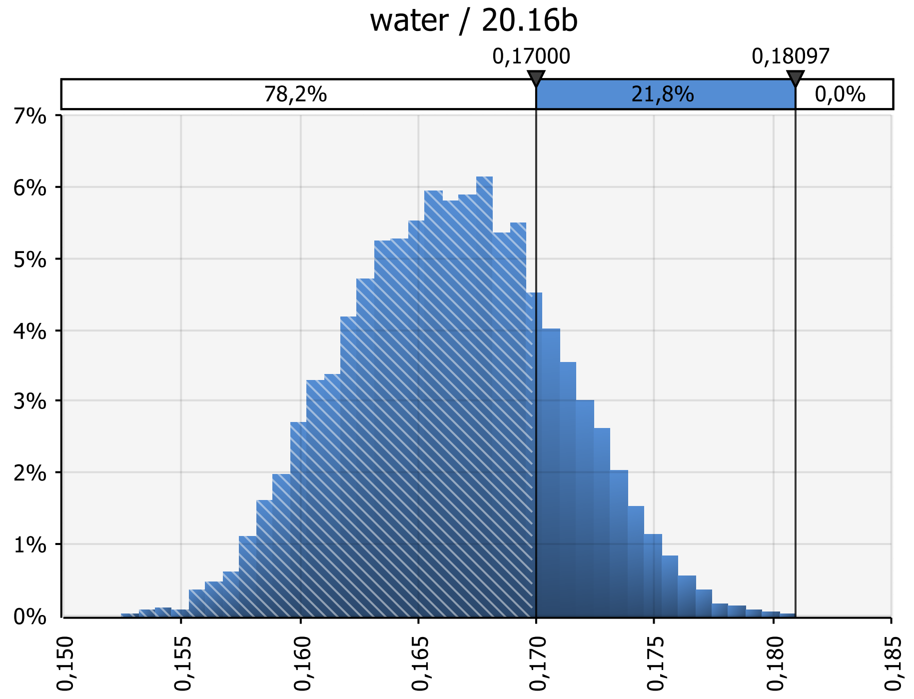


Figure S4. Probability distribution for the water use intensity indicator and probability of higher value compared to the bioplastic model's static value.

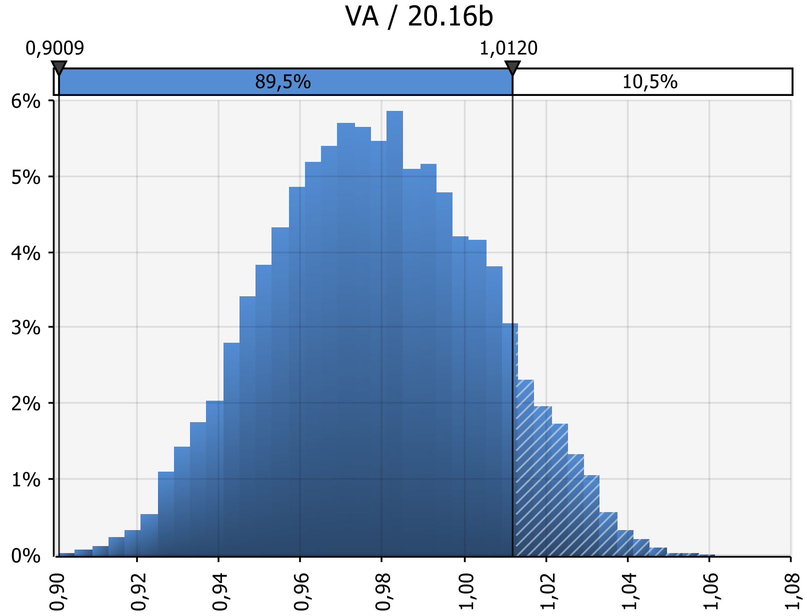


Figure S5. Probability distribution for the value added indicator and probability of lower value compared to the static value of the fossil-based plastic sector.

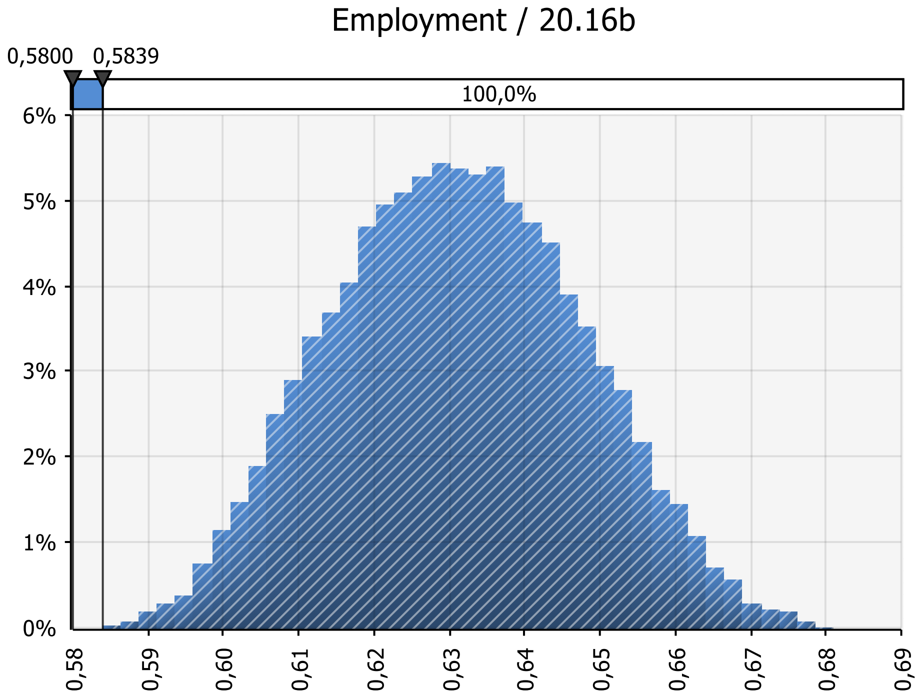


Figure S6. Probability distribution for the employment compensation indicator and probability of lower value compared to the static value of the fossil-based plastic sector.

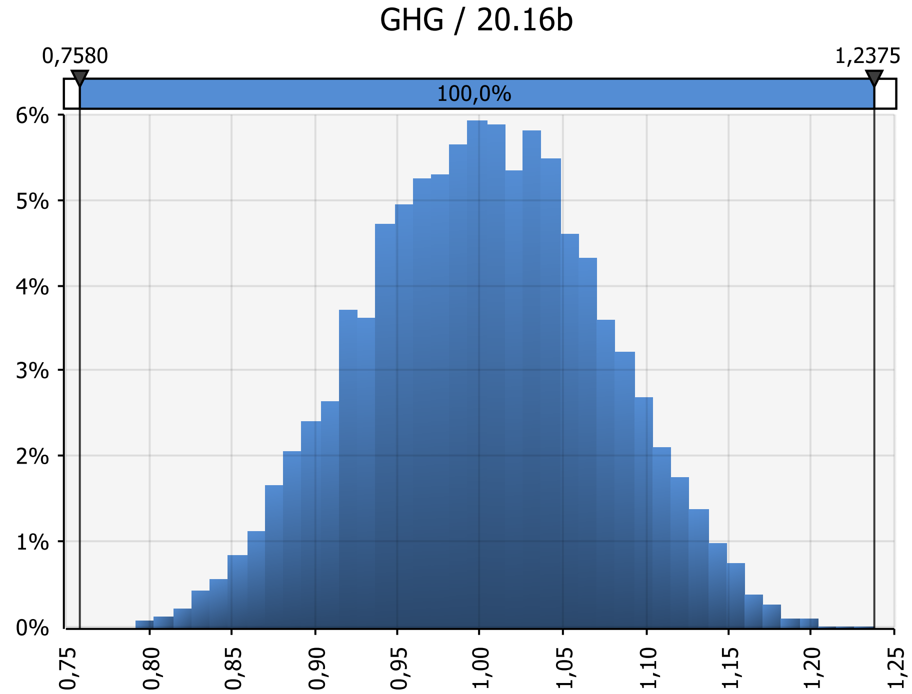


Figure S7. Probability distribution for the GHG emission intensity indicator and probability of higher value compared to the static value of the fossil-based plastic sector.

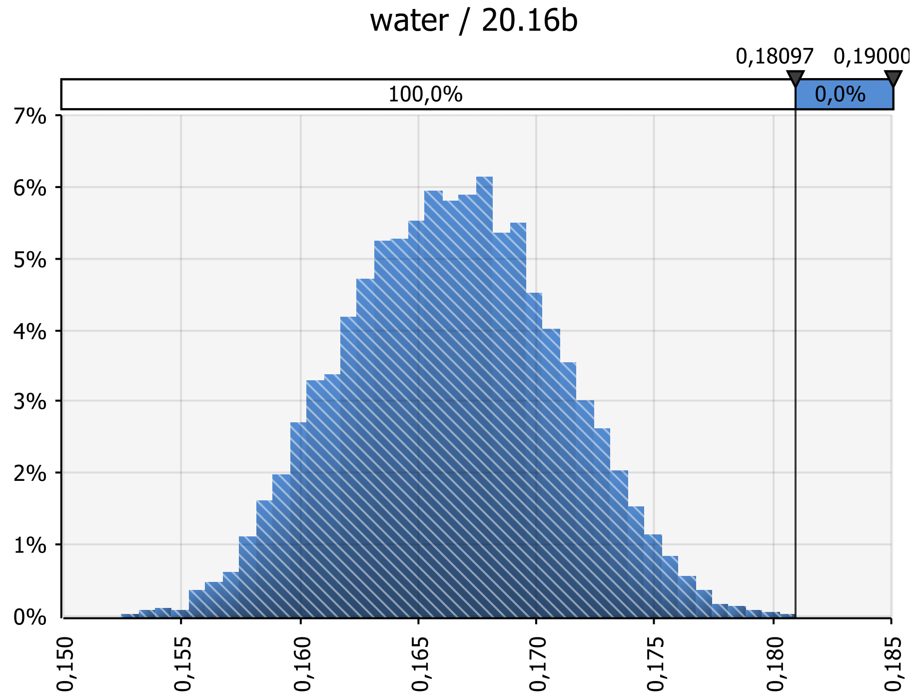


Figure S8. Probability distribution for the water use intensity indicator and probability of higher value compared to the static value of the fossil-based plastic sector.

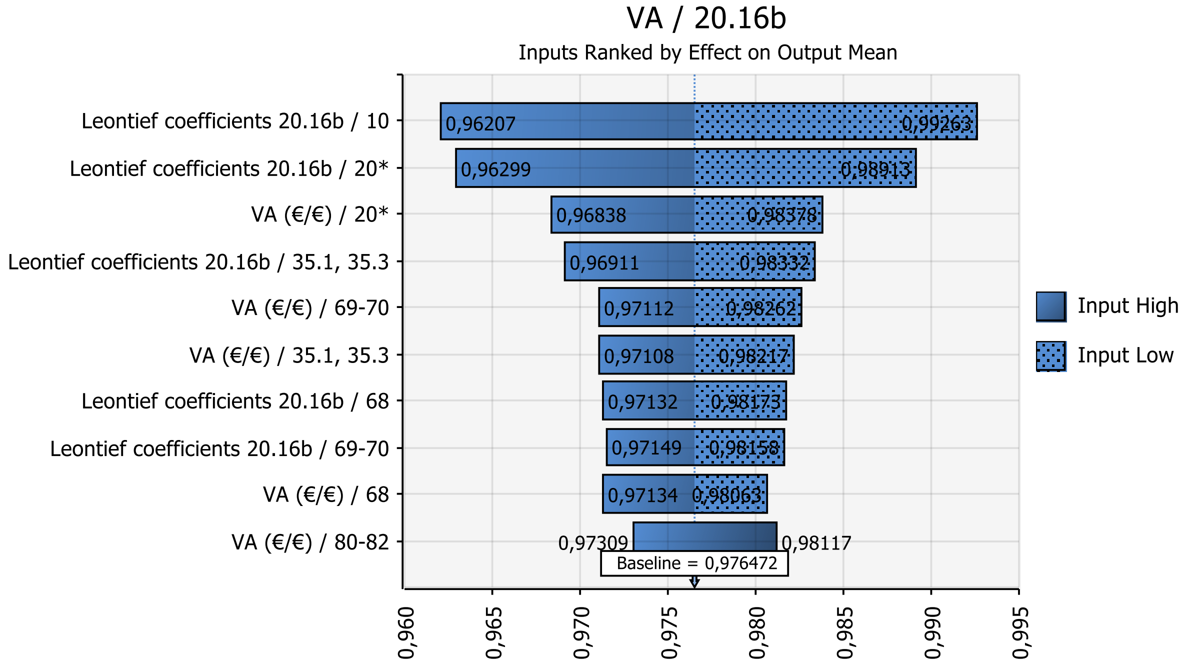


Figure S9. Tornado diagram for the value added indicator.

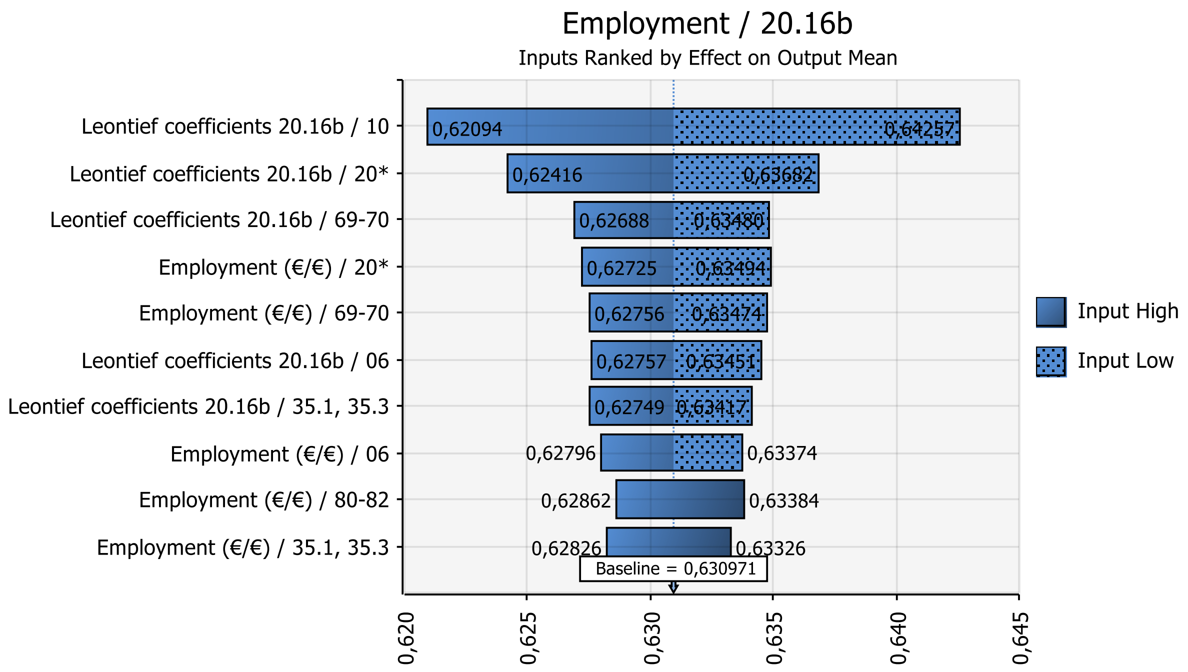


Figure S10. Tornado diagram for the employment compensation indicator.

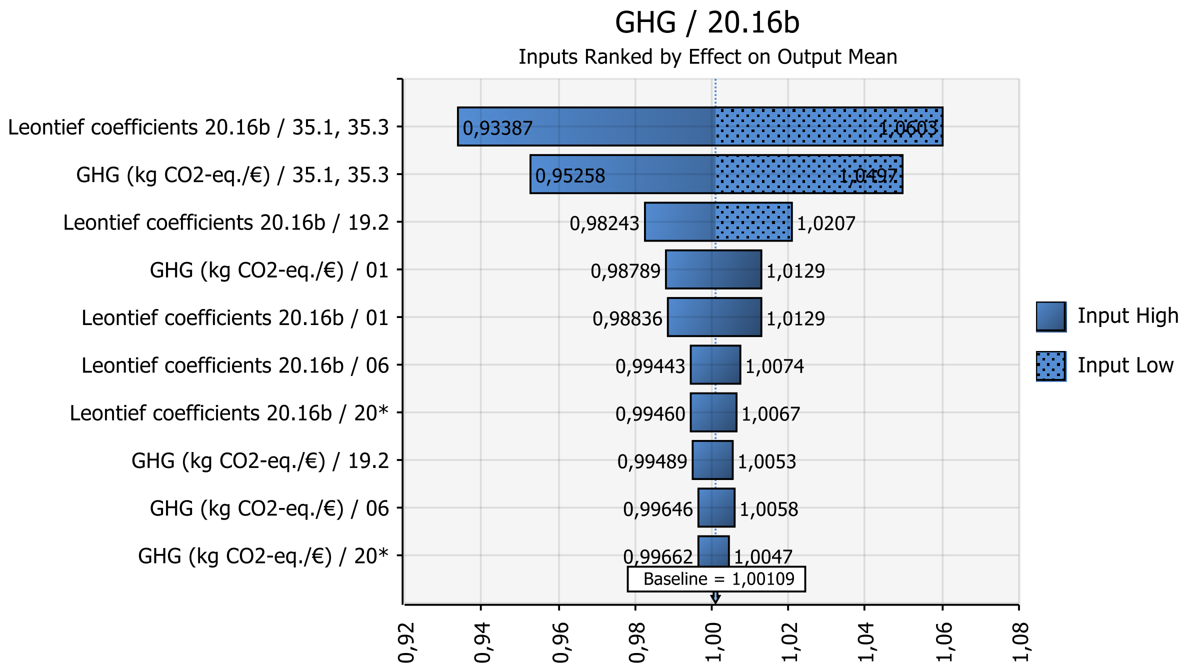


Figure S11. Tornado diagram for the GHG emission intensity indicator.

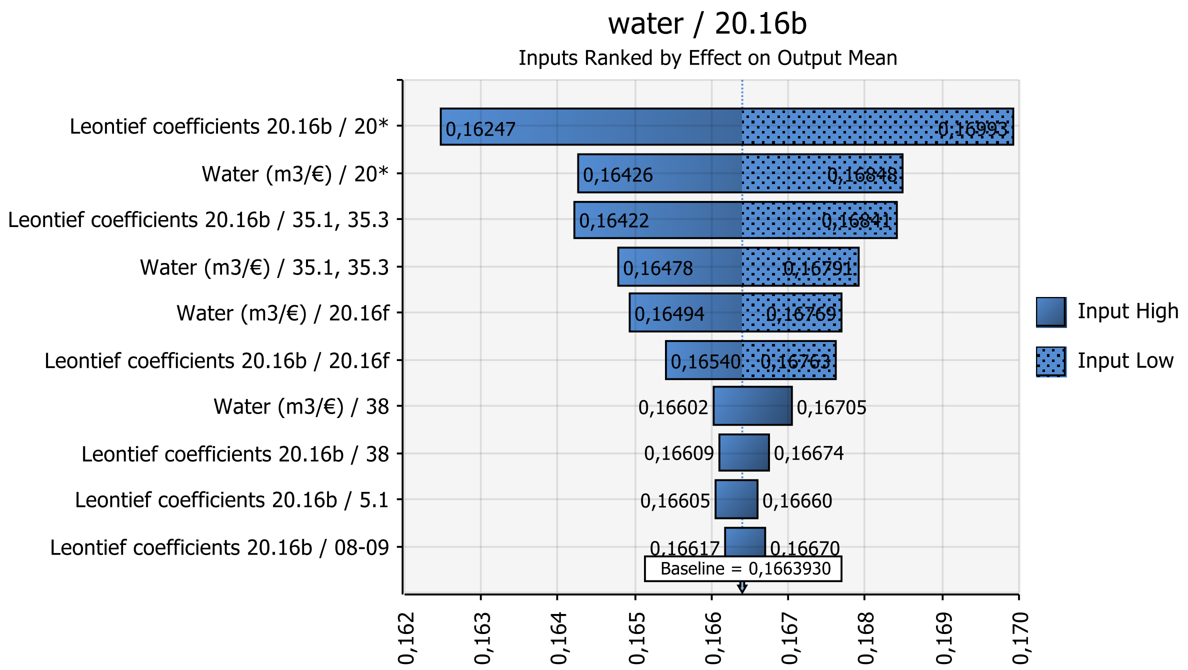


Figure S12. Tornado diagram for the water use intensity indicator.

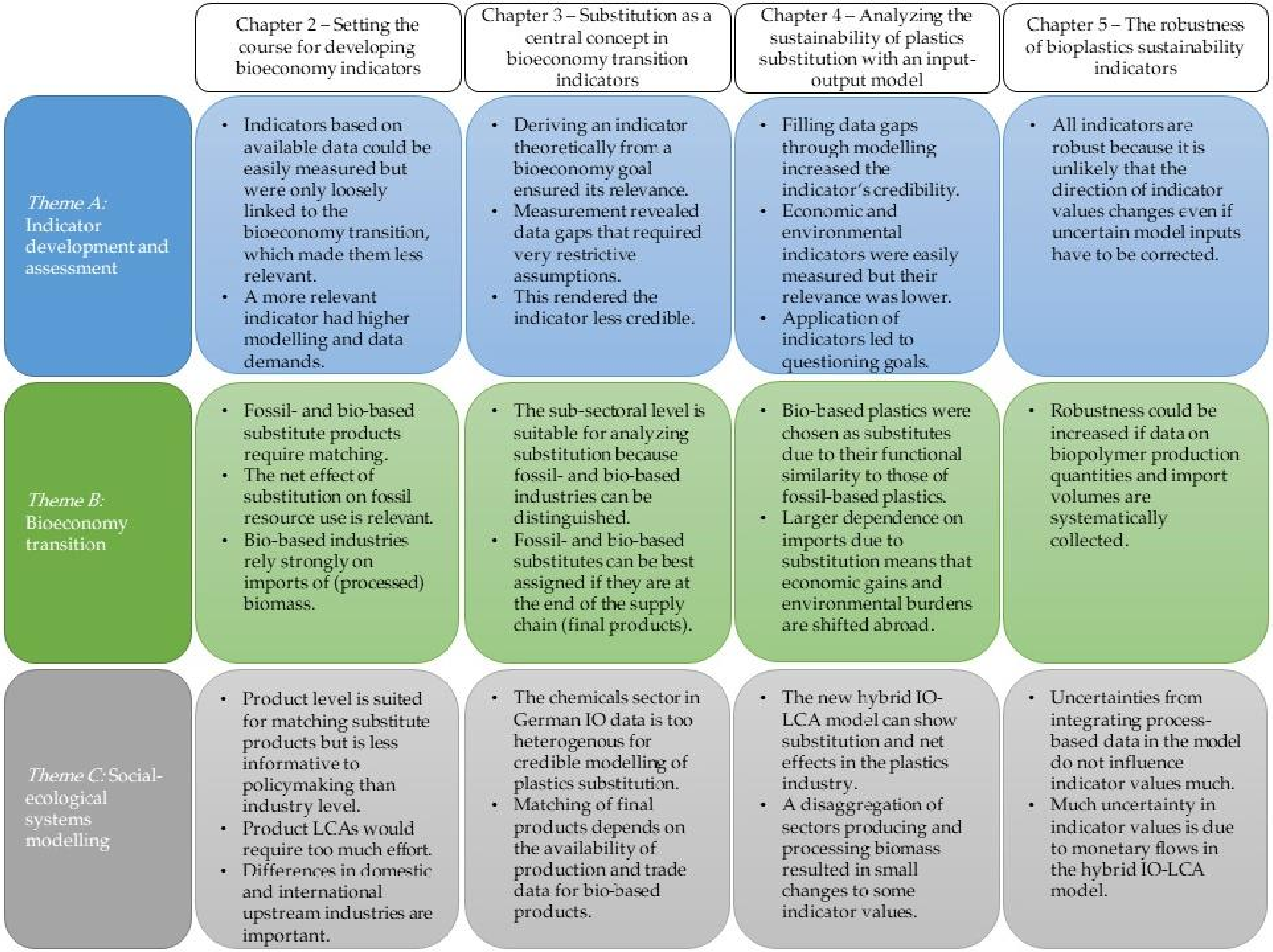
Chapter 6. Summary and integrated discussion

6.1 Summary of research results

Current bioeconomy monitoring systems are intended to provide information on the contributions of bioeconomies towards sustainable development but lack systematically and fully developed indicators for measuring the transition from a fossil-based to a bio-based economy. In chapters 2 through 5, I have sought to fill this gap by proposing how this kind of transition could be monitored while also responding to the general question "What enhancements in bioeconomy monitoring systems are necessary to support evidence-based policymaking oriented towards sustainable bioeconomy transition?" I have also developed and applied a set of indicators for transitioning from a fossil-based to a bio-based economy, thereby gaining insights into possible answers to the following research questions:

> RQ1: How can indicators for bioeconomy monitoring systems be developed so that they adequately fulfill indicator assessment criteria?
>
> RQ2: What are relevant considerations for monitoring transitions from fossil- to bio-based economies?
>
> RQ3: What quantitative model could be suitable for informing indicators for monitoring transitions from fossil- to bio-based economies?

These questions correspond to my general themes A, B, and C, as depicted in Figure 6-1 on the left side. In this chapter I discuss key results of the research presented in the previous chapters, which is also summarized in Figure 6-1.



	Chapter 2 – Setting the course for developing bioeconomy indicators	Chapter 3 – Substitution as a central concept in bioeconomy transition indicators	Chapter 4 – Analyzing the sustainability of plastics substitution with an input-output model	Chapter 5 – The robustness of bioplastics sustainability indicators
Theme A: Indicator development and assessment	• Indicators based on available data could be easily measured but were only loosely linked to the bioeconomy transition, which made them less relevant. • A more relevant indicator had higher modelling and data demands.	• Deriving an indicator theoretically from a bioeconomy goal ensured its relevance. • Measurement revealed data gaps that required very restrictive assumptions. • This rendered the indicator less credible.	• Filling data gaps through modelling increased the indicator's credibility. • Economic and environmental indicators were easily measured but their relevance was lower. • Application of indicators led to questioning goals.	• All indicators are robust because it is unlikely that the direction of indicator values changes even if uncertain model inputs have to be corrected.
Theme B: Bioeconomy transition	• Fossil- and bio-based substitute products require matching. • The net effect of substitution on fossil resource use is relevant. • Bio-based industries rely strongly on imports of (processed) biomass.	• The sub-sectoral level is suitable for analyzing substitution because fossil- and bio-based industries can be distinguished. • Fossil- and bio-based substitutes can be best assigned if they are at the end of the supply chain (final products).	• Bio-based plastics were chosen as substitutes due to their functional similarity to those of fossil-based plastics. • Larger dependence on imports due to substitution means that economic gains and environmental burdens are shifted abroad.	• Robustness could be increased if data on biopolymer production quantities and import volumes are systematically collected.
Theme C: Social-ecological systems modelling	• Product level is suited for matching substitute products but is less informative to policymaking than industry level. • Product LCAs would require too much effort. • Differences in domestic and international upstream industries are important.	• The chemicals sector in German IO data is too heterogenous for credible modelling of plastics substitution. • Matching of final products depends on the availability of production and trade data for bio-based products.	• The new hybrid IO-LCA model can show substitution and net effects in the plastics industry. • A disaggregation of sectors producing and processing biomass resulted in small changes to some indicator values.	• Uncertainties from integrating process-based data in the model do not influence indicator values much. • Much uncertainty in indicator values is due to monetary flows in the hybrid IO-LCA model.

Figure 6-1. Summary of research results by chapters and themes.

In **Chapter 2**, an insight gained into RQ1 is that easily measurable bioeconomy indicators may not be well connected to bioeconomy transition and, thus, are likely to be less relevant than other indicators. Although my co-authors and I show that it is possible with some additional data-collection effort to represent innovative developments in the bioeconomy by concentrating on chemicals industries rather than sectors that have always had a high bio-based share, this sectoral focus is not sufficient to properly represent the transition from a fossil-based to a bio-based economy. Meanwhile, an indicator that is conceptually closer and more relevant – the *fossil resource savings of a bio-based industry* – has higher modelling and data demands than all other indicators presented in Chapter 2. This points to a trade-off between the relevance of indicators and their ease of measurement.

There are two aspects missing in the other indicators that link the indicator *fossil resource savings of a bio-based industry* closer to the transition. First, they do not distinguish between bio-based surfactants that are meant to be substitutes for fossil-based surfactants and conventional bio-based surfactants that have always been bio-based. Growth in bio-based production does not necessarily mean substitution per se – only if fossil- and bio-based substitutes are identified. Second, differences in the use of fossil energy cannot be observed with available indicators. This would be important, however, to see whether substitution of surfactants results in substitution of resources and reduced net fossil resource use. Thus, the links between fossil-based and bio-based substitutes and their fossil resource flows are important considerations for monitoring the transition, which is a central finding related to RQ2.

In addition, the case study illustrates the importance of biomass origin and successive supply chain levels, revealing that (processed) biomass imports are very important to bio-based surfactant production in Germany. This needs to be considered in modelling because imported biomass may involve different production technologies than domestically produced biomass, thereby leading to differences in economic and environmental impacts.

A further issue related to RQ3 is determining the appropriate sectoral level in modelling. On the one hand, matching of substitutes at product level is most credible. On the other hand, aggregation to 4-digit level – a NACE[4] class – in monitoring is necessary because combination with standard economic indicators, based on economic statistics, is only possible at this level, and it is also more informative to policymaking than the product level. However, summing up LCA model results for each product of an industry is not a viable option, as this would require too much effort and unduly increases the cost of monitoring. Thus, a model should provide information for a whole industry but may require input from other available product-specific models.

A different approach to developing indicators was pursued in **Chapter 3**, in order to gain further insights for answering RQ1. Rather than developing indicators from available

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[4] NACE – **N**omenclature statistique des **A**ctivité économiques dans la **C**ommunauté **E**uropéenne (Statistical Classification of Economic Activities in the Euopean Community)

data, an indicator was developed theoretically by quantifying a single bioeconomy goal, which enabled inclusion of relevant dimensions and a more transparent quantification process. The results derived from Chapter 2 for RQ2 – that 1) bio-based substitute goods and 2) net effects of fossil resource use are key aspects of transition – then informed the adapted Bioeconomy Transition Framework (BTF). Focusing on a specific bioeconomy transition entailed changing some elements of the original framework created by van Meijl (2015). First, there was a shift from all bio-based goods to bio-based substitute goods and, second, an emphasis on the goal of reducing fossil resource dependence was added. From this, the *Substitution Share Indicator (SSI)* was developed, which compares bio-based and fossil-based outputs of an industry with their respective fossil resource flows. However, measuring the indicator with existing bottom-up and top-down models revealed its limited credibility, because very restrictive assumptions had to be adopted due to missing data.

This was particularly true for modelling plastics substitution with the top-down approach. The plastics industry was modelled using IO data for the whole chemicals sector due to the low resolution of individual sectors. Thus, with respect to RQ3, modelling substitution with German IO data is only possible for sectors that are relatively homogenous in terms of inputs, processes, and outputs, such as the refined petroleum products sector, which represents fossil-based transport fuels well. A very restrictive assumption was necessary to model primary plastics substitution with the top-down approach because it is part of the quite heterogenous chemicals sector in the IO data. The chemicals sector encompasses a range of very diverse outputs and cannot properly represent bio-based products because they form a small minority. One of two important insights distilled from Chapter 3 for RQ2 regarding transition monitoring is that the sub-sectoral level is necessary for measuring substitution. There are only a few sectors that are either fossil- or bio-based that can be compared directly and without modelling, such as substitution of paper products for plastic products. Most sectors in official German statistics include both fossil- and bio-based products together, especially the chemicals industry. Thus, more relevant and credible information can often be gained by analyzing sub-sectoral levels, which requires modelling. This does not apply to sectors that are homogenous in official statistics, which can be found in high-resolution IO tables of other countries.

The second insight related to RQ2 is concerned with the best supply chain level for measuring substitution. Matching of fossil- and bio-based substitute goods is most credible for final products, that is, at the end of the supply chain, as assumptions become more and more restrictive in upstream industries. For example, substitution of bioethanol for gasoline is plausible as there is no further processing. The biopolymer polylactic acid (PLA) could replace the fossil-based plastics PEHD, PELD, PP or PA, depending on how it is processed. Consumption-related indicators are also more relevant for policymaking because regulating consumption is a common policy target. However, informing RQ3, modelling of consumption-based indicators is only feasible if production and trade data for bio-based products is available. The *SSI* for transport fuels could be easily measured as a consumption indicator by subtracting exports and adding imports. This would not have been possible for plastics because the necessary data for bioplastics products was not available during the study.

In **Chapter 4** and with regard to RQ1, measurement using the theoretically developed *SSI* reveals that a relevant and credible indicator is possible if data gaps are filled through modelling, even though this compromises the indicator's ease of use. By contrast, economic and environmental indicators were easily measurable by extending the new model with available data, but their relevance could be increased with greater modelling efforts. This study also shows that measurement of indicators for one case, here plastics substitution, can lead to questioning the goal from which they were derived and suggest a reconsideration of goals. The *SSI* would be even more relevant if it not only oriented towards reducing dependence on fossil resources, an intermediate bioeconomy goal, but also to pollution reduction, the ultimate goal, for the case of plastics substitution.

Through analyzing the bioeconomy transition in the German plastics industry, characteristics relevant for answering RQ2 have been brought to the fore, which include important information for sub-sectoral monitoring. First, a suitable supply chain level for observing plastics substitution must be found. Building on Chapter 3, which reveals that a consumption-related *SSI* is currently not possible for plastics, I chose the intermediate level for primary plastics production. A requirement for bio-based substitutes is that they fulfill the same functions as their fossil-based counterparts, which is why it was not enough to include biopolymers as substitutes for fossil-based plastics. Rather, because biopolymers are compounded with fossil-based components, bioplastic materials that fulfill similar functions are better substitutes. Thus, this consideration of fossil-based parts in bioplastics production resulted in a lower *SSI* than when only including biopolymers. Descriptions of product groups in official classifications provide good orientation for identifying substitutes. This level downstream from biopolymer production required primary data collection and resulted in a new database for bioplastic material production in Germany. Second, as already indicated in Chapter 2, biomass inputs and import dependences are becoming more significant and require monitoring. The model's results reveal that plastics substitution can result in improved economic performance and lower water use but also in higher process GHG emissions throughout upstream supply chains. As most of the biopolymers for bioplastics production in Germany were imported, this implies that assessment of substitution needs to take into account domestic and foreign economic and environmental impacts of substitution in domestic industries.

Providing an answer for RQ3, the new hybrid IO-LCA model solved the problem of missing representation of fossil- and bio-based plastics industries in German IO data. The model is suitable for measuring indicators for substitution in the plastics industry and its impacts. It enables matching of substitute products at the level of industries, which is more plausible than matching highly aggregated sectors in input-output tables because the assumption of sectoral homogeneity can be relaxed to some extent. The model also accounts for different production technologies involved in imported and domestically produced biopolymers. In a modification of the base model, I modelled the upstream agricultural and food sectors in more detail, which had an impact on some indicators' results but did not change the direction of net effects.

In **Chapter 5** and with respect to RQ1, I have found that, even though measurement of relevant indicators requires modelling and additional data collection, the indicators developed in the study are relatively robust, meaning they cannot be easily manipulated. All of the indicators are robust because it is unlikely that the direction of indicator values would change, even though their magnitude might change if process-based data is corrected. Conclusions drawn from the deterministic model discussed in Chapter 4 are very likely to persist.

An interesting insight related to RQ2 is that biopolymer quantities are most uncertain among the process-based data, which consists of biopolymer prices, input quantities, and input prices, and are very influential according to a sensitivity analysis. Only input prices are more influential, but they are based on solid data and, hence, much more certain. Thus, robustness could be increased significantly if production quantities and import volumes of biopolymers were more certain.

Informing RQ3, the finding that all indicators based on the hybrid IO-LCA model are relatively robust shows that the model is adequate for monitoring. Uncertainties introduced by using process-based data do not affect indicator values much. This is because a wide range of data (sources) is combined in the model, and the indicators are only very sensitive to a few data inputs with lower quality. In the case of the plastics industry, this was only the price of dimethyl carbonate, which greatly determines the value of chemicals used in PHA production. One of the drawbacks of the model is its reliance on monetary flows, exemplified by the lower robustness of the *SSI* compared to the other indicators due to its dependence on naphtha prices. Naphtha is an input to TPS production, which is an important polymer in German bioplastics production, and its price fluctuates strongly. Higher naphtha prices translate into lower or even negative *SSI* values, whereas lower prices result in higher *SSI* values.

For the integrated discussion below, key results regarding the three themes should be kept in mind. Concerning Theme A, I found that bioeconomy transition indicators can be developed starting from a bioeconomy goal and then subsequently balancing trade-offs between indicator assessment criteria. Regarding Theme B, very relevant considerations for monitoring are 1) supply chain level, for matching functionally similar production outputs that are assumed to be substitutes, and 2) changes in the use of fossil and biomass resource inputs and import dependencies. Concerning Theme C, a suitable model could be one at the level of industries that is based on official statistics but includes more detail on a specific bio-based industry.

6.2 Integrated discussion of indicator development, bioeconomy transitions, and hybrid modelling

6.2.1 From data-driven to goal-oriented approaches for developing bioeconomy indicators

In this section, I discuss my results against the background of the overarching *Theme A: Indicator development and assessment*. A common challenge in developing sustainability indicators is that a "well-defined and transparent procedure leading from problem definition to indicator set to interpretation of the indicator values" is still lacking (Niemeijer and Groot 2008, p. 19). This also applies to the development of bioeconomy transition indicators, so here I compare the goal-oriented approach in this work to approaches suggested in the literature on the development of sustainability indicators. Niemeijer (2002) describes two general approaches, depending on the starting point for developing indicators, a "data-driven" and a "theory-driven" approach, acknowledging that there is a wide spectrum of approaches in-between. With data-driven approaches, available data is assessed, and indicators are selected or built from this data. Data-driven indicators are practical because they can be immediately measured. Theory-driven approaches consider first theoretical links between a goal and an indicator and generally result in "best possible" indicators that may have considerable data gaps (Niemeijer 2002, p. 91). While data availability is considered the most important assessment criterion for data-driven indicators and relevance is key for theory-driven indicators, the aim of all fully developed indicators should be to fulfill theoretical, methodological, practical, and political requirements (Meyer 2011). In the research presented here, development of the *Substitution Share Indicator (SSI)* followed a goal-oriented approach, which can be considered theory-driven because theoretical considerations regarding the links between the bioeconomy goal of "reduced dependence on fossil resources" and measurable indicators were explored first, before scanning available databases. I have proposed that the *SSI* sufficiently meets four out of five of the EC's RACER criteria, as it is relevant, credible, easy, and robust. Its relevance to users, or whether it is "accepted" (EC 2017a), requires further attention. By contrast, development of indicators for measuring the German bioeconomy transition's sustainability followed a data-driven approach. They were developed by extending the hybrid model with data on sectoral water use, GHG emissions, employee compensation, and value added, which are easily available from official German statistics. However, they can be considered less relevant than the *SSI*.

The following discussion focuses on the question of how the goal-oriented approach pursued in the research considered here can be improved to result in even more relevant indicators that can be used in the policymaking process. Goal-oriented approaches are also favored in the literature on developing sustainability indicators, which includes some important additions to the approach pursued here, particularly taking into consideration the importance of the planning phase, the interrelated nature of theory- and data-driven approaches and the need for an iterative process, and the involvement of stakeholders.

Frameworks are essential for planning indicator development. Dietz and Hanemaaijer (2012) argue in favor of making significant efforts in planning indicator selection by describing four steps prior to it, including problem definition, specification of goals, assessment of resources available for achieving goals, and analyzing trade-offs between issues, goals, and resources. Similarly, McCool and Stankey (2004, p. 295) emphasize that "what *should be measured* (a normative issue)" should be publicly debated before selecting "what *can be measured* (a technical issue)", though the order is often reversed in practice. In this vein, many sustainability indicator initiatives in rural Canada have been found to be data-driven and do not reflect local priorities and perspectives very well (Lowery et al. 2020). A conceptual framework can summarize the results of this preparatory work, facilitating indicator selection and development. Similarly to the approach taken here, Eisenmenger et al. (2016) show how a comprehensive set of resource efficiency indicators can be derived from a conceptual framework, while Llorente-González and Vence (2019) illustrate how a data-driven approach not using a framework can result in a narrow set of circular economy indicators that does not represent important dimensions of systemic change. By focusing on recycling, current EU circular economy indicators emphasize preservation of materials and not of functions, which woould be sharing for example (Moraga et al. 2019). Frameworks are also powerful tools for assessing and selecting indicator sets that can better represent the state of the environment because they structure the interrelation of single indicators as opposed to unassociated indicators (Niemeijer and Groot 2008; Moraga et al. 2019).

In addition, my research shows that frameworks may require adjustment. Indicator development and exemplary measurement for the plastics industry has revealed the need for specifying frameworks and goals. In the German case study, substitution of bioplastics for fossil-based plastics for reducing fossil resource dependence was shown to only be meaningful if it addresses the largest problem of plastics consumption, which is environmental plastics pollution. By contrast, the contribution of plastics substitution to climate change mitigation is much less relevant compared to energy substitution. Thus, the goal of a "reduced dependence on fossil resources" needs to be related to at least two higher goals – namely, reducing terrestrial and marine pollution and climate change mitigation – each requiring a different set of indicators.

Some intermediate steps combining goal-oriented and data-driven approaches could enhance the approaches taken here. First, existing indicators could be assessed, selected and adjusted before new indicators are developed. "Selection" here means that indicators have already been fully developed previously and have a solid database, which can be considered a data-driven approach. "Development" means that new indicators are designed by taking into account specific criteria. Depending on the criteria chosen, this development process can be data-driven or goal-oriented. Eisenmenger et al. (2016) first select indicators based on RACER assessment, then recommend how they could be adapted to be more relevant to the concept of resource efficiency, and third identify any need to develop new indicators. Pülzl et al. (2012) divide development of sustainability indicators for the forest-based sector into two phases. In the first, indicators are developed or selected from existing sets and, in the second, indicators are redefined based on modelling requirements and data availability.

Apart from such a small loop in indicator development, where theoretical and practical requirements are balanced in an iterative process, a larger loop is recommended between suggesting an indicator and adjusting goals. Developers should allow for repeating all steps of planning and indicator development (Dietz and Hanemaaijer 2012). As argued above, the development and application of the *SSI* revealed that the indicator can support formulation of more specific bioeconomy goals. This, in turn, may require adjustment of the indicator. For example, the *SSI* currently includes biodegradable as well as non-biodegradable bioplastics. If a bioeconomy goal is to reduce pollution, the indicator could focus on those bioplastics that can reduce pollution if substituted for fossil-based plastics. Apart from increasing the relevance or ease of use of indicators, an iterative process allows them to be adjusted "to emerging societal norms and priorities as well as knowledge about the physical system" (Rametsteiner et al. 2011, p. 64). This is especially important because the normative dimension of sustainability has for some time been acknowledged as a challenge to indicator development (Rametsteiner et al. 2011).

Continuous stakeholder involvement in indicator development is important because it makes social norms more explicit and can increase acceptance. If indicators are well accepted, they are more likely to be included in decision-making and have an influence on action, fulfilling their ultimate purpose. Consequently, public opinion and debates should be considered in the planning phase (Dietz and Hanemaaijer 2012), and early stakeholder inclusion already during problem definition could improve quality and acceptance of indicators (Turnhout et al. 2007). An analysis of "science-led" indicator development processes shows that policymakers are underrepresented and that scientists select indicators not based on explicit criteria or their own expertise but rather consensus. This may result in indicators with lower acceptance levels and implicit inclusion of social norms. Meanwhile, norms and political priorities are made more explicit in indicators "led by intergovernmental processes". However, these processes do not automatically lead to better-accepted indicators if the indicators themselves are not directly linked to concrete policy measures (Rametsteiner et al. 2011). It is important to involve scientists, the public, and policymakers because "selecting indicators is a collaborative process and pursuit that represents the best possibility for revealing diverse, often competing, public interests" (McCool and Stankey 2004, p. 304).

With regard to the bioeconomy as such, the importance of stakeholder involvement becomes obvious when comparing bioeconomy visions in official policy papers with those supported by German and Austrian stakeholders from research, business, NGOs, and public administration. They differ quite a bit, with policies tending to support a capitalist vision and many of the other stakeholders favoring a sufficiency vision (Hausknost et al. 2017; Zeug et al. 2021). Another group, primary producers in the agricultural, forestry, and fishery sectors, are currently not being properly taken into consideration in European bioeconomy strategies (Park and Grundmann 2022), although agriculture fulfills important social functions as well as ecological ones (Nowack et al. 2021), implying that their inclusion in developing indicators is all the more important. In more advanced stages of indicator development, data collectors and tool developers should be involved so the process can be a "shared learning experience" (Pülzl et al. 2012, p. 45).

In the initial phase of developing the German monitoring system, stakeholders from research, business, and society were involved in a workshop in 2017 to discuss relationships between the bioeconomy transition and sustainable development goals (Zeug et al. 2019). The outcome of this discussion was considered in a framework that forms the basis of current German monitoring (Egenolf and Bringezu 2019). Similarly, stakeholders were asked in 2018 about their expectations regarding a European monitoring system and what themes and problems it should address (Robert et al. 2020). Later in the development of the German system, researchers were asked via an online survey to evaluate a pilot report containing a preliminary set of indicators (Zeug et al. 2021).

However, there are limits to stakeholder involvement, and what groups are involved at what steps in the process is important. For example, public interest in sustainability indicators in Guernsey only started when indicators had already been developed and were being applied. There, starting "top-down" with an initial development by experts and subsequent refinement by stakeholders proved to be feasible (Mcalpine and Birnie 2007). Another case, analyzing development of quality-of-life indicators in North East England, revealed that participation can lead to struggles and end up severely impeding the process (Scott and Bell 2013). Thus, both "technocratic" and "values-oriented" approaches should be transparent regarding problem definition, indicator development and aggregation, the experts involved, uncertainties and sensitivities, and failings of indicators (Reid and Rout 2020; Saltelli et al. 2020).

What, then, could be a general process for developing bioeconomy transition indicators that are relevant to policymaking? The research presented here is in line with other studies emphasizing the predominant role of relevance in indicator development. This discussion has shown that 1) methodological and practical aspects need to be considered in close conjunction to keep monitoring costs low and 2) frequent interaction with potential users can increase acceptance and lead to indicators that can effectively inform policymaking. Relevant indicators usually require iterative adjustments during their development, considering what is possible in modelling and data collection and what is desired by stakeholders. Ignoring these dimensions of the process is likely to thwart any efforts to develop indicators that will actually be used in policymaking. The nature of the exploratory studies presented here did not allow for large-scale stakeholder involvement or much iteration due to money and time constraints, which is a common challenge in research projects (Rametsteiner et al. 2011). Nevertheless, in Chapter 7.1 I conclude by proposing a general procedure for indicator development for monitoring sustainable bioeconomy transitions that is based on the presented research and discussion.

6.2.2 Bioeconomy: transition or business as usual?

In this section, I discuss my results against the background of the overarching *Theme B: Bioeconomy transition*. "Transition" has become a buzzword in political and scientific discussions (Hölscher et al. 2018). This is also true for discourses on bioeconomy. But what is a bioeconomy transition, as opposed to a bioeconomy that is not really a transition but, rather, business as usual? In section 1.2.2, I summarized three dominant visions of bioeconomy transition found in literature, of which the transition from a fossil-based to a bio-based economy is one. In answering RQ2, summarized in section 6.1, I have found that a central concept of this kind of transition is substitution. Whether substitution can actually support bioeconomy transition is discussed in the following, where I discuss what transition is considered to be in sustainability and bioeconomy research and what views on substitution might support a real transition.

"Transitions" in the context of sustainability research are defined as "radical shifts to new kinds of socio-technical systems" that can contribute towards solving environmental problems – including climate change, loss of biodiversity, chemicals pollution, and resource depletion – rather than "incremental improvements and technological fixes" (Köhler et al. 2019, p. 2) that ultimately maintain the status quo. Socio-technical systems or regimes are meso-level production and consumption sectors that fulfill societal needs, such as food, transport, and housing (Geels 2004) and that cannot be reduced to any specific products or production processes (Audet 2014). Quite to the contrary, these systems are complex, irreversible, characterized by non-linear interactions between many individuals, firms, and organizations, and driven by innovation, new consumption behavior, and changes in governance systems (Markard et al. 2012; Pyka et al. 2022a). Changes in these systems relate to "technology but also changes in consumer practices, policies, cultural meanings, infrastructures, and business models" (Geels 2018). Such radical innovations that can support transitions stand in contrast to incremental innovations, which improve current practice but do not depart from existing paths (van Driel and Schot 2005). An alternative view on transitions focuses less on technological innovation and more on social innovation created by civil society movements and communities (Audet 2014; Silva and Stocker 2018).

Contemporary bioeconomy developments are not considered true transitions in the literature because they do not require significant changes to economic systems. An increased use of biofuels, for example, has not resulted in less fuel consumption and may, on the contrary, have led to growth in the fuels sector through rebound effects (Birch 2019; Bocken et al. 2022). Currently, the bio-based economy relies on management and control by technical experts ("technocratic management") and optimized solutions ("technological fixes"), which increase resource use efficiency and economic gains while reducing emissions to the environment (Blok 2018). There is a danger that ethical considerations are ignored, however, such as alienation between animals, farmers, and citizens in precision livestock farming (Blok 2018). Similarly, innovations in animal production and manure utilization focus on efficiency, technological fixes, and competition being considered inherently desirable (Friedrich et al. 2021). This is also reflected in a review of LCA studies of bio-based products (Talwar and Holden 2022), the authors of which argue that LCA studies often support incremental changes in practice, although more fundamental changes are discussed in their theoretical parts. Béfort et al. (2019, p. 438) found that a "green growth lever", which focuses on increasing profits and economic growth, is not reconcilable with a "transition lever", which requires more fundamental changes in production modes. There are a few businesses, some of them bio-based, that have been pursuing a combined circular and sufficiency strategy, but these cases are rare (Bocken and Short 2020; Bocken et al. 2022).

Bioeconomy transition is oriented towards circularity and sufficiency in order to stay within ecological boundaries while, at the same time, fulfilling societal needs. A circular bioeconomy that includes biological cycles must include sufficiency strategies because current levels of fossil-based consumption cannot be sustained (Giampietro 2019; Bocken et al. 2022; Stegmann et al. 2020). The ability to properly follow the five principles of circular biomass use (safeguarding ecosystems, avoiding non-essential products and waste, prioritizing the fulfillment of basic needs, recycling byproducts, and reducing non-renewable energy use) requires “fundamental changes to policies, technologies, organizations, social behaviour and markets” (Muscat et al. 2021, p. 561). In addition, bioeconomy transitions “not only require technical innovation, but also institutional and organizational innovations” that support sustainable business models (Adamseged and Grundmann 2020, p. 16). Businesses implementing a true bioeconomy transition “make use of the knowledge and networks of the fossil era and are characterized by co-existence, mutual learning, and new forms of collaboration” (Pyka et al. 2022b, pp. 35–36).

All of this requires much negotiation between societal groups because conflicting values and imperfect information make actual implementation difficult. According to some recent studies, stakeholders in Austria, Germany, Sweden, Colombia, Rwanda, and Thailand favor a socio-ecological transformation over continued economic growth (Hausknost et al. 2017; Zeug et al. 2021; Johnson et al. 2022; Zander et al. 2022). Although people surveyed in Germany prefer to undertake such substantial changes, they are also concerned about increasing prices and declining living standards, which shows that it is important to involve civil society in bioeconomy transition discourses (Zander et al. 2022). Another survey has found that views among the German population itself are more diverse than those of experts and that the potential for societal conflict is large, leading to the conclusion that participatory approaches are essential (Eversberg and Fritz 2022). A similar conclusion has been drawn for a circular bioeconomy transition because there are controversies surrounding biorefineries (Starke et al. 2022). A social-ecological transformation requires a fundamental change in “values, imaginaries, and beliefs”, which “must be negotiated and harmonized” (Friedrich et al. 2021, 15;17). In the context of manure utilization within a bioeconomy, for example, this means discussing “self-determination of farmers, future generations’ right to develop and evolve, animal ethics, or indigenous land rights in Southern America” (Friedrich et al. 2021, p. 18). In Germany and India, strong ideas regarding technological fixes are prevalent in two bioeconomic case studies, so the authors suggest replacing these with “socioecological fixes”, which put technical solutions in the context of societal and ecological problems through discourses and transdisciplinary research (Friedrich et al. 2022, p. 593). A “new responsible professionalism” can better solve complex problems than “technocratic management” because values ascribed to nature and those of different stakeholders are acknowledged (Blok 2018).

Based on the foregoing discussion, bioeconomy visions (see section 1.2.2) can be considered to promote more-than-nominal transitions if they are not merely focused on technical innovations to improve resource use efficiency but also consider circularity, sufficiency, and the involvement of society. In the case of transitioning from a fossil-based to a bio-based economy, this essentially depends on the understanding of "substitution", which is discussed next.

A narrow concept of substitution concentrates on substituting inputs where biogenic instead of fossil resources can be used, which is not sufficient for supporting bioeconomy transition. In the German and EU bioeconomy strategies, for example, "replacement of fossil raw materials" (BMEL 2020, p. 10) and enhancement of "our capacity to substitute fossil raw materials" (EC 2018a, p. 6) is envisioned. In the same vein, Linser and Lier (2020, p. 2) point out that "the bioeconomy focus has shifted in the last decade from a relatively narrow economic concept that aims to replace fossil resources with renewable raw materials to a wider sustainable and circular bioeconomy concept". In a typology of bio-based innovations, "substitute products" do not have new functions, are hence not disruptive, and "can be fed into existing value chains" (Bröring et al. 2020, p. 4). Substitution strategies are mostly considered insufficient for a transition, which also requires sufficiency strategies (Bocken et al. 2022). The statement that "a fossil-based industry is replaced by a bio-based industry which takes completely the place of its predecessor offering the same products and services, while economic structures are not affected" (Pyka et al. 2022a, p. 2) is another example of a narrow conceptualization of substitution that supports the business-as-usual vision.

Bioplastics usually do not induce modification of consumption behavior, such as a reduction of single-use plastics, or waste management. "Drop-in innovations", such as bio-based polyethylene or biofuels, are "presented as sustainable" but "maintain the existing paradigm" (Befort 2021, p. 2). A preference for "within-category substitutes", meaning from the same taxonomic category, that are equivalent in quality to conventional products has been observed for food products (Huh et al. 2016). A similar substitute is more likely to be selected than a dissimilar one (Arens and Hamilton 2018), such as the way consumers typically prefer replacing polyethylene bags with bio-polyethylene bags than with paper or canvas bags, because one of the most important functions of plastic bags, impermeability to water, is fulfilled. But this kind of plastics substitution is unlikely to change consumption preferences or behavior. Bioplastics also do not currently contribute to a more circular economy. To the contrary, using PLA, PHA, and PEF poses the risk of lower plastics recycling rates if they disturb established processes (Hiebel et al. 2018; Alaerts et al. 2018; Di Bartolo et al. 2021). There might even be a trade-off for bioplastics between saving fossil resources and circularity.

Substitution of systems that fulfill societal needs, focusing on outputs rather than inputs, is a broader concept that is more consistent with real bioeconomy transition. It can also be described as a replacement of one sociotechnical system by a new one that is more sustainable. Geels and Schot (2007) and Geels et al. (2016) explain in a typology of transition pathways the role that landscape changes in political, economic, or cultural structures and technological niche-innovations play for changing systems. Systems are replaced if pressures on the landscape level give existing niche-innovations the chance to become dominant (“technical substitution path”) or initiate the development of niche innovations (“de-alignment and re-alignment path”). From this perspective, technological innovation leading to input substitution (narrow concept) can still play a major role in the substitution of systems (broader concept). “Substitute products”, as described in Bröring et al. (2020), refer to a narrow concept but from a broader view the innovation types “new products”, “new processes”, and “new behavior” can lead to substitution if they are disruptive. The case of meat and dairy substitutes shows that “substitutionism” (Palmer et al. 2022, p. 2), the replacement of final products that change value chains, can be disruptive to agricultural production and interests. By contrast, “appropriatonism” refers to the replacement of production technologies intended to improve efficiency that is not disruptive, such as feed supplements (Palmer et al. 2022).

Such a systems perspective requires meso-level indicators that are able to show the fulfillment of societal needs and bridge micro indicators, focused on products and services, with macro indicators at the level of economies or sectors, by taking a “function perspective” (Alaerts et al. 2019, p. 365). Products and services provide certain functions that can be fulfilled using many different strategies. For example, a car and related services enable mobility, a function which can be fulfilled through carsharing. Meso-level indicators are more relevant to policymakers within the context of the circular economy because they provide more direct feedback on the impact of policies and innovations but are, unfortunately, missing from current monitoring frameworks (Alaerts et al. 2019). There is some evidence that consumers find “cross-category substitutes” – meaning from a different taxonomic category but serving the same need – more satisfying if substitutes are not exactly the same as conventional products. One explanation is a “negative contrast effect” of “within-category substitutes”, meaning a more obvious replacement with an inferior product (Huh et al. 2016). For the example of plastic bags, this means that consumers might prefer transport of goods via paper or canvas bags or even bike or car to starch-based bags. Dissimilar substitutes are also more effective in terms of replacing consumers’ desire for a given conventional product because differing attributes become more important (Arens and Hamilton 2018).

Taking this broad view of substitution, the transition from a fossil-based to a bio-based economy could thus refer to substitution of “bio-based” systems for “fossil-based” ones. From this perspective, “bio-based” no longer refers to a biogenic resource base but means that production and consumption promote efficient recycling through industrial symbiosis where “non-human ‘natural’ ecosystems [are] models for industrial activity” while at the same time respecting ecological boundaries (Lifset 2009, p. 4; Bijon et al. 2022). “Fossil-based” means “linearization of material and energy flows with the goal to overcome the low pace and density of biological transformations” (Giampietro 2019, p. 143) and a “predominantly linear – extract-use-dispose logic of production” (Starke et al. 2022, p. 1). Substitution in a narrow sense that does not affect consumption behavior or waste management can be considered fossil-based, even if fossil resources are replaced by biogenic ones. From this point of view, it can be argued that bioplastics can contribute to a bioeconomy transition to a limited extent. Consequently, the biopolymer PLA could be considered a “functional innovation”, which “fulfills equivalent functions, from a systemic perspective, favouring low-tech and degrowth options", because its biodegradability offers new possibilities for waste treatment (Befort 2021, p. 2). If composting infrastructures are available and used, this could simplify waste management and return carbon to soils rather than to the atmosphere (Di Bartolo et al. 2021). However, adjusting waste management is currently difficult and, thus, the use of bioplastics is currently not more circular than the use of fossil-based plastics (Alaerts et al. 2018), especially because fossil-based polymers can also be biodegradable. A new indicator for the circularity of bioplastics has been applied to biodegradable mulch films (Razza et al. 2020). The use of some biodegradable plastics products can result in increasing sustainable consumer behavior. For example, the availability of compostable bags for purchasing fruit and vegetables has induced some consumers to reuse these bags for separating organic waste from residual waste (Arbeck et al. 2022). Hence, more compost can be produced and less waste incinerated. In addition, fewer plastic particles have been found in compost when substituting biodegradable bags for polyethylene bags (Kern et al. 2020). Lower absolute consumption levels due to higher prices of bio-based products compared to fossil-based ones is conceivable for some products that are less essential, but evidence for this is not yet available. The role of consumers in bioeconomy transitions, specifically responsible usage and disposal, has not yet gained much attention in research to date (Wilke et al. 2021). Concerning consumption, which is an important "pull factor for a sustainable bioeconomy", two main factors seem to influence decisions: behavioral costs and personal motivations (Otto et al. 2021, p. 8).

Here I have shown how transitions are conceptualized in sustainability and bioeconomy research and that adopting a broader meaning of substitution can support transitions. Meanwhile, a monitoring system that focuses on "with-in category", "drop-in" substitutes hardly challenges existing sociotechnical systems. The example chosen for this study, bioplastic materials, can be considered a "bio-based" product being implemented in a "fossil-based" way of thinking and behaving. Some necessary adjustments to the indicators developed here – which are geared towards circular business models and the consumption perspective (Alaerts et al. 2019) and, thereby, to a genuine bioeconomy transition – are proposed in Chapter 7.

6.2.3 Priorities in hybrid IO-LCA modelling for measuring indicators

In this section, I discuss my results against the background of the overarching *Theme C: Social-ecological systems modelling*. The purposes of monitoring determine the kinds of models suitable for measuring indicators. Models can be used to predict, explain, describe, develop theories, illustrate, draw analogies, and support social learning (Edmonds 2017). Yet, the purposes of the EU and German monitoring systems are not clearly stated in their bioeconomy strategies. The wording "to track […] progress" (EC 2018a, p. 18) and "measuring […] the process of transformation" (BMEL 2020, p. 54) indicates that the main purpose of monitoring is to describe and explain developments. Potential users of a EU bioeconomy monitoring system stated that they need it to prioritize, receive information, persuade, and network (Giuntoli et al. 2020). Hence, I assume within this thesis that this kind of bioeconomy monitoring is first and foremost intended to show past and present rather than future developments. Hybrid IO-LCA models are sufficient to model such developments, have relatively low modelling demands and, thus, have relatively low monitoring costs. Short- to medium-term changes can also be predicted with models integrating a CGE model (Többen et al. 2022; van Meijl et al. 2018; Machado et al. 2020). Long-term structural changes involving alteration of economic structures due to innovation and changing consumer preferences require different models and could be analyzed with system dynamics (Morales et al. 2022) and agent-based modelling (Pyka et al. 2022a). In the following discussion, I explain why the bioplastics hybrid IO-LCA model is suitable for monitoring bioeconomy transitions and explore how it can be further improved to fulfill modelling requirements.

The bioplastics hybrid IO-LCA model is compatible with current monitoring efforts, as it is based on the same official statistical classification systems (SNA, SEEA) and can provide more detail than previous models regarding innovative bio-based industries, which has been identified as a major gap (Mainar-Causapé et al. 2021). Modelling bio-based chemicals industries, such as the bioplastics industry, can improve methods that estimate the bio-based share of downstream industries. Thus far, the bio-based share of an industry has been estimated with the share of input supplied by sectors that are completely bio-based, notably agriculture and food, ("input-based approach") or from expert estimation ("output-based approach") (Kuosmanen et al. 2020; Cingiz et al. 2021). However, the complexity of final products in many sectors makes estimation of their bio-based shares very difficult because there are no direct agricultural and food inputs, and the number of different products is very large. For example, bioplastics and bio-based rubber may be used in the manufacture of cars, but input-output tables only show inputs for plastics and rubber as such, not differentiating by fossil- and bio-based inputs. While experts can estimate the bio-based share of bioplastics, this is much more difficult for cars containing bioplastics elements. The advantage of inserting process-based data into IO tables can be illustrated through the example of the plastics products industry. Cingiz et al. (2021) estimate the value added of bio-based plastics and rubber industry by considering direct inputs of bio-based rubber and cellulose but not bio-based plastics. This results in a value added of bio-based plastics and rubber products that is about 20% lower (EUR 338 million, according to Cingiz et al. 2021) than the value added derived with the bioplastics model developed here (EUR 405 million). By including information from the bioplastics model on the bio-based share in modelling downstream sectors, complex value chains can be sufficiently represented without much additional effort. In this way, bio-based substitute sectors can be compared to corresponding fossil-based sectors with more accuracy, especially consumption sectors such as the one for plastic goods. Thus, disaggregating the chemical sector is key to accounting for bio-based chemicals in the downstream production of almost all industries of an economy. This has also been recognized by recent efforts to represent the EU chemicals sector in more detail by combining official statistics with market and company data as well as data from the literature and expert interviews (Baldoni et al. 2021).

Further developing the bioplastics hybrid IO-LCA model presented here will help to better satisfy the requirements of monitoring and modelling bioeconomies. Broadly speaking, these requirements include the topics of climate change, biodiversity, circular use of biomass, consumer behavior, and innovation and technological change (Pyka et al. 2022a). Within the potential of IO models, representation of carbon cycles and the circular economy can be improved.

Net GHG emissions of substitution is similar to the concept of a "carbon footprint" as defined by Wiedmann and Minx (2007) but include other gases in addition to carbon dioxide, making it a "climate footprint". For the purposes of this study, net GHG emissions of substitution will be defined as emissions generated by the bioplastics industry directly and indirectly through demand for upstream products reduced by the GHG emissions saved due to lowering fossil-based plastics production. Because bioplastics require higher energy use in the model and the German energy sector is fossil-intensive, GHG emissions are higher compared to fossil-based plastics. The chosen primary plastics industry is at the end of the supply chain considered, which is a cradle-to-gate system in which upstream industries are well represented. The carbon footprint of plastics within this system boundary has been found to be considerable, contributing greatly to the GHG emissions of the plastics supply chain, as plastics are mainly produced in coal-based economies (Cabernard et al. 2022). However, although positive and negative emissions in the rest of the life cycle may also be important, they were not considered in the bioplastics model. The model does not include a) direct GHG emissions of downstream sectors such as the plastics products industry, b) biogenic carbon storage in durable final goods and life extension due to consumption behavior shifting towards reuse, c) reduced air emissions due to waste treatment such as composting, and d) biogenic carbon storage in soils and plants. In this regard, the issue of biogenic carbon accounting for bio-based products has been debated among LCA researchers (Pawelzik et al. 2013; Finkbeiner et al. 2013; Brandão et al. 2013).

Major differences between bioplastics and fossil-based plastics in modelling can be expected for waste treatment and carbon sequestration, whereas differences in GHG emissions of downstream industries and consumption are likely to be small because bioplastics can often be processed and used very similarly to fossil-based products. Singh and Bakshi (2014) suggest consideration of carbon sequestration induced by economic activities, where negative emissions due to sinks (farmland, ranchland, forestland, grassland) are combined with the positive emissions of agricultural, forestry, and food sectors, reducing the GHG emissions of biomass-based downstream sectors. They also argue for improving representation of nitrogen cycles by including not only nitrogen losses but also other nitrogen flows (Singh and Bakshi 2015, 2013). Results from comparing fossil- and bio-based plastics in terms of GHG emissions depend very much on end-of-life management of products, according to findings from the process LCA literature (Zheng and Suh 2019; Brizga et al. 2020). In product LCA models, GHG emissions from different end-of-life options could be better compared in LCAs of bio-based and recycled plastics by using corrective terms (Tonini et al. 2021; Spierling et al. 2020). In an IO model, GHG emissions of plastics were calculated for the downstream industry "manufacturing of plastics and rubber products" and three end-of-life options ("recycling", "incineration", "landfill") using EXIOBASE database. End-of-life options provide a minor contribution to the carbon footprint of fossil-based plastics (Cabernard et al. 2022), but IO models comprehensively comparing fossil- and bio-based plastics are currently missing. Apart from climate change, chemicals pollution and biodiversity loss are considered major challenges (UNEP 2021) that are being focused on by few IO models (Persson et al. 2019; Moran et al. 2016; Marques et al. 2017).

Monitoring a bioeconomy transition that is increasingly circular is to some extent possible with hybrid IO-LCA models. Some aspects of circularity have been included in IO models, as summarized by Aguilar-Hernandez et al. (2018). Management of post-consumption waste such as recycling can be analyzed with waste IO models, which are based on tables that have additional rows and columns for waste types and treatment methods (Nakamura and Kondo 2009; Lenzen and Reynolds 2014). In a multiregional analysis, an overview of global solid waste, its treatment, and flows embodied in international trade has been provided by Tisserant et al. (2017). Similarly, waste treatment strategies and their environmental impacts have been assessed in a sub-national analysis for Australia (Fry et al. 2016). Meanwhile, the quality of recycling and the supply-demand balance of secondary materials are analyzed in a dynamic waste IO model (Nakamura and Kondo 2018). Product lifetime extension is accounted for in IO models by adjusting final demand for reduction strategies and input coefficients in production sectors, especially input of maintenance activities. Resource efficiency strategies can be analyzed by reducing input coefficients while keeping output constant. Aguilar-Hernandez et al. (2018) conclude from their overview that waste IO models are the most suitable framework for representing circular economies and call for hybrid monetary-physical tables and higher sectoral resolution.

In an application of a hybrid IO model, Towa et al. (2021) have assessed environmental impacts of different circularity strategies for Belgium and its regions. The strategies reuse, repair, remanufacturing (3R) and use intensification performed best, whereas design improvement and sharing had a smaller impact, and delayed replacement had no effect (Towa et al. 2021). Circularity of fossil-based plastics has also been assessed with a hybrid IO model in which data on the production and end-of-life management of plastic packaging are combined with an IO model for the EU. Plastics waste, only recycled at a rate of about 35%, has been found to be higher than in official statistics and is hardly used for new packaging. Further research is needed regarding the functions of plastics in applications and consumer use of plastic packaging (Cimpan et al. 2021). A material flow analysis of the main fossil-based plastics in the EU and Switzerland has shown that almost half of the primary plastic PET and one fifth of PP is used in textile products. Incineration is still the preferred waste management method for PEHD, PS, and EPS, while both landfilling and incineration are used for the other plastic types. PVC is the most recycled primary plastic (Kawecki et al. 2018). New waste types and treatment methods that arise due to bioplastics production are presented in several reviews of process-based LCAs, including for example industrial composting and anaerobic digestion (Spierling et al. 2020). Thus, process-based LCAs and EW-MFAs can be informative for adjusting the hybrid IO-LCA model for bioplastics to improve representation of circularity.

The hybrid IO-LCA model for bioplastics developed in the research presented here can be a valuable supplement for bioeconomy monitoring systems, but some recent methodological advances need to be included prior to its integration. Based on this discussion of requirements and current approaches to addressing shortcomings, I propose in Chapter 7 how my bioplastics model could be advanced methodologically.

Chapter 7. Conclusions, recommendations, and further research required

7.1 Conclusions regarding how bioeconomy monitoring systems can be enhanced

Based on the foregoing discussion, I propose that the research presented in this thesis forms a sound basis for further advancing bioeconomy monitoring systems so that they can support policymaking that is oriented towards sustainable development. Enhancements in bioeconomy monitoring systems have become necessary in terms of systematic indicator development, agreement on desirable characteristics of bioeconomy transitions, and quantitative modelling. The case study of a transition from a fossil-based to a bio-based plastics industry presented in this thesis reveals that quantification with systematically developed indicators that are both relevant and measurable is possible. Against the background of the research results summarized in 6.1 and the topical discussions in 6.2, here I draw conclusions for each of the three major themes explored throughout the thesis (Theme A: Indicator development and assessment, Theme B: Bioeconomy transition, and Theme C: Social-ecological systems modelling), starting with more practical issues of method development and ending with a systematic procedure for indicator development.

Theme C: Modelling bioeconomies with hybrid IO-LCA models requires improved representation of carbon flows and post-production processes. In my bioplastics model, carbon flows can be better represented by, for example, extending the system boundary from primary plastics production to plastic goods production or even further. More process-based emissions could be accounted for in this way. The bioplastics model in its current form, available plastics material flow analyses, and process information on processing bioplastics can be used to estimate bio-based shares of downstream sectors and related direct GHG emissions. Carbon sequestration and other natural processes can be included in the model by disaggregating the agriculture, forestry, and food sectors and giving credits in the direct GHG emissions data. End-of-life options can be included if the underlying supply and use tables are augmented with waste types and waste treatment sectors. Changing consumption patterns regarding particular plastic products can be represented by adjusting final demand and input coefficients. These advancements would not only have an impact on net GHG emissions of substitution but also enable monitoring of circular product flows.

Theme B: Indicators need to reveal circularity and sufficiency developments in order to support bioeconomy transition. With the *Substitution Share Indicator (SSI)* and related sustainability indicators, these developments can be observed to some extent. The *SSI* shows lower demand for plastics in general if it increases due to declining fossil-based plastics production and constant or increasing bioplastics production. Recycling of plastics means that less input from fossil-intensive industries will be used and more from the waste treatment sector, which is much less fossil-intensive, and will be reflected in a lower fossil resource intensity for the plastics industry. Depending on the use of recycled plastics in fossil-based and bio-based plastics production, the *SSI* could increase or decrease. If fossil-based plastic producers were using recycled material and bioplastics producers virgin material, the *SSI* could decrease and even become negative. Prior to making decisions based on the *SSI*, evaluation with contextual information is necessary, such as whether production has shifted to another industry or country. Contextual information is also necessary for assessing whether a bioeconomy transition from a fossil-based to a bio-based system is fulfilling societal needs while respecting ecological boundaries. As the discussion on bioplastics shows, indicators can either support a "fossil-based" system that is linear and focused on economic growth or a "bio-based" system that supports circularity and sufficiency. Output-oriented indicators for such a bio-based system would require increased attention and could complement the rather input-oriented *SSI* and sustainability indicators, resulting in an even more comprehensive set of indicators. Extending Figure 1-6 (section 1.3.2) in Figure 7-1 below shifts the focus from intermediate production that uses fossil resources, chemicals and chemical products, to final use. It is advisable to observe developments in the construction industry and related impacts on plastics production, for example.

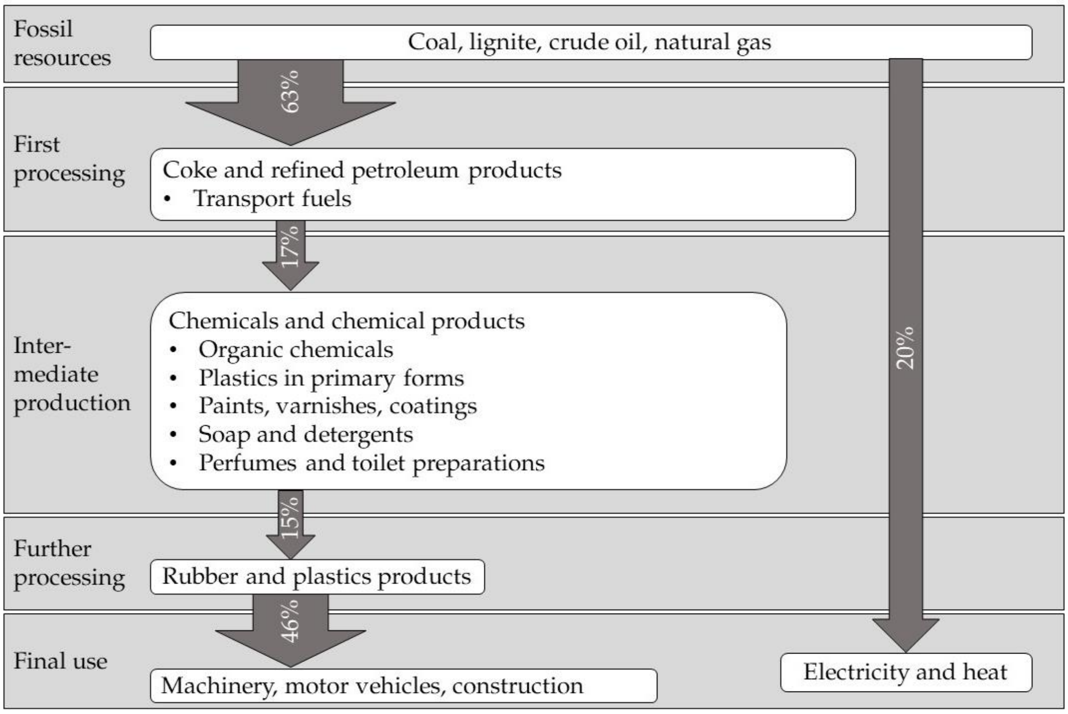

Figure 7-1. Shares of fossil resource use in the German economy, from extraction to final use, in 2014. Source: Own graphic, based on Destatis (2015).

Theme A: Indicator development for a bioeconomy monitoring is a process that needs to be goal-oriented, iterative, and inclusive. Current bioeconomy indicators sets, including the one detailed here, require further development to become even more relevant, as my conclusions regarding themes B and C illustrate. I began this research with a linear approach, illustrated in Figure 1-5 in 1.3.2, and now suggest a recursive one, illustrated in Figure 7-2. A linear approach is shown in Figure 7-2 with the sequence 1-2-3 in black. Blue elements in Figure 7-2 correspond to conceptual aspects, the red one to methodological, and the yellow one to empirical concerns. The elements "stakeholder inclusion" and "selection of available indicators" and linkages between all elements have been added in light of the discussion in Chapter 6. A minimum process consists of the steps along solid arrows, which means that stakeholders are at least informed about indicator development. Additional steps are indicated with dotted arrows, which represent feedback by stakeholders and subsequent adjustments to indicators. This may result in additional smaller or larger loops. The scheme is formulated from the perspective of scientists developing indicators and tools who seek to ensure that other actors become involved in the process as well. Apart from scientists, stakeholders can include statisticians collecting and preparing data, policymakers using developed indicators in decision-making, and other societal groups being affected by policies such as businesses and consumers. Input from the latter group can be particularly important in the planning stages of developing a framework (1a-1b) and theoretical indicator development (1-1d-1e). If collection of new data is necessary, businesses also need to be involved in step 2a-2b, but statisticians usually play the central role in practical indicator development. Policymakers can give important inputs in the planning stage (1a-1b) and at the beginning of indicator development (1-1d-1e). After a pilot phase, indicators should be assessed according to selected criteria and require approval by all stakeholder groups in step 3a-3b. Goals and targets may then be revised, as reflected in an adapted framework (3c). If step 3c is not necessary, the process ends with the "selection of suitable indicators" and completed indicators are ready for continuous monitoring.

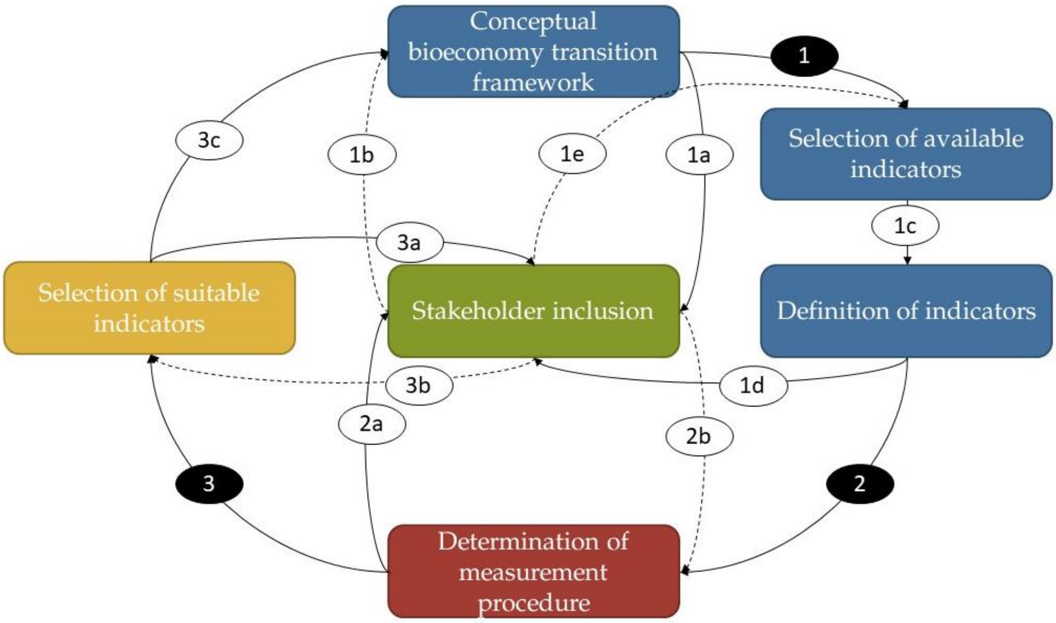

Figure 7-2. Enhanced approach to indicator development. Source: Own graphic, based on Meyer (2011, p. 200).

7.2 Recommendations to bioeconomy monitoring system developers and policymakers

These conclusions have implications for developers of bioeconomy monitoring systems and policymakers. Current bioeconomy monitoring systems could benefit from adjustment of underlying their frameworks. The DIR framework, developed in 2015 (van Meijl 2015), was adapted in Chapter 3 here and by Kardung et al. (2021), but a more fundamental revision of frameworks that reflect specified goals and causal networks is advisable. For example, recent discussions suggest that bioeconomy goals should be more explicitly related to sustainable development goals and targets (Heimann 2019; Linser and Lier 2020; Ronzon and Sanjuán 2020; Calicioglu and Bogdanski 2021). Furthermore, current monitoring efforts assessing and selecting indicators, as described in Giuntoli et al. (2020, p. 51), could focus more on developing new, even more relevant indicators, as attempted with the *SSI* in this research. As time and resources for such monitoring systems are limited, specific questions and user groups could be targeted, with modelling efforts being channeled accordingly. For this, relevant user groups must be identified, and the most important issues need to be discussed in depth with potential users. Although stakeholder workshops and online surveys have been conducted, they have not included specific feedback on the value of available indicators or suggestions for improvement. Also, to my knowledge, none of the stakeholder involvement processes mentioned in the literature describe stakeholder selection, that is, why groups and individuals are considered stakeholders or users of a particular bioeconomy monitoring system.

Furthermore, the success of bioeconomy monitoring systems depends on support from policymakers. First, their involvement is crucial for the development of relevant indicator sets that can provide useful information for decision-making. Second, more funding for setting up such a system can enable increased involvement of stakeholders, harmonization of different monitoring efforts, and automatization of modelling. Current funding for bioeconomy research projects in Germany mainly supports technology development and assessment and not so much inclusion of civil society through transdisciplinary research (Bogner and Dahlke 2022). Funding is necessary if data collected for this thesis and elsewhere is to be added to existing virtual laboratories. The quality of indicators could be much improved by collaborating via open source software (Pauliuk et al. 2015b; Lenzen et al. 2017), especially for Germany where official data is highly aggregated in supply and use tables.

7.3 Further research required regarding the effectiveness of monitoring

Diverse efforts are necessary to ensure that bioeconomy transitions actually do move along a sustainable development trajectory rather than being reduced to business as usual. Carefully designed monitoring systems can be supportive in such efforts by improving the information base for decisions on all levels. This thesis seeks to meaningfully contribute towards improving our understanding of current bioeconomy monitoring systems, while providing a solid foundation for their further advancement. Many questions regarding biomass-related sectoral sustainability strategies and policies and their effective measurement deserve attention in the future. In the center of Figure 7-3, I suggest a different monitoring system that is oriented towards showing the main strategies of sectors fulfilling societal needs to reduce environmental impacts. Sectoral sustainability strategies, for example, could be analyzed along value chains from producers to consumers. One of the strategies of the plastics industry has been taken as an example in this thesis: substitution with bio-based plastics. Another one is use of recycled materials. For other industries, a recent study has shown how companies' organizational strategies try to support sufficiency (Bocken et al. 2022). A new set of indicators, as has been designed to measure achievements made in circular mobility (Alaerts et al. 2019), could make visible industrial environmental strategies and enable comparisons between sectors. For this, the major challenges revolve around identification of the needs fulfilled with plastic products, the value networks associated with them, and the strategies being pursued to make them (more) sustainable. Furthermore, relevant indicators need to be developed that can provide direct feedback for policymakers.

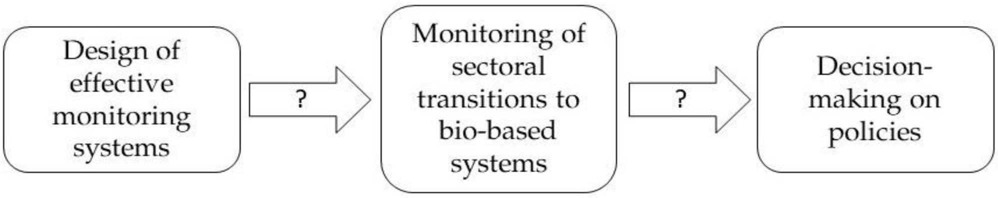

Figure 7-3. Three promising points of departure for further research.

Complementary to the development of new sets of indicators, a deeper understanding of the design and impact of monitoring systems in general is urgently needed, as illustrated by the left- and right-side boxes of Figure 7-3. What are the impacts of monitoring systems on decision-making? What design factors influence such impacts? These questions are already being addressed to some extent within the research field known as sociology of quantification (Espeland and Stevens 2008), which investigates "when and how do numbers matter?" and "who gets to decide what we quantify and how we do it?" (Berman and Hirschman 2018, p. 258).

The role of indicators and monitoring systems in decision-making, the right side of Figure 7-3, is not clear. Direct impacts are often assumed but have been seldom researched (Lehtonen 2012; Schoenefeld and Rayner 2019). Sustainability and energy indicators have been used rather indirectly and have only played a limited role in policy formulation (Lehtonen 2012; Lehtonen et al. 2016), mainly influencing discussions on sustainability during indicator development (Sébastien et al. 2014). Hence, this process should receive more attention (Scott and Bell 2013). Similarly, a forest monitoring system has contributed to agenda-setting, definition of solutions, and evaluation of outcomes (Neeff and Piazza 2020). This confirms that indicators not only have an instrumental function but also conceptual, tactical, symbolic, and political ones (Hezri and Dovers 2006). Indicators can have unintended side effects if misused (Lyytimäki et al. 2013), or they may only play a minor role next to other influences, such as emotions, beliefs, and habits (Cairney 2016). Lehtonen (2015, p. 95) claims that "the true power of indicators as policy formulation tools lies in their indirect, unintended, and partly intractable long-term impacts through learning, political advocacy and systemic effect".

As this thesis has attempted to demonstrate in various ways, design of monitoring systems, the left side of Figure 7-3, very likely influences their impacts. In essence, development of monitoring systems entails a series of decisions about "*who* monitors, *what, why, when, and with what effect(s)*" (Schoenefeld 2021). Policy monitoring can be considered a “governance activity” that is influenced by “overarching rules, the institutional support for implementation, and the criteria governing the quality of the information they deliver” (Schoenefeld et al. 2019, p. 719). A monitoring system’s success depends on the “trust, credibility and reputation of the different organizations producing indicators” (Lehtonen 2015, p. 95) as well as many other factors – power relations, interests, and norms – which produce particular storylines (Saltelli and Giampietro 2017; Espeland 2015). Thus, (re)investigating and drawing conclusions about well-established monitoring systems can inform emerging monitoring efforts related to advancing bioeconomy, circular economy, and biodiversity efforts, making it a crucial task for future research.

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Research Methods Annex

The annex includes a detailed description of the model that was used to generate results in Chapters 4 and 5.

The published methods paper has been added to this thesis in the next pages.

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Method Article

An extended hybrid input-output model applied to fossil- and bio-based plastics

Wiebke Jander

Department of Technology Assessment and Substance Cycles, Leibniz Institute for Agricultural Engineering and Bioeconomy e.V. (ATB), Potsdam, Germany

ABSTRACT

Matrix augmentation method is developed further and described transparently for enabling more specific input-output analyses of bio- vs. fossil-based sectors. A number of economic and environmental effects of substitution can be estimated, compared, and managed. While the model was applied for the first time to the German plastics industry, it can be well integrated into existing bioeconomy monitorings to represent substitution in sectors and countries.

- Original matrix augmentation method is described in much detail for the first time considering available data for bio- and fossil-based industries.
- Particular attention is paid to balancing cost and benefit in model building so that indicators can be integrated in a continuous monitoring of the bioeconomy. Hence, industry data is prefered to process data whenever possible.
- Input structures of bio-based imports are considered in single-region input-output analysis.

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E-mail address: wjander@atb-potsdam.de

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Specifications table

Subject Area	Economics and Finance
More specific subject area	Industrial Ecology
Method name	Matrix augmentation of supply and use tables to represent bio-based value chains
Name and reference of original method	Model III: Disaggregating an Existing Industry Sector (Joshi, 1999, see [1]) based on Input-Output Analysis (Leontief, 1936, see [2]) and Environmental Input-Output Analysis (Leontief, 1970, see [3])
Resource availability	Supply and use table, Source: Destatis [4] Energy use by production sector, Source: Destatis [5] Material- und Wareneingangserhebung (MWE), Source: Destatis [6] Life cycle inventory database, Source: Ecoinvent 3.4 [7]

Motivation

Considerable efforts are currently under way to establish bioeconomy monitorings to advice policy-makers on potential economic, social, and environmental trade-offs, especially in the EU [8–11]. Approaches partially rely on input-output data with a resolution of 65–200 sectors and on methods for estimating bio-based shares of these sectors [12]. Although research on net effects comparing bio-based sectors to the rest of the economy has begun [13,14], a significant challenge is to adequately represent bio-based sectors and to clearly distinguish them from other sectors in input-output modelling. Because national input-output data refers to broad sectors, such as chemicals and chemical products, different inputs and processes can only be analyzed if uncertainties of aggregation are accepted. This leads to rather broad overviews as in [14] rather than to analyses relevant for practical policy-making.

Hybrid input-output models have been proposed to reduce the aggregation error in input-output analyses. Joshi (1999) suggests 'Model III' to analyze environmental effects of product groups that are already included in existing sectors of input-output tables. Model III consists of a disaggregation of one sector into two sectors. Input structures of the more detailed sectors may be derived from cost sheets of representative products [1]. Input shares that are known can be added manually to the new use table columns while unknown input shares require an allocation method [15]. In literature, values are often allocated analogous to the original (aggregate) sector (see Supplementary Information p.16ff. in [15] or p.4ff. in [16]).

Although hybrid models have been created for some bioeconomy sectors, such as the biotechnology [17], biofuels [16,18–20], and wood [21] sectors, different methods have been applied making it difficult to compare their strengths and weaknesses and study results [22]. More specifically, it is rarely reported (1) how process data, detailed industry data, or input data of the aggregate sector are combined to create new sectors in input-output tables and (2) how to deal with non-competitive imports of inputs. These questions are addressed against the background that there should be a balance between cost of model building/data collection and benefits in terms of meaningful results. Concering question 1, using industry data is most preferable because process data introduces a new source of uncertainty while the proportionality assumption inherent in aggregate data may imply large errors as well. The existing sector, in this case chemicals and chemical products, contains a large variety of basic and processed products that are dissimilar to plastics. Hence, the model builds on plastics industry data from Destatis [6] for modelling the (new) fossil-based plastics industry, for bioplastics process data from Ecoinvent [7] for modelling parts of the (new) bio-based plastics industry, and on aggregate sector data from Destatis [4] for all remaining inputs. In a first step, a fossil- and bio-based plastics sector is extracted from the aggregate chemicals sector included in input-output tables. Information on the plastics sector is used to model the fossil-based part of the bio-based industry because bioplastics are at present based on biopolymers and fossil-based polymers to achieve certain product functionalities [23]. It can be assumed that the input structure of fossil-based polymer inputs is similar to that of the plastics industry as long as bio-based production is very low. Concerning question 2), the domestic technology assumption (DTA) may be applied or the input-output model can be extended to further regions that are relevant trading partners [24]. DTA holds for imports that are produced in a similar way as domestic products. Errors may be large in the case

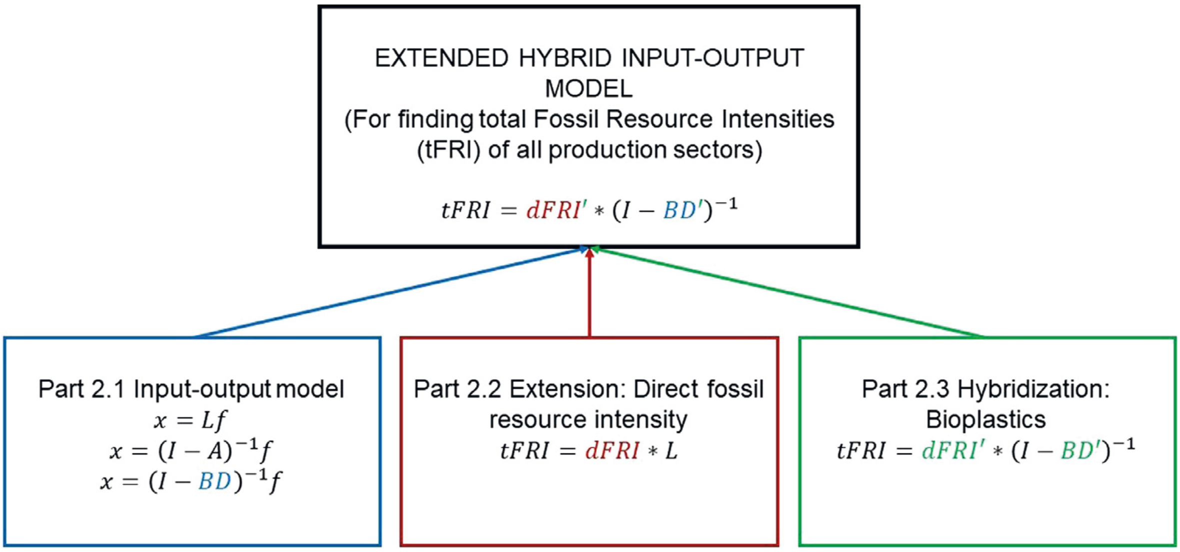

Fig. 1. Approach to building an extended hybrid input-output model in three steps. Source: own illustration.

of bioplastics because many biopolymers are imported without being produced in Germany. Setting up a multi-regional input-output (MRIO) model requires much effort because input-output data for biopolymers in other countries is hardly available. In this model, biopolymer input information draws on process data for domestically produced and imported biopolymers in order to represent non-competitive biopolymer imports that are used in bioplastics production. However, pretending that all biopolymers are produced domestically using foreign input structures is only plausible for small amounts as in the bioplastics case. If the bio-based industry because more significant, a MRIO model is more appropriate but has higher modelling demands.

This article presents a transparent method for augmenting supply and use matrices with a bioeconomy sector by integrating available process and alternative economic data, called hybridization. Special attention is paid to the challenges explained above in section 2.3.2.2. One central aim is to contribute to normalization of the matrix augmentation method while recognizing that exact procedures depend on data availability. The case chosen here, fossil resource intensity of bioplastics in Germany, relies on relatively few information and data, which makes it more complex to account for missing values. Thus, the method proposed here specifically relates to novel bio-based value chains in countries having a low resolution of their input-output data. A better representation of other value chains in input-output models or analyses for countries with high-resolution input-output tables may require different/fewer steps.

The extended hybrid input-output model starts with a basic input-output model (Part 2.1, see Fig. 1) explaining methodological choices and alternatives and continues with the environmental extension to account for fossil resource use (Part 2.2) before showing the hybridization process (Part 2.3). The method is validated for the case of bioplastics in Part 3.

Method details

Building a basic input-output model

Leontief quantity models measure the effects on the output supplied by each sector due to a change in final demand [25]. Through multiplication of a Leontief inverse matrix L with a final demand vector f, changes in sectors' outputs x can be obtained (Eq. (1)). Leontief inverse matrix L is derived from an identity matrix I and a technology coefficients matrix A.

$$x = Lf = (I - A)^{-1} f \tag{1}$$

Table 1
Scheme of notations and relationships between matrices and vectors. Dark grey – information derived from supply table V (q^{do}, x^{do}, q', x) and additional information (q^{m}, (T – S), tt). Light grey – information derived from use table U (x^{di}, q^{di}, x', q) and additional information (va, f_{hh}, f_{gov}, f_{po}, I, Δs, q^{x}).

	Industries (i)	Commodities (j)	Total input of j to all i	Total output of i of all j	Final demand	Invest-ments	Stock change	Exports	Total input of j
Industries (i)		V		$x^{do} = x$					
Commodities (j)	U		q^{di}		f_{hh}, f_{gov}, f_{po}	I	Δs	q^{x}	q
Total output of j by all i		q^{do}							
Total input to i of all j	x^{di}								
Imports		q^{m}							
Taxes minus subsidies		(T – S)							
Trade and transport margin		tt							
Total output of j		q'							
Value added	va								
Total input to i	x'								

V – supply table (commodity output produced by an industry)

x^{do}, x – total output of commodities by an industry
x – total output of commodities by an industry

q^{do} – total output of a commodity by domestic industries
q^{m} – imports of a commodity
(T – S) – taxes minus subsidies of a commodity
tt – trade and transport margins of a commodity
q' – total output of a commodity including imports

U – use table (commodity input used by an industry)

x^{di} – total intermediate input of commodities to an industry
va – value added by an industry
x' – total input of commodities and value added to an industry

q^{di} – total input of a commodity by all domestic industries
f_{hh}, f_{gov}, f_{po} – final demand for a commodity by households, government, and private organizations
I – investments in buildings and equipment for the production of a commodity
Δs – stock change of a commodity
q^{x} – exports of a commodity
q – total input of a commodity to domestic industries, final demand, and exports (and investments and stock change)

Matrix A, showing input structures, is based on an input-output table (IOT) or on supply and use tables (SUT), which are commonly provided by national statistical offices. An IOT is a model of interrelations between sectors of an economy and is derived from SUT. Four main types of IO models have been identified that are based on (strong) assumptions about input structures or (weak) assumptions about sales structures of secondary products [26]. To allow for greater flexibility regarding the way multiproduct processes are represented, the bioplastics model starts from SUT for integrating data [15,25–27]. While statistical offices prefer to use a model with weak assumptions because they are closer to observed data [26], these result in industry-by-industry IO models. For the purpose of this research, however, the IO model chosen is in the form product-by-product because, first, changes in products rather than industries are of interest, and, second, data for environmental extensions refer to production sectors rather than industries [28,29]. There are two ways for building a product-by-product IO model relying on either product technology or industry technology assumption. The former is better suited for subsidiary production, while the latter applies better to by-production [26]. In the bioeconomy, both forms of production are relevant but it was decided that a good representation of by-production is advantageous with regard to future bioeconomy analyses that will increasingly consider input of residues and by-products. Eq. (2) implies that all commodities produced by an industry have the same input structure [25]. Matrix *B* is called a technology matrix, which is values in a use table *U* divided by respective industry output *x'*. *D* is a market shares matrix, calculated by dividing values in a supply table *V* by the value of commodity inputs *q* [4].

$$A = BD = [U/x\prime][V/q\prime] \tag{2}$$

Table 1 gives an overview of matrices and vectors that are available from national statistical offices and serve as a basis for the hybridization process. Prior to a description of changes to industries *i* and commodities *j* in Part 2.3, I shortly recapitulate how to estimate total environmental effects triggered by a change in final demand through environmentally extended input-output models and show how direct intensities were split for disaggregated sectors.

Extending the basic model with direct fossil resource use data

The basic input-output model is extended with a vector for direct fossil resource intensities (*dFRI*) in order to find out how much more or less fossil energy is necessary if changes in demand occur. In my research, I wanted to calculate net fossil energy use due to substitution, i.e. reduced demand for fossil-based plastics and increased demand for bio-based plastics.

$$tFRI = dFRI * L \tag{3}$$

Calculation of total fossil resource intensities (*tFRI*) follows the established method of extending the basic IO model by environmental information to obtain so-called multipliers [25]. Thus, further effects of substitution can be measured using sector-specific data. Relating to bioeconomy objectives as stated in bioeconomy strategies [30,31] and having a reliable data base, value added, employer compensation, greenhouse gas emissions and water use were selected to exemplify trade-offs with fossil resource substitution [23]. As value added and employment multipliers rely on economic data collected from firms and refering to economic sectors (industries) rather than production sectors, the assumption that value added and employment data is similar for production and economic sectors for the selected case must be plausible to use this data in a product-by-product model [29]. Production sectors refer to homogenous products that are not empirically observable while economic sectors refer to a mixed bundle of goods produced by a certain industry, which is classified by its main activity [32].

Data for direct Fossil Resources Consumption (*dFRC*) in Joule (coal, lignite, crude oil, natural gas) by German production sectors is part of Environmental Accounting [5,33]. Intensity is *dFRC* divided by total output value of a commodity by domestic industries q^{do} (Eq. (4)). As data is available for fewer production sectors than in the IO model (48 compared to 85), it was split based on output value of the production sector j and the aggregate sector *agg* for which data is available (Eq. (5)). More detailed information is available for splitting aggregate *dFRC* of coke and petroleum products as well as of electricity and gases [34].

$$dFRI = dFRC/q^{do} \tag{4}$$

$$dFRC = dFRC_{agg} * \left(\frac{q_j^{do}}{q_{agg}^{do}} \right) \tag{5}$$

In the absence of data for the disaggregated sectors, it was assumed that no direct fossil resource consumption is required in bio-based plastics production and that fossil-based plastics production only sources natural gas directly (no crude oil, coal or lignite). Natural gas use was estimated based on output values of the fossil-based plastics sector and the (aggregate) chemicals sector.

Hybrid model using matrix augmentation

Disaggregation is performed for the commodity group j “chemicals and chemical products” and the industry i “manufacturing of chemicals and chemical products” (C20 according to CPA - Statistical Classification of Products by Activity, Version 2.1), resulting in fossil- and bio-based primary plastics sectors ($\mathrm{C20.16_f}$ and $\mathrm{C20.16_b}$) and an other chemicals and chemical products sector ($\mathrm{C20^*}$).

The following sections show adjustments to the supply table first and then to the use table. Factors that are marked in bold indicate the use of primary or secondary data. All factors not explained here are part of the basic model and described above in Table 1.

Supply table

Industry output. This section shows how information is added to supply table rows so that total output of bio-based, fossil-based and other chemicals industries (x_b, x_f, x_o) of all commodities, main and by-products, can be estimated (Eq. (6), Table 2).

$$x = \sum_{j=1}^{n} v_{ij} \tag{6}$$

Table 2
Augmentation of supply table rows, in relation to Table 1.

	V		$x^{do} = x$					
U		q^{di}		f	I	Δs	q^x	q
	q^{do}							
x^{di}								
	q^m							
	T – S							
	tt							
	q‘							
va								
x‘								

Table 3
Augmentation of supply table columns, in relation to Table 1.

	V		$x^{do} = x$					
U		q^{di}		f	I	Δs	q^x	q
	q^{do}							
x^{di}								
	q^m							
	T – S							
	tt							
	q‘							
va								
x‘								

Information on the kinds of commodities produced by new bio- and fossil-based economic sectors is required. For the case of bio- and fossil-based plastics, it is assumed that the respective industry only produces its main products that are classified as plastics and does not engage in other economic activity because information was not available. This is a reasonable assumption considering that, in the aggregate chemicals sector, more than 80% of its activity was related to chemicals products in Germany in 2016. Thus, commodities other than chemicals produced by the chemicals sector were fully assigned to the other chemicals and chemical products sector. Supply of bio- and fossil-based plastics and other chemicals (v_{oo}, v_{bb}, v_{ff}) is derived in the next section 2.3.1.2.

Commodity output. This section shows how information is added to supply table columns so that total output of bio-based, fossil-based and other chemical commodities (q_b', q_f', q_o') by all domestic and foreign industries, i.e. including imports, can be estimated (Eq. (7), Table 3).

$$q\prime = q^{do} + q^m + (T - S) + tt \tag{7}$$

For the bio-based sector, factors are determined in the following way:

$$q_b^{do} = \sum_{c=1}^{n} (\boldsymbol{q_c} * \boldsymbol{p_c}) = v_{bb} \tag{8}$$

q_c – production quantity of a bio-based product c (in tons) p_c – price of a bio-based product c (in €/ton)

An underlying assumption in Eq. (8) is that bio-based plastics are only produced by the bio-based plastics industry and not by other industries. If they were also produced by other industries, $q^{do}{}_{b}$ would also have to equal the sum of supply table column values (v_{ib}).

Information on imports of bio-based plastic are not available. Based on expert interviews, imports of bioploymers were estimated but not considered in modelling because the focus was on building a bio-based plastic sector, i.e. processed biopolymers (for further information see [23]). Nevertheless, the input structure of imported biopolymers is considered in section 2.3.2.2.

$$q_b^m = \sum_{c=1}^{n} (\boldsymbol{m_c} * \boldsymbol{p_c}) \tag{9}$$

m_c – imports of a bio-based product c (in tons)

$$(T - S)_b = (\boldsymbol{T} - \boldsymbol{S})_{\boldsymbol{agg}} / \boldsymbol{q^{do}_{agg}} * q_b^{do} \tag{10}$$

$(T - S)_{agg}$ – taxes minus subsidies of commodities in aggregate production sector $q^{do}{}_{agg}$ – total output of commodities in aggregate production sector by domestic industries, basic price

$$tt_b = \boldsymbol{tt_{agg}} / \boldsymbol{q^{m}_{agg}} * q_b^{m} \tag{11}$$

tt_{agg} – trade and transport margin of aggregate commodities $q^{m}{}_{agg}$ – imports of aggregate commodities

For the fossil-based sector, factors *(T – S)* and *tt* are determined in the same way by multiplying specific commodity output with aggregate sector shares as in Eqs. (10) and (11). Fossil-based imports $q^{m}{}_{f}$ are calculated by subtracting bio-based imports from known plastics imports (Eq. (11)). Output of fossil-based commodities by domestic industries $q^{do}{}_{f}$ depends on values in the respective use table column (u_{fj}), which are described in section 2.3.2.2. Here, again, it is assumed that fossil-based plastics are only produced by the fossil-based plastics industry ($q^{do}{}_{f} = v_{ff}$).

$$q_f^m = \boldsymbol{q^{m}_{f+b}} - q_b^m \tag{12}$$

$q^{m}{}_{f+b}$ – imports of fossil- and bio-based commodities

For the other chemicals and chemical products sector, factors *(T – S)* and *tt* are determined in the same way by multiplying specific commodity output with aggregate sector shares as in Eqs. (10) and (11). Other imports $q^{m}{}_{o}$ are calculated by subtracting known bio- and fossil-based plastics imports from known aggregate sector imports $q^{m}{}_{agg}$ (Eq. (13)). Output of other commodities by domestic industries $q^{do}{}_{o}$ is aggregate sector supply $q^{do}{}_{agg}$ minus the supply of fossil- and bio-based commodities (Eq. (14)). Entries in supply table columns for this sector, i.e. v_{io}, are assumed to be the same as for the aggregate sector, except for v_{oo}, which is calculated with Eq. (15) (v_{aggagg} is the intersection of the aggregate sector in the supply table).

$$q_o^m = \boldsymbol{q^{m}_{agg}} - \boldsymbol{q^{m}_{f+b}} \tag{13}$$

$$q_o^{do} = \boldsymbol{q^{do}_{agg}} - q_b^{do} - q_f^{do} \tag{14}$$

$$v_{oo} = \boldsymbol{v_{aggagg}} - v_{bb} - v_{ff} \tag{15}$$

Use table

Commodity input. This section shows how information is added to use table rows so that total input of bio-based, fossil-based and other chemicals commodities (q_b, q_f, q_o) to all industries (q^{di}), final demand (f), and exports (q^x) as well as investemnts (I) and stock change (Δs) can be estimated (Eq. (16), Table 4).

$$q = q^{di} + f + I + \Delta s + q^{x} \tag{16}$$

Information on bio-based export quantities is based on expert interviews and calculated with Eq. (17). As total exports of fossil- and bio-based plastics is known, fossil-based exports can be easily

Table 4
Augmentation of use table rows, in relation to Table 1.

	V		$x^{do} = x$					
U		q^{di}		f	I	Δs	q^x	q
	q^{do}							
x^{di}								
	q^m							
	T – S							
	tt							
	q‘							
va								
x‘								

calculated with Eq. (18).

$$q_b^x = \sum_{c=1}^{n} (\boldsymbol{q_c^x} * \boldsymbol{p_c}) \tag{17}$$

$q^x{}_c$ – export quantity of bio-based product c (in tons) p_c – price of a bio-based product c (in €/ton)

$$q_f^x = \boldsymbol{q_{f+b}^x} - q_b^x \tag{18}$$

In the absence of more detailed information, values for *f*, *I*, and Δs for bio- and fossil-based commodities are proprtional to aggregate sector values Eqs. (19)–((23)).

$$\Delta s_{b,f} = \left(q_{b,f} - q_{b,f}^x\right) * \left(\boldsymbol{\Delta s_{agg}} / \left(\boldsymbol{q_{agg}} - \boldsymbol{q_{agg}^x}\right)\right. \tag{19}$$

$$I_{b,f} = \left(q_{b,f} - q_{b,f}^x\right) * \left(\boldsymbol{I_{agg}} / \left(\boldsymbol{q_{agg}} - \boldsymbol{q_{agg}^x}\right)\right. \tag{20}$$

$$f_{b,f}^{hh} = \left(q_{b,f} - q_{b,f}^x\right) * \left(\boldsymbol{f_{hh,agg}} / \left(\boldsymbol{q_{agg}} - \boldsymbol{q_{agg}^x}\right)\right. \tag{21}$$

$$f_{b,f}^{po} = \left(q_{b,f} - q_{b,f}^x\right) * \left(\boldsymbol{f_{po,agg}} / \left(\boldsymbol{q_{agg}} - \boldsymbol{q_{agg}^x}\right)\right. \tag{22}$$

$$f_{b,f}^{gov} = \left(q_{b,f} - q_{b,f}^x\right) * \left(\boldsymbol{f_{gov,agg}} / \left(\boldsymbol{q_{agg}} - \boldsymbol{q_{agg}^x}\right)\right. \tag{23}$$

f^{hh} – final demand of households f^{po} – final demand of private organizations f^{gov} – final demand of government

Values for other chemicals and chemical commodities in use table rows are found by subtracting values for bio- and fossil-based sectors from aggregate sector values.

Because *q* is equal to *q’*, which is known from section 2.3.1.2, and all other factors are derived above, q^{di} can be calculated as shown in Eq. (24). It is the sum of sales of a commodity group to all industries.

$$q^{di} = q - f - I - \Delta s - q^x \tag{24}$$

Values in the use table (u_{ji}) can be estimated with q^{di} (Eq. (25)). Bio-based plastics (sector 20.16b) are sold to the rubber and plastics industry (sector 22) only so that $q^{di}{}_{20.16b} = u_{20.16b,22}$. This assumption holds because only biopolymers that are processed into plastics products, including plates, sheets, foils, packaging, plastic parts for vehicles, and household goods were included while biopolymers that are used in other sectors (e.g. polyurethane in mattress production) were excluded. Fossil-based plastics are sold to the fossil-based plastics, bio-based plastics, and other chemicals sectors (see section 2.3.2.2), as well as to the pharmaceutical industry (sector 21) and the rubber

Table 5
Augmentation of use table columns, in relation to Table 1.

	V		$x^{do} = x$					
U		q^{di}		f	I	Δs	q^x	q
	q^{do}							
x^{di}								
	q^m							
	T – S							
	tt							
	q'							
va								
x'								

and plastics industry (sector 22) according to official statistics [6]. Other chemicals are sold to other industries based on information for the aggregate chemicals sector, to sectors 21 and 22 based on aggregate chemicals sector values minus sales of fossil- and bio-based plastics, and to fossil-based plastics, bio-based plastics, and other chemicals sectors as described in section 2.3.2.2.

$$q^{di} = \sum_{i=1}^{n} u_{ji} \tag{25}$$

Industry input. This section shows how information is added to use table columns so that total input into bio-based, fossil-based and other chemicals industries (x'_b, x'_f, x'_o) can be estimated (Eq. (26), Table 5). Input consists of the sum of inputs from all industries (x^{di}) and value added (va).

$$x\prime = x^{di} + \boldsymbol{va} \tag{26}$$

Value added of bio-based plastics production (va_b) is not available and was estimated to be 25% of total input x'_b. It is a rough estimation and, thus, associated with high uncertainty. Value added of the aggregate chemicals sector (va_{agg}) was 36% of total inputs (x'_{agg}) in Germany in 2016 [4], which is assumed for the fossil-based plastics sector. Hence, value added of the other chemicals sector is aggregate value added minus value added by bio- and fossil-based sectors.

Information on commodity inputs to bio- and fossil-based industries (u_{jb}, u_{jf}), as well as to the adjusted aggregate sector (u_{jo}), has to be inserted in use table columns in order to build their sum (Eq. (27)). Estimating input structures for the three new sectors is the most complex step in the model and is illustrated in Fig. 2.

$$x^{di}_{b,f,o} = \sum_{j=1}^{n} u_{jb,f,o} \tag{27}$$

Bio-based plastic industry (C20.16b) uses biopolymers as well as fossil-based polymers in production, which requires splitting the bio-based industry again into a bio-based intermediate industry *bb* and a fossil-based intermediate industry *bf* to represent different input structures (Steps 1–3). These are then combined to build input structures of the bio-based industry (Eq. (28)). With information on the bio-based industry, the fossil- based and other chemicals industries can be modelled (Steps 4 and 5).

$$u_{jb} = u_{jbb} + u_{jbf} \tag{28}$$

u_{jbb} – input of commodity j into bio-based intermediate industry u_{jbf} – input of commodity j into fossil-based intermediate industry

Some of the inputs to the bio-based intermediate industry, i.e. to biopolymer production, are known from process data (u_{pbb}) while the majority of input relations was estimated based on

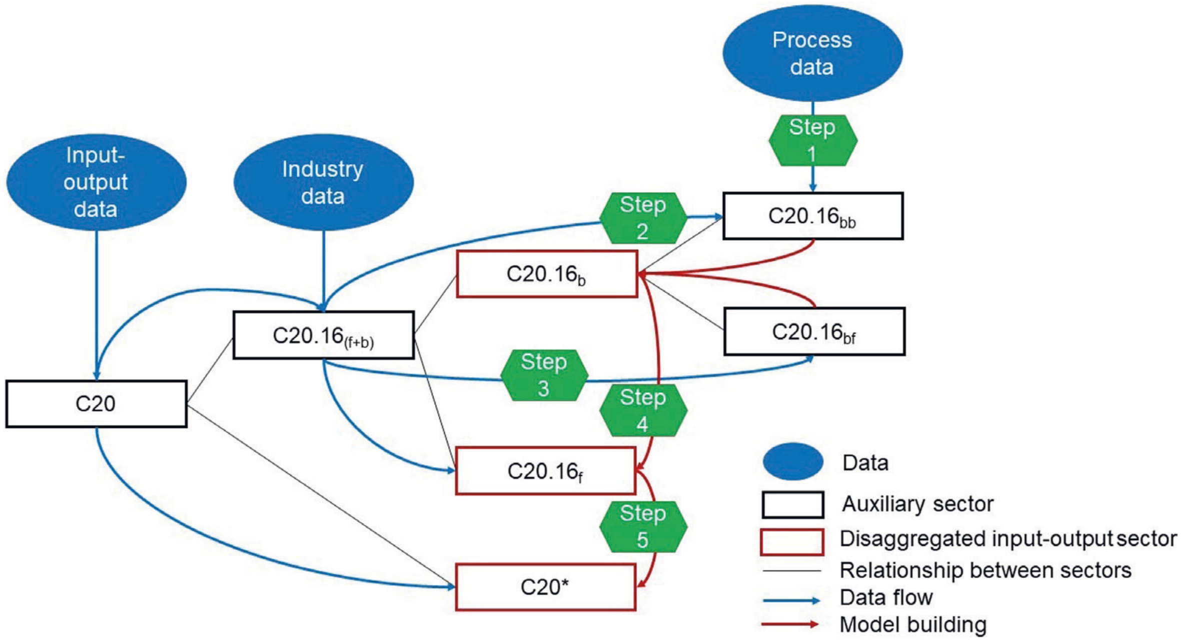

Fig. 2. Steps in estimating input structures of disaggregated sectors. Source: own illustration.

information of the combined bio- and fossil-based plastics industry (u_{rbb}) Eq. (29)). Eqs. (30)–((34) describe the procedure using process data and Eqs. (35)–(43) using plastics industry information. By using process data of imported and domestically produced biopolymers, the domestic technology assumption (DTA) is relaxed.

$$\sum_{j=1}^{n} u_{jbb} = \sum_{p=1}^{n} u_{pbb} + \sum_{r=1}^{n} u_{rbb} \tag{29}$$

u_{pbb} – input of commodity *p* into bio-based intermediate industry *bb* where information from technical literature is available; for the case of plastics, *p* refers to CPA 10, 17.2, 19.2, 20, 35.1, 35.3
u_{rbb} – input of residual commodity *r* into bio-based intermediate industry *bb* where no information from technical literature is available

Step 1

$$u_{pbb} = s_{pbb} * x_{bb}^{di} \tag{30}$$

s_{pbb} – share of commodity *p* in bio-based intermediate production *bb* where information from technical literature is available; for the case of plastics, p refers to CPA 10, 17.2, 19.2, 20, 35.1, 35.3
x^{di}_{bb} – total input of commodities to bio-based intermediate industry

$$s_{pbb} = \sum_{c=1}^{n} \left(s_{pcbb} * s_{cbb} \right) \tag{31}$$

s_{pcbb} – share of commodity *p* in bio-based intermediate product *c* that is part of bio-based intermediate industry *bb* s_{cbb} – share of bio-based intermediate product *c* in production value of bio-based intermediate industry

$$s_{pcbb} = \left(\boldsymbol{q_p} * \boldsymbol{p_p} \right) * (\boldsymbol{q_{cb}} * \boldsymbol{p_{cb}}) / ((\boldsymbol{q_{cb}} * \boldsymbol{p_{cb}}) - \boldsymbol{va_{cb}}) \tag{32}$$

q_p – quantity of input commodity *p* into product *c*, in physical units per € p_p– price of input commodity *p*, in € per physical unit q_{cb} – quantity of bio-based intermediate product *cb*, in tons p_{cb} – price of bio-based intermediate product *cb*, in € per ton va_{cb} – value added of bio-based intermediate product *cb*

$$s_{cbb} = \left(\boldsymbol{q_{cb}} + \boldsymbol{q^{m}_{cb}}\right) * \boldsymbol{p_{cb}} \Bigg/ \sum_{cb=1}^{n} \left(\left(\boldsymbol{q_{cb}} + \boldsymbol{q^{m}_{cb}}\right) * \boldsymbol{p_{cb}}\right) \tag{33}$$

qmcb – import quantity of bio-based intermediate product cb, in tons

$$x^{di}_{bb} = \sum_{cb=1}^{n} \left(\boldsymbol{p_{cb}} * \boldsymbol{q_{cb}}\right) - \boldsymbol{va_{cb}} \tag{34}$$

Step 2

$$u_{rbb} = rs_{rbb} * R_{bb} \tag{35}$$

$\mathrm{rs}_{\mathrm{rbb}}$ – share of residual commodity *r* according to industry information

R_{bb} – residual input value for bio-based intermediate industry *bb*

$$R_{bb} = x^{di}_{bb} - \sum_{p=1}^{n} u_{pbb} \tag{36}$$

$$rs_{rbb} = s_{(f+b)r} \Bigg/ \sum_{r=1}^{n} s_{(f+b)r} \tag{37}$$

$\mathrm{s}_{\mathrm{(f+b)r}}$ – share of input commodities *r* to the aggregate fossil- and bio-based industry *f+b* for which no process information on bio-based intermediate industry inputs is available

Information on the fossil- and bio-based industry *f+b* is available on a detailed basis for some input commodities *w* from Destatis [6] Eq. (38)) but not for others (residual shares *rs* of input commodities *z*). For the latter case, shares are estimated based on aggregate industry residual shares rs_{agg} (Eqs. (39)–((43).

$$s_{w(f+b)} = \boldsymbol{s_{wagg}} * \left(\boldsymbol{d_{w(f+b)}} \Bigg/ \sum_{w=1}^{n} \boldsymbol{d_{w(f+b)}}\right) \Bigg/ \left(\boldsymbol{d_{wagg}} \Bigg/ \sum_{w=1}^{n} \boldsymbol{d_{wagg}}\right) \tag{38}$$

$\mathrm{s}_{\mathrm{w(f+b)}}$ – share of input of commodity *w* into fossil- and bio-based industry *f+b*, from detailed industry data $\mathrm{s}_{\mathrm{wagg}}$ – share of input of commodity *w* into aggregate industry *agg* $\mathrm{d}_{\mathrm{w(f+b)}}$ – input of commodity *w* into fossil- and bio-based industry *f+b* $\mathrm{d}_{\mathrm{wagg}}$ – input of commodity *w* into aggregate industry *agg*

$$rs_{z(f+b)} = u_{z(f+b)} / \boldsymbol{x^{di}_{(f+b)}} \tag{39}$$

$\mathrm{rs}_{\mathrm{z(f+b)}}$ – residual share of input of residual commodity *z* into fossil- and bio-based industry *f+b* $\mathrm{u}_{\mathrm{z(f+b)}}$ – input of residual commodity *z* into fossil- and bio-based industry *f+b* $\mathrm{x}^{\mathrm{di}}{}_{\mathrm{(f+b)}}$ – total input value of fossil- and bio-based industry *f+b*

$$u_{z(f+b)} = rs_{zagg} / R_{(f+b)} \tag{40}$$

$\mathrm{rs}_{\mathrm{zagg}}$ – residual share of input of residual commodity *z* into aggregate industry *agg*

$\mathrm{R}_{\mathrm{(f+b)}}$ – residual input value for fossil- and bio-based industry

$$rs_{zagg} = \boldsymbol{s_{zagg}} \Bigg/ \sum_{z=1}^{n} \boldsymbol{s_{zagg}} \tag{41}$$

$\mathrm{s}_{\mathrm{zagg}}$ – share of input of residual commodity *z* into aggregate industry *agg*

$$R_{(f+b)} = \boldsymbol{x^{di}_{(f+b)}} - \sum_{w=1}^{n} u_{w(f+b)} \tag{42}$$

$\mathrm{x}^{\mathrm{di}}{}_{\mathrm{(f+b)}}$ – total input of fossil- and bio-based commodities by all domestic industries $\mathrm{u}_{\mathrm{w(f+b)}}$ – input of commodity *w* into fossil- and bio-based industry *f+b*

$$u_{w(f+b)} = s_{w(f+b)} / \boldsymbol{x^{di}_{(f+b)}} \tag{43}$$

Step 3

Recalling from Eq. (28) that the bio-based industry has fossil-based intermediate inputs, Eq. (45) shows that this aspect is accounted for by using input values from the fossil- and bio-based industry *f*+*b*. How input shares of this aggregate industry $s_{j(f+b)}$ were modelled is described in Eqs. (37)–(42).

$$u_{jbf} = s_{jbf} * x^{di}_{bf} \tag{44}$$

u_{jbf} – input of commodity j into fossil-based intermediate industry s_{jbf} – share of commodity *j* in total fossil-based intermediate industry *bf* inputs $x^{di}{}_{bf}$ – total input of commodities to fossil-based intermediate industry

$$s_{jbf} = s_{j(f+b)} \tag{45}$$

$$\sum_{j=1}^{n} s_{j(f+b)} = \sum_{w=1}^{n} s_{w(f+b)} + \sum_{r=1}^{n} rs_{r(f+b)} \tag{46}$$

$$x^{di}_{bf} = \sum_{cf=1}^{n} \left(\boldsymbol{p_{cf}} * \boldsymbol{q_{cf}}\right) - \boldsymbol{va_{cf}} \tag{47}$$

q_{cf} – quantity of fossil-based intermediate product *cf*, in tons p_{cf} – price of fossil-based intermediate product *cf*, in € per ton va_{cf} – value added of fossil-based intermediate product *cf*

Step 4

Having built the bio-based industry, based on process data and plastics industry data, inputs to the fossil-based industry are aggregate fossil- and bio-based industry inputs corrected for bio-based industry inputs (Eq. (48)).

$$u_{jf} = u_{j(f+b)} - u_{jb} \tag{48}$$

u_{fj} – input of commodities into fossil-based industry $u_{(f+b)j}$ – input of commodities into fossil-and bio-based industry u_{bj} – input of commodities into bio-based industry

Step 5

Other chemicals industry inputs, in turn, are modelled based on inputs to the aggregate sector u_{jagg} and to the fossil- and bio-based industry $u_{j(f+b)}$ (Eq. (49)).

$$u_{jo} = u_{jagg} - u_{j(f+b)} \tag{49}$$

Method validation

Net effects on fossil resource use of substituting disaggregated product groups can be derived from the model described above. These net effects indicate a transition from a fossil-based to a bio-based economy, which is one of the main objectives in current bioeconomy strategies [30,31] and should be measured with an indicator in order to make visible trade-offs with other objectives [13]. The plastics sector is currently transitioning towards a bioeconomy at a relatively low rate of 0.1% [23]. Apart from the fact that bio-based plastics production is low and prices are high compared to fossil-based plastics production, total Fossil Resource Intensities of bio-based ($tFRI_b$) and fossil-based plastics ($tFRI_f$) are similar (14.8 MJ/$€_f$ and 13.6 MJ/$€_b$). One Euro more of bio-based plastics production and one Euro less of fossil-based plastics production saves only 8% of fossil energy [23].

Intensity of bio-based plastics is high because 40% of bio-based plastics inputs are fossil-based intermediate products [23]. Thus, for most inputs, shares do not differ much between bio- and fossil-based industries, especially for fossil resource intensive sectors including coke oven and refined petroleum products, basic iron and metals, gas, and transport services (see Table 6, columns 5 and 6). Although much less fossil-based plastics and other chemicals that also have above average fossil resource intensities are used in the bio-based industry, higher electricity input increases the bio-based industry's production intensity.

Table 6
Modelling results: Share of input commodities j (columns 1 – 2) in bio- and fossil-based industry output (columns 3 – 5) and total fossil resource intensities (column 6) for Germany in 2016.

Commodities j	*CPA 2008*	*Input share bio-based plastics industry* s_{jb}	*Input share fossil-based plastics industry* s_{jf}	*Difference in input shares* $s_{jb} - s_{jf}$	*Total fossil resource intensity (MJ/€)* *tFRI*
Products of agriculture, hunting (…)	01	0.02%	0.02%	0.00%	11.46
Products of forestry, logging (…)	02	0.02%	0.02%	0.00%	7.27
Fish and other fishing products	03	0.00%	0.00%	0.00%	8.60
Hard coal	5.1	0.02%	0.02%	0.00%	9.97
Lignite	5.2	0.01%	0.01%	0.00%	10.33
Crude petroleum and natural gas	06	2.06%	1.91%	0.15%	14.25
Metal ores	07	0.00%	0.00%	0.00%	0.00
Stone, sand and clay	08,09	0.29%	0.27%	0.02%	10.43
Food products	10	20.86%	0.00%	**20.86%**	7.49
Beverages	11	0.02%	0.02%	0.00%	7.75
Tobacco products	12	0.00%	0.00%	0.00%	7.49
Textiles	13	0.02%	0.02%	0.00%	6.72
Wearing apparel	14	0.00%	0.00%	0.00%	6.62
Leather and related products	15	0.00%	0.00%	0.00%	6.60
Wood and of products of wood	16	0.32%	0.30%	0.02%	6.54
Pulp, paper and paperboard	17.1	0.00%	0.00%	0.00%	6.96
Articles of paper and paperboard	17.2	1.61%	2.29%	-0.67%	11.41
Printing and recording services	18	0.12%	0.11%	0.01%	4.81
Coke oven products	19.1	0.15%	0.14%	0.01%	**532.41**
Refined petroleum products	19.2	3.23%	4.23%	-1.00%	**117.02**
Other chemicals and chemical products	20*	15.75%	34.92%	**-19.17%**	**15.59**
Fossil-based plastics	20.16f	7.70%	19.99%	**-12.29%**	**14.80**
Bio-based plastics	20.16b	0.00%	0.00%	0.00%	13.57
Basic pharmaceutical products (…)	21	0.02%	0.01%	0.00%	5.39
Rubber products	22.1	0.09%	0.08%	0.01%	7.13
Plastic products	22.2f	2.26%	2.09%	0.17%	7.23
Glass and glass products	23.1	0.04%	0.04%	0.00%	12.60
Clay building materials	23.2–23.9	0.50%	0.46%	0.04%	12.57
Basic iron and steel and ferro-alloys	24.1–24.3	0.01%	0.01%	0.00%	**29.31**
Basic precious and other non-ferrous metals	24.4	0.19%	0.17%	0.01%	**29.00**
Casting services of metals	24.5	0.00%	0.00%	0.00%	**29.02**
Fabricated metal products	25	0.76%	0.70%	0.06%	7.46
Computer, electronic and optical products	26	0.01%	0.01%	0.00%	3.96
Electrical equipment	27	0.19%	0.18%	0.01%	5.10
Machinery and equipment n.e.c.	28	0.45%	0.42%	0.03%	5.16
Motor vehicles, trailers and semi-trailers	29	0.05%	0.05%	0.00%	5.16
Other transport equipment	30	0.00%	0.00%	0.00%	4.67
Furniture	31	0.01%	0.01%	0.00%	4.28
Other manufactured goods	32	0.01%	0.01%	0.00%	4.38
Repair and installation of machinery (…)	33	1.55%	1.44%	0.12%	5.01
Electricity, transmission and distribution (…)	35.1, 35.3	13.36%	3.87%	**9.49%**	**46.59**
Manufactured gas	35.2	0.24%	0.22%	0.02%	**17.01**
Natural water	36	0.20%	0.19%	0.02%	8.50
Sewerage services	37	0.55%	0.51%	0.04%	5.04
Waste collection, treatment and disposal (…)	38	1.18%	1.09%	0.09%	4.67
Remediation services and waste (…)	39	0.12%	0.11%	0.01%	4.57
Buildings and building construction works	41	0.04%	0.04%	0.00%	5.57
Constructions (…) for civil engineering	42	0.00%	0.00%	0.00%	6.51
Specialised construction works	43	1.16%	1.07%	0.09%	5.60
Wholesale and retail trade: motor vehicles (…)	45	0.16%	0.15%	0.01%	3.50
Wholesale trade services	46	0.31%	0.29%	0.02%	5.32
Retail trade services	47	0.00%	0.00%	0.00%	3.96
Land transport services (…)	49	2.05%	1.90%	0.15%	9.43
Water transport services	50	0.10%	0.10%	0.01%	**18.49**
Air transport services	51	0.14%	0.13%	0.01%	**30.11**
Warehousing (…) for transportation	52	0.95%	0.88%	0.07%	9.21

(*continued on next page*)

Table 6 (*continued*)

Commodities j	*CPA 2008*	*Input share bio-based plastics industry* s_{jb}	*Input share fossil-based plastics industry* s_{jf}	*Difference in input shares* $s_{jb} - s_{jf}$	*Total fossil resource intensity (MJ/€)* *tFRI*
Postal and courier services	53	1.34%	1.24%	0.10%	7.05
Accommodation services (…)	55,56	0.35%	0.33%	0.03%	4.50
Publishing services	58	0.40%	0.37%	0.03%	2.04
Motion picture, video and television (…)	59,60	0.00%	0.00%	0.00%	2.33
Telecommunications services	61	0.31%	0.29%	0.02%	2.66
Computer programming (…)	62,63	1.72%	1.59%	0.13%	1.72
Financial services	64	0.92%	0.85%	0.07%	1.40
Insurance, reinsurance and pension (…)	65	0.81%	0.75%	0.06%	1.68
Services auxiliary to financial services (…)	66	0.02%	0.01%	0.00%	1.54
Real estate services	68	1.29%	1.19%	0.10%	1.25
Legal and accounting services (…)	69–70	2.39%	2.21%	0.18%	1.93
Architectural and engineering services	71	2.05%	1.89%	0.15%	2.19
Scientific research and development (…)	72	0.00%	0.00%	0.00%	3.93
Advertising and market research (…)	73	2.01%	1.86%	0.15%	1.91
Other professional, scientific and technical (…)	74	0.69%	0.64%	0.05%	3.26
Veterinary services	75	0.00%	0.00%	0.00%	3.19
Rental and leasing services	77	1.58%	1.46%	0.12%	1.97
Employment services	78	0.77%	0.71%	0.06%	0.86
Travel agency (…)	79	0.07%	0.06%	0.00%	9.16
Security and investigation services (…)	80–82	2.83%	2.62%	0.21%	3.36
Administration services of the State (…)	84.1,84.2	0.99%	0.92%	0.07%	2.95
Compulsory social security services	84.3	0.00%	0.00%	0.00%	2.95
Education services	85	0.19%	0.18%	0.01%	1.65
Human health services	86	0.03%	0.03%	0.00%	2.38
Residential care services (…)	87–88	0.00%	0.00%	0.00%	2.82
Creative, arts and entertainment services (…)	90–92	0.00%	0.00%	0.00%	2.48
Sporting services (…)	93	0.01%	0.01%	0.00%	2.95
Services (…) membership organisations	94	0.16%	0.15%	0.01%	2.18
Repair services of computers (…)	95	0.06%	0.05%	0.00%	2.43
Other personal services	96	0.12%	0.11%	0.01%	3.59
Services of households as employers (…)	97,98	0.00%	0.00%	0.00%	0.17

Summary

This extended hybrid input-output model was developed based on prior conceptual work addressing bioeconomy monitoring challenges [13,35]. Substitution of bio-based for fossil-based products can be analyzed by comparing net effects of two matching sectors. This requires hybridization of national input-output tables. In the article, a method for augmenting tables with bio-based, fossil-based, and other products industries using process, industry, and input-output data was described. During model building, the aim of a detailed representation of domestic and imported processes and products that enables specific analyses was carefully weighed against the effort of collecting and integrating data that is not available in official statistics. Reproduction of the method to other sectors and countries in bioeconomy monitorings that seek to show substitution of bio-based for fossil-based products and its effects is thereby facilitated. Results for the case of bio- and fossil-based plastics are discussed intensely in [23].

Declaration of Competing Interest

The author declares that she has no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Erklärung / Declaration

Erklärung:
Hiermit erkläre ich, die Dissertation selbstständig und nur unter Verwendung der angegebenen Hilfen und Hilfsmittel angefertigt zu haben.

Declaration:

I hereby declare that I completed the doctoral thesis independently based on the stated resources and aids.

Date / Datum: 25.09.2022

Signature / Unterschrift: