EISEVIED

Contents lists available at ScienceDirect

Science of the Total Environment

journal homepage: www.elsevier.com/locate/scitotenv



A methodology for integrating the biomass balance approach into life cycle assessment with an application in the chemicals sector



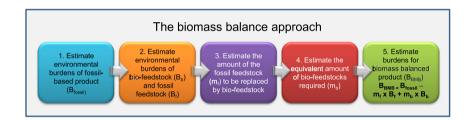
Harish K. Jeswani ^a, Christian Krüger ^b, Andreas Kicherer ^b, Florian Antony ^c, Adisa Azapagic ^{a,*}

- ^a Sustainable Industrial Systems, School of Chemical Engineering and Analytical Science, The University of Manchester, Manchester M13 3PL, UK
- ^b BASF SE, CDS/S, 67056, Ludwigshafen am Rhein, Germany
- ^c Oeko-Institut e.V, Institute for Applied Ecology, P.O. Box 17 71, 79017 Freiburg, Germany

HIGHLIGHTS

- A methodology integrating the biomass balance (BMB) approach with LCA was developed.
- It helps to establish biomass content in complex supply chains, reducing data needs.
- Helps to incentivise industry to increase the production of bio-based products.
- It also helps to identify the effect on impacts of biofeedstock and biogenic carbon.
- The application is illustrated through a case study in the chemicals industry.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 26 April 2019
Received in revised form 5 June 2019
Accepted 5 June 2019
Available online 7 June 2019

Editor: Damia Barcelo

Keywords: Biochemicals Biomass balance Life cycle assessment Sustainability Certification

ABSTRACT

Driven by the need to reduce greenhouse gas emissions and dependence on fossil resources, the chemical and other industries are gradually starting to develop bio-based products. For the introduction of bio-feedstocks in existing production pathways in a cost-effective way, a simplified approach based on mass balance has been proposed. This concept is known as the biomass balance (BMB) approach and the resulting products are called BMB products. They do not necessarily contain biomass material but can contribute to sustainable sourcing and production of bio-based products in the supply chain without any performance loss in comparison to the same products derived from fossil resources. The aim of the study is to show how the BMB approach can be used in life cycle assessment (LCA) while following the requirements set out in the ISO 14040 and 14044 standards. To demonstrate that, the proposed BMB approach has been used to estimate life cycle environmental impacts of a polymer product, which can be produced using fossil or bio-feedstocks. For the polymer derived from bio-feedstocks, bionaphtha and biogas are considered as replacement to naphtha and its impacts are compared with the fossil-based alternative. The paper demonstrates that the BMB approach provides a quick and pragmatic method for establishing the biomass content in chemical and related products while incentivising the industry to continue increasing the proportion of bio-based products in their product portfolio. It also shows that the environmental performance of BMB products is highly dependent on the particular bio-feedstock used, the way it is sourced and on key modelling assumptions, including the assumptions on biogenic carbon uptake in the bio-feedstocks. Crown Copyright © 2019 Published by Elsevier B.V. This is an open access article under the CC BY-NC-ND license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

1. Introduction

During the past two decades, a number of initiatives have been developed to address some of the environmental and social concerns

^{*} Corresponding author.

E-mail address: adisa.azapagic@manchester.ac.uk (A. Azapagic).

associated with the agriculture- and forest-based products (Mol and Oosterveer, 2015). This has led to a steady growth of markets for organic, Fairtrade® and 'eco-friendly' products (Lernoud et al., 2018). With the increasing demand for sustainable products, the need for independent verification of sustainability-related claims associated with commodities and products has also increased. As a result, a number of schemes have been developed to improve the traceability and transparency of agro-industrial and food supply chains (e.g. timber, cotton, bananas, coffee, cocoa, fish, palm oil, sugar) as well as of bioenergy (electricity and biofuels) (UNGC, 2014). Producers of such products are using these schemes to support sustainability claims through certification. At the same time, the information provided by such certification and labels on otherwise invisible characteristics of products help consumers to make more informed choices (Gassler and Spiller, 2018).

There are four models in terms of how certification schemes trace sustainability claims: *identity preservation*, *product segregation*, *mass balance*, and *book and claim* (Mol and Oosterveer, 2015). The first two models require that certified products are physically separated from non-certified at each stage along the value chain. In the identity preservation model, mixing of certified materials from other producers is not permitted. This enables the traceability of products back to the originating farm, forest or production site. However, owing to the complexity of supply chains, it is often difficult for companies to trace each and every step in the journey of a given product.

The product segregation model reduces this complexity by allowing mixing of products from different certified producers. This model is important to the organic produce sector, where organic and non-organic products are strictly separated. However, for other complex supply chains, maintaining complete segregation is not only difficult and expensive, but in many cases not essential or simply impossible due to technological or other reasons. In such cases, the mass balance model is often used, which allows for the controlled mixing of certified and non-certified materials at any stage of the supply chain. However, the exact quantities of the certified material entering the supply chain must be controlled and equivalent quantities of the product leaving the supply chain can be sold as certified. Both product segregation and mass balance models are currently being used for certification of biofuels and biomaterials, including by the European Union's Renewable Energy Directive (EU RED) (EU, 2018) and the organisation for International Sustainability and Carbon Certification (ISCC, 2019).

The book and claim model, on the other hand, is very different from all other models and does not require any physical or material link between the certified raw materials and the certified end-product. In this model, the producers of sustainable products obtain tradable certificates for their products and sell them to the interested companies via trading platforms. This type of system is widely used in the energy market for trading of renewable energy products and in carbon emissions

trading schemes. In both mass balance and book and claim models, the end products do not necessarily contain certified material but have contributed to the sourcing and production of the certified material by ensuring that a similar quantity has been produced according to the certification criteria.

With the drive to reduce greenhouse gas (GHG) emissions and dependence on fossil resources, the chemical industry has been developing bio-based products. However, replacing fossil feedstocks with biofeedstocks is a challenging task for the industry. Large investments are required in R&D and production facilities to produce bio-based chemicals. Moreover, due to technological limitations, currently only some products can be produced from bio-feedstocks alone. In an attempt to overcome some of these difficulties and improve traceability in their supply chain, BASF has proposed a simplified approach based on the above-mentioned mass balance model (Krüger et al., 2018). This concept is known as the biomass balance (BMB) approach (Fig. 1) and the resulting products are called BMB products. BMB products are chemicals that are produced using both fossil and biomass feedstocks in an integrated chemical production facility. The output is a mix of fossil- and bio-based products which are not distinguishable on the basis of their composition or technical characteristics. To allocate the specific characteristics of fossil or bio-feedstocks to the final product, the producers declare a certain share of their production to be from renewable resources, in proportion to the share of bio-feedstocks used as

Several studies have assessed life cycle environmental impacts of bio-polymers; for a review, see Spierling et al. (2018) and Hottle et al. (2013). In almost all of these studies, the segregation method is employed, whereby all inputs and emissions in the supply chain of the bio-products are accounted for, assuming that the bio-product supply chain is segregated. However, in reality, many companies are coproducing chemical products with varying proportions of bio- and fossil feedstocks in integrated production facilities. Therefore, collection of all the required data for life cycle assessment (LCA) for a segregated product becomes challenging. As a result, such data are often obtained based on simulation models instead of actual production data. In this regard, this study aims to show how the BMB approach can be used in LCA to simplify the data-related requirements for bio-products. A further goal is to find out if the BMB approach can be used in compliance with the requirements set out in the ISO standards for LCA (ISO, 2006a, 2006b). The application of the methodology is demonstrated through a real case study in the chemicals sector. The case study focuses on assessing life cycle environmental impacts of a polymer product, which is produced in an integrated production facility where a small proportion of fossil feedstocks is replaced by bio-feedstocks. The details of the case study are provided in Section 3. This is followed by the discussion of the results in Section 4 and the conclusions in Section 5. Prior to that,

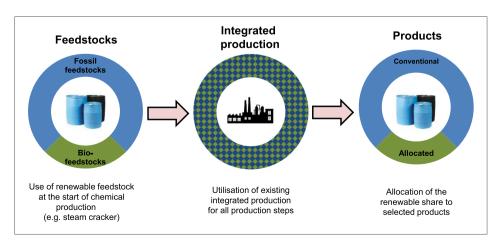


Fig. 1. The biomass balance (BMB) approach.

the next section describes the BMB approach and how it can be applied

2. Biomass balance methodology

The main fossil feedstocks in the chemical industry are naphtha and natural gas, which are further processed either by cracking or partoxidation at high temperatures. In BMB products, these feedstocks are replaced by bio-feedstocks, i.e. bio-naphtha and biogas (bio-methane). The amount of the fossil feedstocks and the quantities of biofeedstocks required to replace the fossil inputs are calculated through a material flow analysis.

To conduct an LCA of a BMB product, an existing ISO 14040/14044 compliant LCA model for the fossil-based product is used as a starting point. The life cycle environmental burdens for BMB products are determined in the Inventory phase according to Eq. (1):

$$\begin{array}{l} B_{BMB} = B_{fossil} + a_1 \left(c v_{N/BN} \times B_{BN} - B_N \right) + a_2 \left(c v_{N/BG} \times B_{BG} - B_N \right) \\ + b_1 \left(c v_{NG/BG} \times B_{BG} - B_{NG} \right) + b_2 \left(c v_{NG/BN} \times B_{BN} - B_{NG} \right) \end{array} \tag{1}$$

where:

B_{BMB} environmental burdens of biomass balanced products B_{fossil} environmental burdens of fossil-based products

a₁ amount of naphtha substituted by bio-naphtha

cv_{N/BN} chemical value factor for naphtha/bio-naphtha

B_{BN} environmental burdens of bio-naphtha

B_N environmental burdens of naphtha

a₂ amount of naphtha substituted by biogas

cv_{N/BG} chemical value factor for naphtha/biogas

B_{BG} environmental burdens of biogas

b₁ amount of natural gas substituted by biogas

cv_{NG/BG} chemical value factor for natural gas/biogas

B_{NG} environmental burdens of natural gas

b₂ amount of natural gas substituted by bio-naphtha cv_{NG/BN} chemical value factor for natural gas/bio-naphtha.

The "chemical value factor" cv is defined by Eq. (2) and is discussed further below:

$$cv = LHV_{fossil\ feedstock\ (substituted)}/LHV_{biofeedstock}$$
 (2)

where:

LHV lower heating value.

The sum of a_1 and a_2 in Eq. (1) represents the total amount of fossil naphtha substituted while the sum of b₁ and b₂ is the total amount of natural gas substituted by bio-feedstocks.

The LCA modelling is relatively straightforward if the bio-feedstocks have the same chemical properties as their fossil counterparts, hence being totally interchangeable. In such cases, the life cycle environmental burdens of naphtha or natural gas are subtracted from the total burdens of the fossil-based product and the burdens of bio-naphtha or biogas are added to the LCA model. However, some bio-feedstocks may have different carbon content, energetic value or other chemical properties from the fossil feedstocks to be replaced. This could lead to higher or lower requirements for bio-feedstock quantities compared to the quantities of fossil feedstocks. In such situations, it is necessary to consider the equivalent quantities of bio-feedstocks. For these purposes, it is suggested to use an equivalent factor, based on the lower heating value (LHV) of fossil and bio-feedstocks as an approximation of the chemical properties. This ratio in the context of the BMB approach is termed as the 'chemical value factor' of the feedstock (Eq. (2)). Although it is not necessarily related to chemical parameters, it is used to denote the use of feedstocks as chemicals rather than energy sources. The reason for using LHV is that these feedstocks are also used as energy sources and the LHV values are easily available and comparable across the feedstocks, unlike their differing chemical properties.

It is important to mention that this simplified LCA methodology for BMB products is only applicable when there are no other differences between fossil and bio-alternatives in terms of the production processes as well as in the use of auxiliaries and utilities. Also, the resulting fossil and bio-products must have the same properties and be completely interchangeable in terms of their further use.

The next section demonstrates through a real case how the BMB approach can be applied in LCA following the requirements of the ISO standards.

3. Application of the BMB method

The BMB approach is applied to a commercial polymer product produced by BASF from two monomers, here referred to as Monomer 1 and Monomer 2 to preserve confidentiality. Currently, the main feedstocks for these monomers are fossil naphtha and natural gas. To illustrate the BMB method and reduce the complexity, the focus is on the feedstock changes for Monomer 1, considering only the substitution of naphtha used for its production by bio-naphtha and biogas. In congruence with the LCA methodology, the goal and scope of the study are outlined first, followed by the inventory data and life cycle impact assessment methodology.

3.1. Goal and scope

The main goals of the study are to demonstrate how the BMB method can be used in LCA in congruence with the ISO standards and how it can help in simplifying the data requirements for bio-products. Through that, the study also aims to identify and discuss the environmental implications of using bio- instead of fossil feedstocks. Adhering to the 'accounting' perspective of the BMB approach and heeding the requirements of most business users of the product considered, an attributional modelling approach is applied.

The functional unit is defined as the production of 1 t of a polymer product. Since the physical and chemical properties (hence, the functions) of the polymer under study are not affected by the type of feedstock used, the selected functional unit is appropriate for comparing the different production routes. In order to have a clear focus on the different feedstocks and production processes, the scope of the study is from 'cradle to gate'. Thus, the use stage and end-of-life treatment of the product are not considered. Infrastructure-related processes, such as production of facilities, equipment and vehicles, as well as storage of products and production of packaging materials, are omitted from the assessment. The system boundaries are shown in Fig. 2, including the relevant foreground and background processes for the production of the considered product. In addition, Figs. 3 and 4 show the simplified production system of the two bio-feedstocks considered in the study. In the base case, it is assumed that production of monomers and polymers occurs on the same site. However, to represent relevant and typical supply chain alternatives, other scenarios are also considered for the production at different locations, taking into account transport between the production sites in a sensitivity analysis.

3.2. Inventory data

Life cycle inventory (LCI) data for the production of Monomer 1 from the fossil feedstock have been obtained from an industry association database (confidential), based on data from six plants in four European countries. This relates to 100% of the European production capacity in 2012.

It is assumed that the bio-naphtha and fossil naphtha have the same properties and are fully interchangeable. The former has been modelled according to a mix of bio-feedstocks, 64% of which is produced from palm oil and the rest from tallow. Crude palm oil is imported from

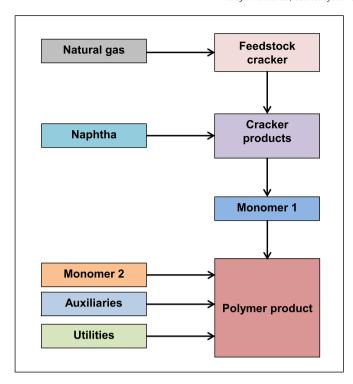


Fig. 2. System boundaries for production of the polymer considered in the study [For the BMB polymer, naphtha is assumed to be replaced by either bio-naphtha or biogas.]

Indonesia and tallow from Australia. Oceanic transport for both feedstocks is considered as specified in Table 1. Since supplier-specific LCI data for these feedstocks were not available, LCI data have been

Table 1LCI data for the production of bio-naphtha.

Inputs	Amount (per kg of bio-naphtha)	Notes
Palm oil	0.76 kg	To produce 0.64 kg of bio-naphtha (84% yield)
Tallow	0.4 kg	To produce 0.36 kg of bio-naphtha (91% yield)
Oceanic transport (bulk commodity carrier; 200,000 DWT)	10 t∙km	Palm oil from Indonesia and tallow from Australia.
Barge transport		
Hydrogen (from natural gas)	0.03 kg	For hydrogenation
Steam	0.07 kg	
Electricity	0.01 MJ	

obtained from the GaBi database (Thinkstep, 2017). In the case of tallow, LCI data for the production of tallow fatty acid (C16-C18 fatty acid from tallow) are used as proxy. For crude palm oil, GHG emissions from direct land use change (dLUC) from palm fruit plantations are also considered. These feedstocks are further processed via a hydrogenation process to produce bio-naphtha. The estimated quantities of steam, electricity and hydrogen used for the hydrogenation step are shown in Table 1.

For the polymer derived from biogas, the fossil naphtha in Monomer 1 is substituted by bio-methane, which is assumed to be produced from food (kitchen) waste via anaerobic digestion. It should be noted that, as kitchen waste contains both biomass and non-biomass materials, biogas is also mass-balance rather than bio-based. This is congruent with the definition of bio-based materials according to EN 16575 (CEN, 2014).

The differences in properties of bio-methane in comparison to naphtha are taken into account by introducing the chemical value factor as explained in Section 2 (Eq. (2)). LCI data for bio-methane have been

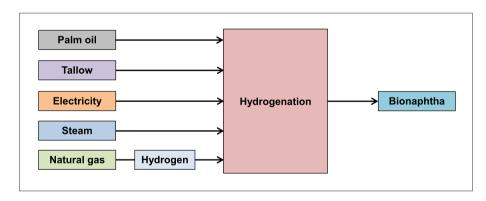


Fig. 3. System boundaries for production of bio-naphtha used as a feedstock for the BMB product.

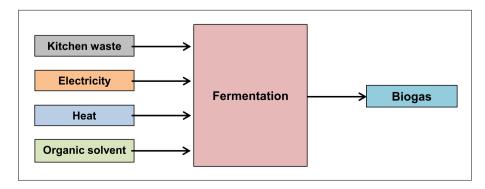


Fig. 4. System boundaries for production of biogas used as a feedstock for the BMB product.

Table 2Lower heating values (LHVs) of different feedstocks (Thinkstep, 2017).

Feedstock	LHV (MJ/kg)	
Naphtha	44.3	
Bio-naphtha	44.3	
Biogas	49.8	

sourced from the GaBi database (Thinkstep, 2017). In this model, food waste is considered as burden-free. The LHV of the feedstocks can be found in Table 2.

The inventory data for all upstream processes, such as the production of Monomer 2 and auxiliaries as well as the production of polymer, are based on primary data from BASF. The GaBi database (Thinkstep, 2017) has been used for the background data, including for the production of naphtha, natural gas, palm oil and tallow, as well as for transportation. An overview of the data used is given in Table S1 in Supplementary Information (SI). A data quality rating (DQR) in accordance with the EU product environmental footprint (PEF) (EC-JRC, 2011a) guide has been applied (see Table S2 in the SI for details), which shows that the considered datasets are of a good quality level.

Considering that the polymer product is manufactured in an integrated industrial plant along with various other products, production-related burdens have been allocated among the products using mass allocation. Exergy allocation has been applied for steam and electricity, which are co-produced in an on-site combined heat and power (CHP) system.

3.3. LCA modelling of BMB products

The LCA modelling has been carried out in the GaBi 7.3 software (Thinkstep, 2017), using a model for the fossil-based product as a starting point and applying Eq. (1) to estimate the environmental burdens of the BMB product. For bio-naphtha based BMB polymer, only the material use of naphtha in the fossil-based product is substituted as mentioned earlier. The product-specific consumption of naphtha to be substituted for the production of BMB products (a_1 for bionaphtha-based BMB and a_2 for biogas-based BMB) is calculated using the material flow analysis. Considering that the functional properties of naphtha and bio-naphtha are the same (Table 2), the chemical value factor cv is assumed to be 1. For the biogas-based BMB product, the cv is estimated by Eq. (2) at 0.89 (44.3 MJ/49.8 MJ) to account for the differences in the chemical properties of naphtha and biogas. The simplified equations for both cases, based on Eq. (1), are as below:

$$B_{BMB-BN} = B_{fossil} + a_1 (1 \times B_{BN} - B_N)$$
 (3)

$$B_{BMB-BG} = B_{fossil} + a_2 (0.89 \times B_{BG} - B_N)$$
 (4)

where:

 $B_{\text{BMB-BN}}\quad\text{environmental burdens of the bio-naphtha-based BMB}$ product

 B_{BMB-BG} environmental burdens of the biogas-based BMB product.

3.4. Sensitivity analysis

To gauge the robustness of the results and the validity of key assumptions described above, a sensitivity analysis has been carried out for the following three parameters that could affect the results:

- i) CO₂ uptake and the biogenic carbon;
- ii) assumptions on the land-use change; and
- iii) the production of the BMB product at different locations involving transport of Monomer 1.

3.5. Life cycle impact assessment

Various impact assessment methodologies are applicable for use in the respective regional contexts, including CML (Guinée et al., 2002), ReC-iPe (Huijbregts et al., 2016) and methods recommended by the ILCD (ECJRC, 2011b). This assessment is predominantly based on the compilation of impact categories recommended by the EU PEF guidelines, which follow the characterisation factors published in May 2016 based on EC-JRC (2011a). These impacts, applicable to the European context, include some widely used indicators but also others which are still under discussion in the scientific community. However, since the EU PEF framework has gained broad attention from industry and academia, due to its potential application in future EU regulations, it is deemed to contain an appropriate set of impacts for a study whose main audience is expected in the EU market. Table 3 presents the impact assessment categories considered along with the methods used for their estimation.

PEF guidelines also include some other categories, i.e. ozone depletion, water depletion, particulate matter, ionizing radiation and the toxicity (USEtox) related impacts, but these are not considered in the study for the following reasons. Ozone depletion potential is not assessed as no ozone-depleting substances are emitted in the foreground system. For water depletion and particulate matter impacts, relevant information for assessing these impacts according to the goal and scope of the study is lacking in most of the datasets. Ionizing radiation is not an internationally accepted indicator and there are large uncertainties associated with ecotoxicity. Finally, toxicity according to independent methods like USEtox has not been determined because of the lack of appropriate data for the foreground processes. Instead, the BASF human toxicity method, developed by Landsiedel and Saling (2002), is considered in the study.

4. Results and discussion

The LCA results applying the BMB approach are detailed in Figs. 5–13, which show the impacts for each of the nine impact categories considered, along with the contributions of different life cycle stages.

4.1. Climate change

The climate change impact has been estimated as global warming potential (GWP) for a 100-year perspective based on characterisation factors from the Intergovernmental Panel on Climate Change (IPCC,

Life cycle impact assessment categories.

Impact category	Unit	LCIA indicator	Reference
Climate change	kg CO ₂ eq.	Radiative forcing	IPCC (2013)
Depletion of elements	kg Sb eq.	Scarcity	Guinée et al. (2002)
Depletion of fossil resources	MJ	Scarcity	Guinée et al. (2002)
Acidification	mol H ⁺ eq.	Accumulated exceedance	Seppälä et al. (2006) and Posch et al. (2008)
Eutrophication - freshwater	kg P eq.	EUTREND model	Goedkoop et al. (2009)
Eutrophication - marine	kg N eq.	EUTREND model	Goedkoop et al. (2009)
Human toxicity	Tox points	Model based on H-phrases of GHS system	Landsiedel and Saling (2002)
Land use	kg C deficit eq.	Soil organic matter	Milà et al. (2007)
Summer smog	kg NMVOC eq.	Tropospheric ozone concentration increase	van Zelm et al. (2008)

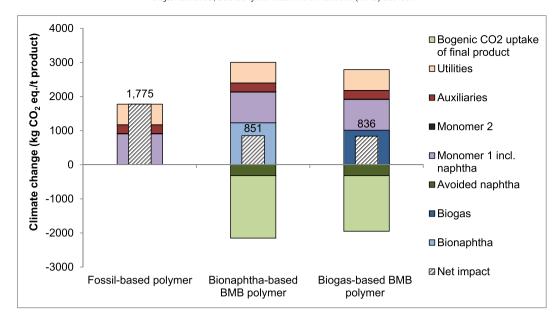


Fig. 5. Climate change impact of the fossil-based and BMB polymer.

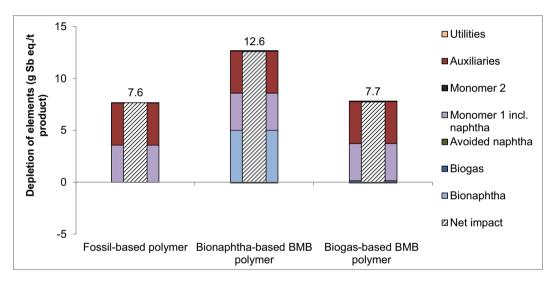


Fig. 6. Depletion of elements for the fossil-based and BMB polymer.

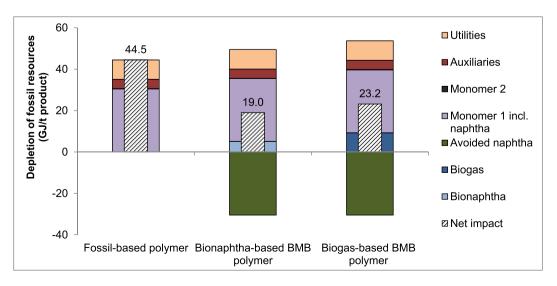


Fig. 7. Depletion of fossil resources for the fossil-based and BMB polymer.

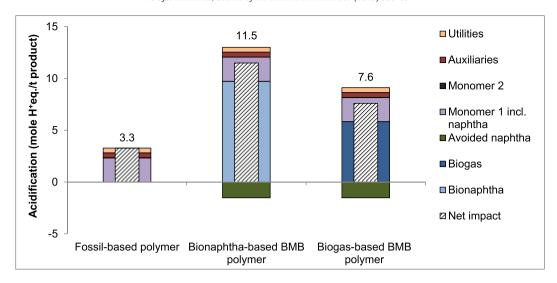


Fig. 8. Acidification of the fossil-based and BMB polymer.

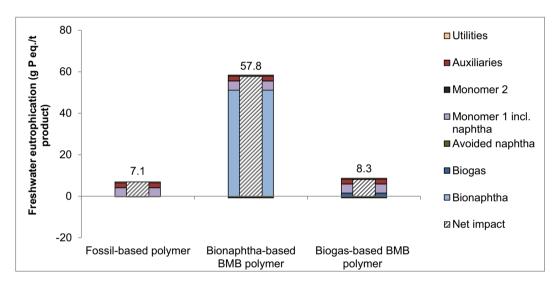


Fig. 9. Freshwater eutrophication of the fossil-based and BMB polymer.

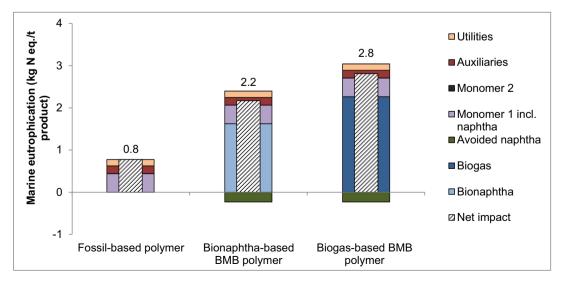


Fig. 10. Marine eutrophication of the fossil-based and BMB polymer.

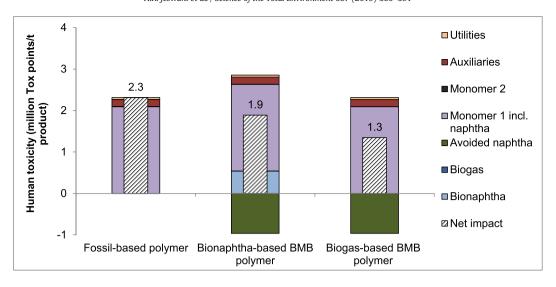


Fig. 11. Human toxicity of the fossil-based and BMB polymer.

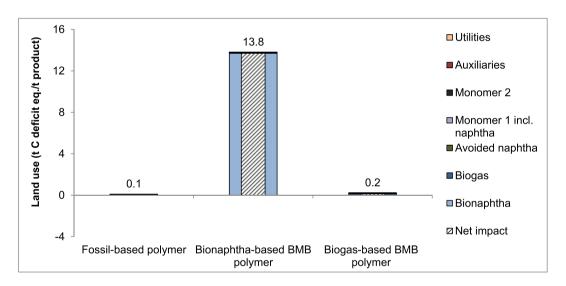


Fig. 12. Land use of the fossil-based and BMB polymer.

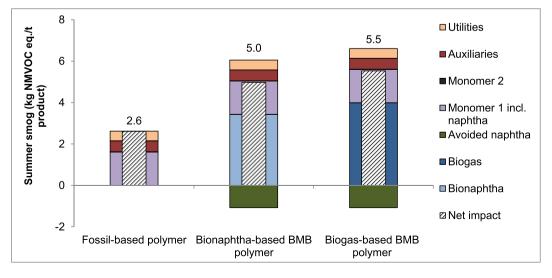


Fig. 13. Summer smog of fossil-based and BMB products.

2013); the results are displayed in Fig. 5. It is important to emphasise that this study has considered the storage of biogenic carbon in the bio-feedstocks by crediting the system for the uptake of CO₂ from the atmosphere. Also, given that the production of palm oil could involve dLUC, its effects are considered for the BMB polymer from bionaphtha. For dLUC-related emissions, land use changes caused by palm oil plantation during the last 20 years are considered. The impacts of the palm oil without dLUC as well as with indirect land use change (iLUC) are considered in the sensitivity analysis.

The cradle-to-gate climate change impact of the fossil-based polymer is estimated at 1775 kg CO₂ eq./t. Production of Monomer 1 and the use of utilities are the hotspots, with the contribution of 51% and 34%, respectively. As shown in Fig. 5, the BMB alternatives exhibit a better performance in the climate change impact in comparison to the fossil alternative. The lowest impact is found for the biogas-based option (836 kg CO₂ eq./t), 53% below that of the fossil alternative. Replacing fossil naphtha by bio-naphtha also reduces the impact substantially (851 kg CO₂ eq./t). This reduction in the impact for the BMB alternatives is mainly due to the credits for biogenic CO₂ uptake in the final product. Therefore, if the BMB alternatives are considered in cradle-to-grave LCA studies, any emissions of the corresponding biogenic CO₂ emissions must be considered in the end-of-life modelling. However, if the uptake of carbon is excluded, then the BMB products would have a higher cradle-to-gate climate change impact than the fossil alternative (see Fig. 5).

Bio-naphtha production has a higher climate change impact than biogas, partly due to the dLUC emissions and partly due to the assumption that biogas is derived from burden-free kitchen waste. At the same time, the $\rm CO_2$ uptake of biogas-based product is slightly lower than that derived from bio-naphtha due to the lower chemical value factor for biogas (see the explanation in Section 3.3). As a result, the difference in the climate change impact between the two BMB alternatives is very small.

4.2. Abiotic resources depletion (elements and fossil)

The abiotic resources depletion has been determined according to Guinée et al. (2002). As shown in Fig. 6, the auxiliaries and Monomer 1 are the hotspots for element depletion for the fossil-based polymer, with contributions of 53% and 47%, respectively. It can also be seen that there is no notable difference in element depletion for biogas-based BMB and its fossil counterpart. However, bio-naphtha-based alternative has a substantially (64%) higher impact than the fossil-derived polymer. This increase is almost entirely caused by palm oil production, largely due to the use of fertilisers.

In the case of fossil depletion, the main hotspot for the fossil polymer is the production of Monomer 1, which accounts for 68% of the impact (Fig. 7). This is due to the use of naphtha as a feedstock. Therefore, as expected, the exchange of naphtha with bio-naphtha or biogas leads to a significant decrease (48% and 57%) in the impact for the BMB polymer. Fossil depletion for the production of biogas is double that of bionaphtha production due to the use of electricity in biogas production.

4.3. Acidification

For the evaluation of acidification, the accumulated exceedance method according to Seppälä et al. (2006) and Posch et al. (2008) has been used. As shown in Fig. 8, the substitution of naphtha by bionaphtha leads to a factor of three increase in the impact from the BMB product compared to the fossil-based alternative (11.5 vs. 3.3 mol $\rm H^+$ eq./t). Using biogas instead, increases the impact around two times (7.6 mol $\rm H^+$ eq./t). The impact of biogas production is lower than for bio-naphtha due to the burden-free kitchen waste used for biogas production.

The main influencing factors for the polymer from bio-naphtha are ammonia emissions from the production of tallow and palm oil, along

with the nitrogen oxide emissions from palm fruit plantations. For the biogas-based alternative, nitrogen monoxide and sulphur dioxide emissions from biogas production are the most important contributors. The former contributes 71% to the impact from biogas production, while the latter accounts for 21%. For the fossil-based product, 70% of the impact is associated with the production of Monomer 1, while the auxiliaries and utilities account for 15% each.

4.4. Eutrophication (freshwater and marine)

The eutrophication impacts are assessed based on the EUTREND model (Goedkoop et al., 2009) and the results are displayed in Figs. 9 and 10. As can be seen, the fossil-based polymer performs better in comparison to the BMB alternative for both impacts. For freshwater eutrophication, the bio-naphtha-based polymer has an eight times higher impact than the fossil-based option, while the difference between the biogas and fossil counterparts is relatively small (~15%). The latter is probably due to the burden-free kitchen waste. For the polymer from bio-naphtha, 89% of the impact is caused by bio-naphtha production, largely due to tallow production (70%).

The fossil alternative has around three times lower impact than the bio-naphtha and biogas polymer (Fig. 10). Again, the production of bio-naphtha and biogas are the major contributors, accounting for 75% and 81% of the total, respectively. For bio-naphtha, 59% of the impact comes from the production of tallow and the rest from the palm oil. The main burdens are nitrogen emissions to freshwater (for both tallow and palm oil) and air emissions of nitrogen oxides (for palm oil). For biogas, 96% of the total impact is caused by nitrogen monoxide emitted in anaerobic digestion to produce biogas. The contribution of Monomer 2, all other auxiliaries and the utilities is very small.

4.5. Human toxicity

Fig. 11 shows the human toxicity potential of the three alternatives considered in the study, determined using the afore-mentioned BASF method. In the case of the fossil-based polymer, the impact is estimated at 2.3 million Tox point/t, 90% of which is associated with the production of Monomer 1. The biogas alternative has the lowest human toxicity, 42% below that of the fossil counterpart. Bio-naphtha-based BMB also performs better than the polymer from the fossil feedstock, with an 18% lower impact, because the production of bio-naphtha has a 78% lower human toxicity than naphtha.

4.6. Land use

Land use is considered to determine whether the agricultural activities related to bio-naphtha production have an influence on the overall results. The soil organic matter method (SOM) from Milà et al. (2007) has been chosen for this purpose as recommended in the ILCD handbook (EC-JRC, 2011b).

Exchanging fossil naphtha by bio-naphtha would increase land use by a factor of 137 (Fig. 12). This is due to the high demand of land in agricultural production of palm oil. All other materials and processes, including transport, have negligible contribution to land use. Although the biogas-based alternative has a much lower land requirements than the bio-naphtha-based product, its impact is still twice as high as that of the fossil counterpart (Fig. 12).

4.7. Summer smog

The potential for the formation of summer smog has been estimated using the model of van Zelm et al. (2008) related to an increase in the tropospheric ozone concentration. As can be seen in Fig. 13, summer smog for the fossil-based polymer is estimated at 2.6 kg NMVOC eq./t. The majority of this (61%) is associated with the production of Monomer 1, with the auxiliaries and utilities contributing around 20% each.

The substitution of naphtha by bio-naphtha or biogas leads to a two times higher summer smog for the BMB polymer. For the bio-naphtha, the production of palm oil accounts for 58% of the total impact, mainly due to nitrogen oxide emissions associated with the cultivation. Much of the remaining impact is due to tallow production, largely due to NMVOC emissions. For the biogas alternative, nitrogen monoxide emissions from fermentation are the main contributor, accounting for 91% of the impact from biogas production. Summer smog of biogas production is higher than that of bio-naphtha production due to the higher emissions from the fermentation process.

4.8. Sensitivity analysis

4.8.1. CO₂ uptake: Chemical value vs biogenic carbon content

In the base case, the CO_2 uptake in the biogas-based BMB product has been calculated based on the chemical value of biogas. Here, the CO_2 uptake is estimated on the basis of the biogenic carbon content of the final product. Fig. 14 shows the climate change impact for both approaches; the other impacts considered in the study are not affected by this assumption. The results show that there is a substantial (24%) decrease in the impact if the chemical value of the feedstock is not considered. This is because the use of the chemical value factor (as in the base case) leads to lower estimates of the CO_2 uptake in comparison to the carbon content of the final product. If the difference in the chemical value is higher, the influence on the impact would be higher. Thus, it is recommended to use the worst case approach, as considered in the base case.

4.8.2. LUC in palm oil production

As mentioned earlier, the LCI data for palm oil have been obtained from the GaBi database which includes GHG emissions related to dLUC. Given that the palm oil used in the production of the BMB product considered here is certified and does not involve dLUC, the effect on climate change of excluding it is investigated here. Without dLUC, the impact of the bio-naphtha-based BMB product would decrease by 54%, from 851 kg CO₂ eq./t to 390 kg CO₂ eq./t (Fig. 15). This finding is congruent with a recent consequential LCA study on palm oil (Schmidt and De Rosa, 2018) which claimed that certified palm oil has 40% lower GHG emissions than non-certified palm oil.

However, it is possible that palm oil from certified sources can still cause iLUC. To investigate its potential effect on the climate change impact, the EU RED (2009) default iLUC value of 55 g CO₂ eq./MJ palm oil (corresponding to 2 kg CO₂ eq./kg palm oil with a LHV of 36.3 MJ/kg) is considered instead of dLUC. The results show that the impact of bionaphtha BMB product would increase by 36%, from 851 kg CO₂ eq./t to 1159 kg CO₂ eq./t. However, it would still have 34% lower impact than

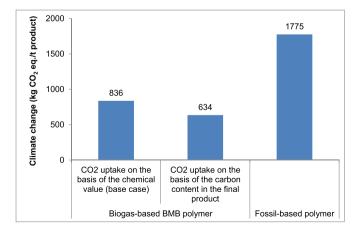


Fig. 14. Effect of the CO_2 uptake and biogenic carbon on the climate change impact from the biogas-based BMB polymer.

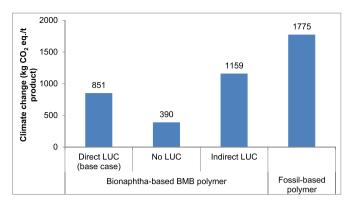


Fig. 15. Effect of land use change in palm oil production on the climate change impact from bio-naphtha-based BMB polymer.

the fossil-based product. Nevertheless, it should be noted that it is uncommon to consider iLUC in an attributional LCA study.

4.8.3. Production at different sites

In the base case, it has been assumed that the production of Monomer 1 and the BMB product occur on the same site. However, it is possible that substitution of naphtha in the bio-naphtha-based Monomer 1 occurs in one facility, while the BMB product is produced at another production site. Although this does not necessary involve transport of bio-naphtha-based Monomer 1, in this scenario, an option of transporting to a North American production site (as a worst case) is considered. This would involve a 500 km barge transport and a 9500 km ocean-tanker transport. Other data are assumed to be the same as in the base case. Table 4 compares the results for this scenario with the base case for all the considered impact categories.

The results show that the consideration of transport would lead to a small increase (2%-4%) in climate change and fossil depletion. For summer smog, acidification and marine eutrophication, sea transport has some effect (8%-14%), while there is no change in the values for freshwater eutrophication, land use, depletion of elements and human toxicity.

4.9. Summary of the findings

The results of the study reveal that in comparison to their fossil-based counterpart, the BMB product performs better on climate change (considering biogenic carbon storage), fossil depletion and human toxicity due to the avoided production of fossil naphtha for Monomer 1. On the other hand, the use of biogas or bio-naphtha instead of naphtha for the production of the monomer leads to an increase in acidification, depletion of elements, eutrophication, summer smog and land use. These findings relate to the assumption that the production processes, auxiliaries, utilities and Monomer 1 are identical for the fossil and biomass alternatives.

The results of the sensitivity analysis show that the assumptions on the CO_2 uptake and LUC have a significant influence on the climate change impact. Additional transport of Monomer 1 between the production sites is less influential, increasing the impacts by 2%-14%.

One of the important limitations of the study is the use of secondary datasets for naphtha and the feedstocks for the production of bionaphtha and biogas. Specifically, the background dataset for palm oil are estimates. These results might change if country-specific primary datasets are used for these processes. Furthermore, if the food waste used for the biogas production is not assumed burden-free and/or not credited for the uptake of CO₂ from the atmosphere during food production, the overall impacts of the biogas-based BMB product might change substantially.

Table 4 Effect of transport on the impacts.

Impact category	Unit (per t product)	Bio-naphtha BMB polymer (base case)	Production at different sites	Difference
Climate change	kg CO ₂ eq.	851	883	4%
Acidification	mol H ⁺ -eq.	11.5	12.5	9%
Eutrophication – freshwater	g P eq.	57.8	57.9	_
Eutrophication – marine	kg N eq.	2.2	2.4	12%
Summer smog	kg NMVOC eq.	5.0	5.7	15%
Abiotic resources - elements	g Sb eq.	12.6	12.6	-
Abiotic resources - fossil	GJ	19.0	19.4	2%
Land use	t C deficit eq.	13.8	13.8	_
Human toxicity	Million Tox points	1.9	1.9	-

5. Conclusions and recommendations

The biomass balance (BMB) approach is an innovative and simple method allowing evaluation of life cycle environmental impacts of bio-based products without the need for building up the whole value chains separately from the fossil-based routes. Thus, it can support rapid estimations of environmental implications of substituting fossil with bio-feedstocks in the chemical and related industries.

Its application to a real case study demonstrates that the approach can be used efficiently and effectively in LCA while following the requirements of the ISO standards. The main characteristic of the BMB method is the process chain, which is also a basic requirement of these standards to build up an inventory on a unit process level. This is also reflected in the case considered in this study.

The study highlights the influence of some key methodological and modelling aspects related to LCA of bio-based products. Given that the system boundary in the study is from cradle-to-gate, the system is credited for the uptake of biogenic carbon by the bio-feedstocks. However, this will require consumers of the BMB products to account for the release of the biogenic carbon at the end of the product life cycle. Therefore, it is necessary to report transparently the CO₂ uptake so that for subsequent cradle-to-grave studies, the carbon emissions can be taken into account accordingly.

The analysis also highlights the methodological challenges in treating feedstocks derived from biogenic waste. Such feedstocks are often considered burden-free as any impacts arising up until waste treatment/resource recovery are assigned solely to the product responsible for the waste generation. Therefore, consideration of the uptake of biogenic carbon for BMB products for burden-free waste streams needs further deliberation.

Furthermore, based on the findings of the study, it is suggested that the estimation of the CO_2 uptake in biomass-balanced products should be adjusted on the basis of the lower heating value of the feedstocks if there are differences in the chemical properties of fossil and biofeedstocks. This approach needs further refinement and should be addressed in future BMB LCA studies, possibly considering an alternative approach. It is also suggested that future studies apply this methodology for BMB products in other sectors, such as agro-industrial and bioenergy. This will help in identifying any other methodological issues that need addressing, hence enhancing the methodology.

For some bio-feedstocks, such as palm oil, GHG emissions from dLUC and iLUC could significantly affect the overall climate change impact of bio-based products. Therefore, it is important to consider such emissions in LCA studies of BMB products. Bio-feedstocks procured from certified sources are not associated with dLUC but can still contribute to iLUC. However, iLUC related emissions are not considered in an attributional LCA so it may be necessary to switch to consequential LCA. However, in that case, a new BMB approach may be needed which could be considered as part of future work.

It is often difficult to obtain primary data for some bio-feedstocks (e.g. for palm oil) because of complex supply chains. The use of secondary data for bio-feedstocks can be a source of major uncertainty in the results. Thus, it is recommended to consider improved and more

detailed LCI data, especially for raw materials, in future BMB-related studies. Also, all uncertainties in inventory data should be identified and reported along with a detailed uncertainty analysis.

In conclusion, this study can help in improving the understanding of the suitability of the BMB approach being used in relation to the requirements of existing LCA standards. However, considering the influence of the above aspects, it is of utmost importance that the corresponding assumptions and their influence on the results and conclusions be described and communicated transparently whenever the study, or parts thereof, are disclosed to any stakeholders to avoid possible misinterpretation of the study.

Acknowledgements

This work was funded by BASF. The authors are grateful to Dr Carl Vadenbo of Aveny GmbH and Professor Konrad Hungerbuehler of ETH Zürich for their advice and comments on the methodology development. We also acknowledge Dominik Müller of TÜV Rheinland for his contribution to LCA modelling.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.scitotenv.2019.06.088.

References

CEN, 2014. European Standard EN 16575: 2014. Bio-Based Products –Vocabulary. European Committee for Standardization, ftp://ftp.cen.eu/CEN/Sectors/List/bio_basedproducts/DefinitionsEN16575.pdf.

EC-JRC, 2011a. Analysis of Existing Environmental Footprint Methodologies for Products and Organizations: Recommendations, Rationale, and Alignment. First ed. European Commission- Joint Research Centre - Institute for Environment and Sustainability, Italy

EC-JRC, 2011b. International Reference Life Cycle Data System (ILCD) Handbook- Recommendations for Life Cycle Impact Assessment in the European Context. First ed. European Commission- Joint Research Centre - Institute for Environment and Sustainability. Luxemburg.

EU, 2018. Directive (EU) 2018/2001 of the European Parliament and of the council of 11 December 2018 on the promotion of the use of energy from renewable sources (text with EEA relevance.) PE/48/2018/REV/1. OJ L 328, 82–209 21.12.2018.

Gassler, B., Spiller, A., 2018. Is it all in the MIX? Consumer preferences for segregated and mass balance certified sustainable palm oil. J. Clean. Prod. 195, 21–31.

Goedkoop, M., Heijungs, R., Huijbregts, M., De Schryver, A., Struijs, J., Van Zelm, R., 2009. ReCiPE 2008: A Life Cycle Impact Assessment Method which Comprises Harmonised Category Indicators at the Midpoint and the Endpoint Level- First Edition. Report I: Characterization. Ruimte en Milieu. Ministerie van Volkshuisvesting, Ruimtelijke Ordening en Milieubeheer, The Netherlands.

Guinée, J.B., Gorrée, M., Heijungs, R., Huppes, G., Kleijn, R., Koning, A.d., Oers, L.v., Wegener Sleeswijk, A., Suh, S., Udo de Haes, H.A., Bruijn, H.d., Duin, R.v., Huijbregts, M.A.J., 2002. Handbook on Life Cycle Assessment. Operational Guide to the ISO Standards. Kluwer Academic Publishers, Dordrecht.

Hottle, T.A., Bilec, M.M., Landis, A.E., 2013. Sustainability assessments of bio-based polymers. Polym. Degrad. Stab. 98, 1898–1907.

Huijbregts, M.A.J., Steinmann, Z.J.N., Elshout, P.M.F., Stam, G., Verones, F., Vieira, M.D.M., Hollander, A., Zijp, M., Zelm, R.V., 2016. ReCiPe 2016 - a harmonized life cycle impact assessment method at midpoint and endpoint level; report I: characterisation. www. rivm.nl/bibliotheek/rapporten/2016-0104.pdf.

IPCC, 2013. Anthropogenic and natural radiative forcing. Climate Change 2013: The Physical Science Basis. Contribution of Working Group I to the Fifth Assessment Report.

- Intergovernmental Panel on Climate Change https://www.ipcc.ch/pdf/assessment-report/ar5/wg1/WG1AR5_Chapter08_FINAL.pdf.
- ISCC, 2019. International sustainability & carbon certification. https://www.iscc-system.
- ISO, 2006a. ISO 14040: Environmental Management Life Cycle Assessment Principles and Framework (Geneva. Switzerland).
- ISO, 2006b. ISO 14044: Environmental management Life cycle assessment Requirements and guidelines (Geneva, Switzerland).
- Krüger, C., Kicherer, A., Kormann, C., Raupp, N., 2018. Biomass balance: An innovative and complementary method for using biomass as feedstock in the chemical industry. In: Benetto, E., Gericke, K., Guiton, M. (Eds.), Designing Sustainable Technologies, Products and Policies: From Science to Innovation. Springer International Publishing, Cham, pp. 101–107.
- Landsiedel, R., Saling, P., 2002. Assessment of toxicological risks for life cycle assessment and eco-efficiency analysis. Int. J. Life Cycle Assess. 7, 261–268.
- and eco-efficiency analysis. Int. J. Life Cycle Assess. 7, 261–268.
 Lernoud, J., Potts, J., Sampson, G., Schlatter, B., Huppe, G., Voora, V., Willer, H., Wozniak, J.,
 Dang, D., 2018. The State of Sustainable Markets 2018: Statistics and Emerging
 Trends. ITC, Geneva.
- Milà i Canals, L., Romanyà, J., Cowell, S.J., 2007. Method for assessing impacts on life support functions (LSF) related to the use of 'fertile land' in Life Cycle Assessment (LCA). I. Clean. Prod. 15, 1426–1440.
- Mol, A.P.J., Oosterveer, P., 2015. Certification of markets, markets of certificates: tracing sustainability in global agro-food value chains. Sustainability 7, 12258.

- Posch, M., Seppälä, J., Hettelingh, J.-P., Johansson, M., Margni, M., Jolliet, O., 2008. The role of atmospheric dispersion models and ecosystem sensitivity in the determination of characterisation factors for acidifying and eutrophying emissions in LCIA. Int. J. Life Cycle Assess. 13, 477.
- Schmidt, J., De Rosa, M., 2018. LCA of certified palm oil. 11th International Conference on Life Cycle Assessment of Food 2018 (LCA Food), Bangkok, Thailand.
- Seppälä, J., Posch, M., Johansson, M., Hettelingh, J.-P., 2006. Country-dependent characterisation factors for acidification and terrestrial eutrophication based on accumulated exceedance as an impact category indicator. Int. J. Life Cycle Assess. 11, 403–416.
- exceedance as an impact category indicator. Int. J. Life Cycle Assess. 11, 403–416.

 Spierling, S., Knüpffer, E., Behnsen, H., Mudersbach, M., Krieg, H., Springer, S., Albrecht, S., Herrmann, C., Endres, H.-J., 2018. Bio-based plastics a review of environmental, social and economic impact assessments. J. Clean. Prod. 185, 476–491.
- Thinkstep, 2017. GaBi ts V 7.2 software and database. https://www.thinkstep.com/.
- UNGC, 2014. A Guide to Traceability a Practical Approach to Advance Sustainability in Global Supply Chains. United Nations Global Compact Office, New York.
- van Zelm, R., Huijbregts, M.A.J., den Hollander, H.A., van Jaarsveld, H.A., Sauter, F.J., Struijs, J., van Wijnen, H.J., van de Meent, D., 2008. European characterization factors for human health damage of PM10 and ozone in life cycle impact assessment. Atmos. Environ. 42, 441–453.