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# Biosurfactant-containing products from an environmental perspective – life cycle assessment of a liquid laundry detergent and a personal care product

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This study evaluates the environmental impacts of products containing a biotechnologically produced biosurfactant in a prospective cradle-to-grave life cycle assessment (LCA). To gain better understanding of the product system and enhance the product sustainabilty, we analysed two potential applications of the glycolipd biosurfactant mannosylerythritol lipid (MEL) in a liquid laundry detergent (LLD) and a cosmetic cream. Although MEL manufacturing is currently conducted at laboratory scale and several aspects have been upscaled for the LCA, we anticipate further enhancements as the production scale and technology readiness rise. For LLD, the LCA results in 0.44 kg CO<sub>2</sub>-eq. for the category climate change (CC) per wash load of 4.5 kg textile. The electricity demand for washing at 40 °C and the production of formulation components are identified as the main contributing processes. The cosmetic cream contributes 0.12 kg CO2-eq. to CC per tube of 50 g cream, which is mainly influenced by the production of the cream ingredients and packaging. To identify potential improvements and address uncertainties in surfactant efficiency, a scenario analysis was carried out. For LLD, improving the washing performance is found to be particularly important, as a reduced washing temperature combined with optimistic assumptions revealed a potential reduction of 65% in CC. The impact of the cosmetic cream can be improved primarily through the type of ingredients used and improving their production, as well as packaging design, resulting in 32% reduction in CC in an optimistic case. In conclusion, the findings indicate that biosurfactants may significantly influence the environmental performance for both products considered. They highlight the need for continued research on both further process development for biosurfactant production and on tailored formulations.

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#### Sustainability spotlight

To achieve the transition from a fossil to a biobased economy, it is necessary to develop alternative materials and production routes, including for surfactants. To evaluate biosurfactants regarding their environmental sustainability, it is important to not only assess their production, but also their use and disposal, which significantly depend on the application, the surfactant's chemical properties and the performance in a formulation. The prospective character of this LCA study provides an improved understanding of the role of biosurfactants in two application cases and can be used to guide product development. It therefore contributes to SDG 12 (Responsible consumption and production) and SDG 9 (Industry, innovation, technology and infrastructure), while also addressing further SDGs, such as Goals 13, 14 and 15.

#### Introduction

The challenge of tackling climate change demands the shift from fossil resources to biogenic alternatives. This transition to a bioeconomy is promoted by the European Union through various programs and initiatives, such as the European Green Deal, the Circular Economy Action Plan, the Farm to Fork Strategy, the Biodiversity Strategy, and the Chemical Strategy.¹ This transition also concerns the use of surfactants, which are versatile substances, due to their amphiphilic structure. Their functions as emulsifiers, wetting and dissolving agents have made them essential components in washing, care, and cleaning products since their discovery. Surfactants facilitate the removal of dirt from soiled surfaces by reducing surface tension and allowing water to permeate the soil. They function through adsorption at interfaces and can also inhibit the re-deposition of dirt on the cleaned surface.² The global market size for surfactants is estimated to be 18.25 million tons³ in 2024 and is

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expected to grow to 70.13 billion US dollars<sup>4</sup> in 2032. To date, they are predominantly chemically synthesized from petrochemical and oleo sources. An alternative is provided by biobased and biotechnologically produced surfactants, referred to as "biosurfactants".<sup>5,6</sup>

As early as 1996, a Life Cycle Inventory (LCI) of the non-ionic surfactants alkyl polyglycosides (APGs) of renewable raw materials had been provided by Frank Hirsinger.7 This LCI gives a comprehensive inventory of the environmental impacts and resource consumption of alkyl polyglycosides as part of the life cycle analysis. To evaluate not only the environmental aspects of biosurfactant production but also the application of biosurfactants, two potential products containing mannosylerythritol lipids (MEL) are considered with Life Cycle Assessment (LCA) within the scope of this research. For a first application, a liquid laundry detergent (LLD) is evaluated in this article. The second application for biosurfactants under consideration is as an emulsifier in a cosmetic cream. This way, this study builds upon the research gap identified in the review paper on LCA of biosurfactants by Briem et al., specifically regarding the use phase and end-of-life of biosurfactants in product applications.8

The production design, such as substrate type, production strains and process conditions significantly influence the molecular structure of hydrophobic side chains. These effects were characterized for MELs in the publications by Beck et al. 9-11 The modified molecular structure of MEL results in correspondingly varying physiochemical properties, which could be tailored this way according to their application. For instance, the production of a particularly hydrophilic MEL structure through targeted design of the production process may result in advantages for certain applications, such as laundry detergents. practical applications, multi-surfactant systems are commonly used for many applications, such as laundry detergents, to benefit from synergistic effects. Valuable insights into the enhanced washing performance resulting from the combination of specific MELs with sophorolipids and/or anionic surfactants are mentioned in patent DE 10 2023 212 849 A1.12 It indicates that the washing performance of MEL is generally in a comparable range to that of the mentioned surfactants and can even surpass them when co-formulated.12 Further information regarding the structure, functions, and applications of MELs, as well as their potential within the context of a circular economy, can be found in the review articles by W. N. F. W. M. Zulkifli, et al.13 and J. D. de Almeida, et al.14 These studies provide a comprehensive analysis of the structural characteristics of MELs, highlighting their diverse biochemical properties and versatility as biosurfactant, additionally, they explore various applications of MELs in industries such as cosmetics, pharmaceuticals, and agriculture, emphasizing their antimicrobial and antiadhesive properties. The articles also discuss innovative production methods, including the utilization of waste materials, which present significant opportunities for enhancing sustainability and promoting a circular economy. 13,14

Additionally, the European Platform on Life Cycle Assessment (EPLCA) supports the methodological development of LCA as an essential integrated environmental assessment to support to the EU policy making process and the ambition of

Green Deal, and many other policy initiatives.1 To assess the environmental impact of products the European Commission proposed the Product Environmental Footprint (PEF) as a LCAbased method. Its aim is to establish a common, harmonized approach to measure and communicate the life cycle environmental performance of products and organizations.<sup>15</sup> Therefore, the development of product-specific calculation rules (Product Environmental Footprint Category Rules, PEFCRs) and sector-specific rules (Organisation Environmental Footprint Sector Rules, OEFSRs) was tested in the pilot phase running from 2013 to 2018 with the active participation of stakeholders, such as the International Association for Soaps, Detergents and Maintenance Products (AISE), resulting in the finalisation of 19 PEFCRs and 2 OEFSRs published in the Commission Recommendation (EU) 2021/2279. AISE evaluated the application of the PEF methodology for heavy-duty liquid laundry detergents for machine applications, which provides one of the main references for this research. AISE concludes that the EF method is overall moving into the right direction, while recognizing its mid- to long-term potential. However, the methodology and life cycle inventory data availability are considered to be not yet sufficiently robust.16 Therefore, AISE found that some limitations apply to this first PEFCR version, such as the finding that several EF impact methods are not yet ready for comparative testing.17 For this reason, AISE recommends to use the available PEFCR to engage with upstream businesses, such as suppliers, in order to improve relevant processes, but not to use product specific PEF results for communication with retailers and costumers, given the complexity, remaining challenges and methodological limitations.17 Nevertheless, the PEF pilot project facilitated the identification of the relevant impacts of a European representative liquid laundry detergent, which will be discussed in more detail in the following section.

This pilot PEFCR study provides fundamental data for modelling and conducting LCAs for LLDs. The updated data regarding the definition of the functional unit (FU) and the modelling of the use phase of LLDs is published in the Commission Recommendation (EU) 2021/2279.15 The EPLCA recommends assuming a larger washing machine (8 kg) with higher energy consumption (0.81 kWh) and lower water consumption (39.5 litres) per washing cycle compared to the pilot study.15 Furthermore, specific information about washing machine models has been published, which can be used for modelling. The results of the pilot study and AISE's conclusions indicate that the use phase of the LLD, particularly the energy demand, has the most significant environmental impact over the product lifecycle.17 Concluding in a high degree of dependency of the PEF profile on consumer's behaviour and the country-specific electricity mix in the use phase.17 Additionally, AISE emphasizes the necessity of evaluating cleaning performance even at low washing temperatures, when successfully applying the PEF climate change indicator.17 It should also be considered that the formulation of the reference product, as defined in 2013, is no longer considered up-to-date and would therefore require updating.17

Insights for modelling and conducting LCA in the application example of cosmetic cream are provided by the comprehensive LCA analysis of an APG-containing cosmetic cream based on palm kernel oil by Guilbot et al. in 2013 and a subsequent study by Martinez et al. in 2017.18,19 Both studies identify transport to retailers and consumers, as well as packaging, as the main contributing processes. According to Guilbot et al., the influence of purchasing is relatively easy to anticipate (the shorter the distance, the more environmentally friendly the transport mode and the lower the impacts).18 To reduce the impact of packaging on production and transport, Martinez et al. propose an eco-design with reduced packaging weight.19 Furthermore, both research groups found that industrial transformation processes and the production of other vegetable oils, followed by refined palm kernel oil and wheat derivatives, are the main contributing processes in the production of cosmetic cream. 18,19 This is directly related to the quantity used and the cultivation conditions of the plant from which the oil is extracted.18 The use of palm oil primarily affects the impact categories of climate change and land use, due to deforestation and the transformation of peat soils.19

Briem et al.8 analysed publicly available literature on LCA of microbial biosurfactants and give an overview on main aspects of the LCA studies and findings. Only a limited number of publicly available LCA studies on microbial biosurfactants was identified in this review, and none specifically for MEL. In 2023, the research group of Schonhoff et al.20 investigated sustainability aspects of MEL and rhamnolipid production from sugar industry substrates, conducting an LCA to evaluate environmental impacts, while also addressing social and economic considerations. Further, Bippus et al.21 conducted a prospective LCA to accompany the development of the fermentation of MEL from rapeseed oil and glucose in an aerated bioreactor and downstream purification. Using experimental data scaled up to a 10m<sup>3</sup> reactor and prospective assumptions, the findings from a scenario analysis highlight opportunities for process optimization related to substrate use, bioreactor aeration and solvent use in downstream processing. These studies offer a compressive analysis of recent developments in MEL production, however, the availability of environmental data for microbial biosurfactant production, but particularly for applications of microbial biosurfactants remains limited.

For the considered application examples, no other publicly available comprehensive LCA studies examining the entire life cycle of the products were found, aside from those mentioned above, particularly none involving the use of biotechnologically produced surfactants, such as MEL. Most studies focus on conventional and/or bio-based surfactants, as well as an exclusive examination of product packaging. For these reasons, this cradle-to-grave LCA study on biosurfactant-containing products aims to address this research gap and contribute to closing it.

#### Materials and methods

To assess the potential environmental impacts associated with the entire life cycle of the biosurfactant-containing products under consideration the internationally recognized LCA method is applied, based on the ISO standards 14040 and 14044.22,23 The goal of the assessment is to identify

environmental hotspots at an early development and product design stage to help enhancing the environmental performance and to derive process optimization potentials from the results. The description of the product system and the methods applied are described in this section.

#### Goal, functional unit, and system boundaries

The goal of this study is to quantify the potential environmental impacts and identify the main contributing process steps of biosurfactant-containing products at an early development stage for the application of a biosurfactant for the examples of a liquid laundry detergent (LLD) and a facial cosmetic cream. Based on the results and findings, process optimization approaches are derived to improve the environmental performance of the investigated product systems.

The functional unit and the corresponding reference flow for the liquid laundry detergent under consideration are based on the PEFCR study.24 They are defined as "washing of 4.5 kg dry normally soiled fabric with medium water hardness in a 6 kg capacity machine wash (75% loading)" and a recommended dosage of 75 g detergent per wash cycle. The previously mentioned updated data regarding the definition of the functional unit (FU) and the modelling of the use phase of the LLD, published in Commission Recommendation (EU) 2021/2279, were taken into account in the scenario analysis. The consideration of both FU definitions facilitates a comparison of the results with the reference product and underscores the differences that arise from the updated version. For the cosmetic cream under consideration, the functional unit is defined as "moisturizing facial skin by applying 50 g cosmetic cream" with the corresponding reference flow of one tube of cosmetic cream.

The system boundaries were defined as cradle-to-grave. This includes the extraction and cultivation of precursors, processing, production, use phase and end-of-life of both application examples. The system boundaries also include primary packaging and national transport of 400 km in case of the LLD and 150 km for the cosmetic cream from a potential production site to Stuttgart, Germany by truck.

The assumed primary packaging of the LLD per packaged product includes a stand-up pouch made of LDPE (polyethylene low density) with a filling volume of 1.5 L and an empty weight of 380 g, plus a 2 g screw cap made of PP (polypropylene). For the cosmetic cream the same assumptions apply to the screw cap. In addition, a 50 mL tube made of HDPE (polyethylene high density) with an empty weight of 8 g is assumed. The filling volume of the primary packaging is in both product systems assumed to be approximately 1 L  $kg^{-1}$  respectively. While more and more manufacturers adopt recycled plastics for their packaging of such products, primary polymers remain a major packaging material. Studies specially addressing packaging design the use of recycled materials provide insights into their environmental aspects and demonstrate that use of recycled plastic can significantly reduce the environmental impacts. 25-27 Nevertheless, primary material is assumed for the packaging for this LCA, as the focus is on the formulation and its ingredients, as well as potential implications of the performance on the

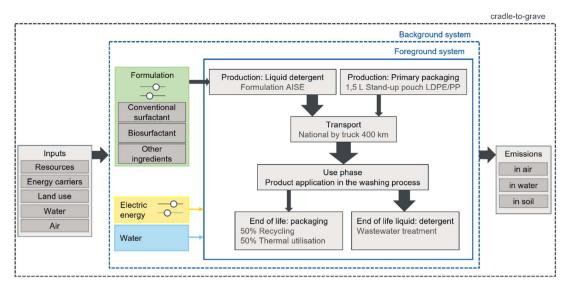


Fig. 1 Process flowchart for the analysed product system of the liquid laundry detergent (LLD), cradle-to-grave.

product life cycle. Secondary packaging such as trays, storage and retail facilities and individual transport by the consumer during product purchase are excluded from the system boundary. Additionally, in the case of LLD, the manufacturing of the washing machine and the fabrics to be washed will be not considered further in the analysis. The geographical scope was defined for Germany for all life cycle stages.

#### Product systems and data collection

The background system includes the upstream chains. Process parameters, such as the choice of surfactant and energy source, are part of the foreground system and vary in the scenario analysis. A graphical representation of the process flow, the system boundaries, and the corresponding life cycle phases is shown in Fig. 1 for the LLD under consideration and in Fig. 2 for the cosmetic cream under consideration.

For modelling the foreground system, the software "LCA for Experts (GaBi)" Version 10.9.1.17 was used.<sup>28</sup> The data for the background system was provided by Sphera's Managed LCA Content (MLC, formerly known as GaBi Professional databases) in the content version 2025.1. Due to the current state of research, the prospective study is mainly based on literature for the product formulations and partly supplemented by our own measurements and assumptions.

Corresponding to the geographical scope, the German grid mix for the most recent available reference year 2020 was applied to the foreground system. In addition to the current German grid mix in the use phase of the LLD, the German green electricity grid mix 2021 was assessed as a renewable energy source. The LLD formulation is based on the AISE PEFCR study<sup>24</sup> and the technical book on cosmetics and hygiene by Umbach<sup>29</sup> provides the basic formulation for the cosmetic cream as an oil-in-water emulsion. For both products, minor adjustments were made to the reference formulation in relation to the original formulation in the literature for improved alignment with the current state of the art for a currently typical

reference products. To reflect the trend of modern formulations, silicones were removed from the LLD reference formulation used in the AISE PEFCR study and the other components were increased proportionally. Additionally, perfume, optical brighteners (FWA1, FWA5) and dye NC-80% removal were also excluded from the analysed formulation, assuming that these components have a minor influence on the surfactant system and are used in a similar way in both product systems. For the cosmetic cream, the original lipophilic component paraffin oil is approximated with the LCI for white mineral oil. As an alternative bio-based oil component sunflower oil was analysed.

The considered washing machine during the use phase of the LLD was assumed to require 50 litres of water per wash cycle. The electricity demand varied based on the washing temperature: 0.3 kWh per cycle for 30 °C, 0.5 kWh per cycle for 40 °C and 0.75 kWh per cycle for 60 °C. These values are assumptions based on literature and verified by own measurements. The use phase of the cosmetic cream under consideration includes the application of the cream to the skin. Within the use phase, no cosmetic, pharmacological, or medical effects of the cream are considered. The LCA does not account for any benefits or harms or the positive or negative effects of the cosmetic cream on the skin or body of a person. The use phase of the cosmetic cream is considered without direct or indirect emissions in the system. The end-of-life of both products is modelled using a wastewater treatment data set with sewage sludge incineration with the assumption that the facial cream is metabolized through oxidation to CO2. For the primary packaging a recycling rate of 50% is assumed. For the recycled share, a cut-off approach is selected, and the burdens of processing and material credits are allocated to the next product's life cycle. The remaining part is sent to incineration. Material-specific data sets were used for the disposal of polyethylene in a municipal incineration plant in Germany, which include credits for electrical and thermal energy. In the scenarios not otherwise indicated, the German electricity grid mix and thermal energy from natural gas were credited for these. Also

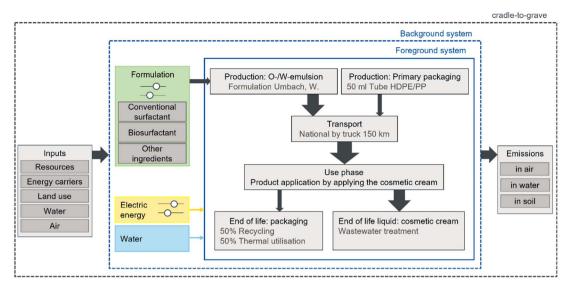


Fig. 2 Process flowchart for the analysed product system of the cosmetic cream, cradle-to-grave.

considered at the end-of-life is the biogenic carbon content of the products to separately account for the carbon released by the fossil and biogenic formulation components in the impact assessment.

The biosurfactant MEL was selected for this study because it is currently being investigated for the considered applications. Comprehensive information of its manufacturing and LCA models is available. The manufacturing of MEL and the LCA modelling for MEL manufacturing is described in detail in previous publications. The LCA model for MEL manufacturing is based on upscaled experimental data. The experimental fermentations and process modelling were carried out at Fraunhofer IGB. They are described in the corresponding publication by Beck *et al.* 2022 (ref. 10) from a process engineering perspective. For the LCA modelling and environmental

aspects of MEL manufacturing, Bippus *et al.* 2024 (ref. 21) conducted a prospective LCA accompanying the process development of MEL. The publication provides the methodology, inventory data, results of the impact assessment and a discussion of the findings on the environmental aspects for MEL production. The model for MEL production in this study on biosurfactant-containing products is based on scenario "FB1 Enhanced projection",<sup>10</sup> only the fermentation parameters aeration rate (0.3 vvm) and energy demand for compressed air (0.3 MJ m<sup>-3</sup>) deviate from this scenario. Hence, it represents a slightly more conservative version of an enhanced projection scenario "FB1 Enhanced projection". To analyse the maximum effects of a potential formulation adaption, a 1:1 replacement of conventional surfactants with MEL was chosen, due to the

Table 1 Overview of the analysed scenarios for the application example LLD, with  $\uparrow$  = higher or  $\downarrow$  = lower LLD-dosage and/or temperature per wash cycle in comparison to the base case scenario. The scenario code is comprised of a reference to the surfactant type, the dosage and the washing temperature

Sc. No.	Scenario code	Description	Surfactant	Washing temperature [°C]	Energy source	Dosage [kg per wash cycle]
1a	B75-40	Base case	MEL <sup>21</sup>	40	German grid mix	0.0750
1b	B90-40	↑ dosage	$\mathrm{MEL}^{21}$	40	German grid mix	0.0900
1c	B50-40	↓ dosage	$\mathrm{MEL}^{21}$	40	German grid mix	0.0500
2	C75-40	Reference conventional	Reference	40	German grid mix	0.0750
		surfactant	formulation <sup>24</sup>		e e e e e e e e e e e e e e e e e e e	
3a	B75-60	↑ temperature	$\mathrm{MEL}^{21}$	60	German grid mix	0.0750
3b	B50-60	↓ dosage +	$\mathrm{MEL}^{21}$	60	German grid mix	0.0500
		↑ temperature			-	
4a	B37.5-30	↓ dosage +	$\mathrm{MEL}^{21}$	30	German grid mix	0.0375
		↓ temperature			-	
4b	B37.5-30-EE	↓ dosage +	$\mathrm{MEL}^{21}$	30	German green electricity	0.0375
		↓ temperature + EE			grid mix	
5	B70 PEFCR	PEFCR guidance FU:	$\mathrm{MEL}^{21}$	_	German grid mix	0.0700
	guidance	8 kg load,				
		0.81 kWh per cycle,				
		9.5 L wash water per cycle				

Table 2 Overview of the analysed scenarios for the application example cosmetic cream, with  $\uparrow$  = higher or  $\downarrow$  = lower dosage of MEL in comparison to the base case scenario. The scenario code is comprised of a reference to the surfactant type, and the mass share of surfactant in the formulation

Sc. No.	Scenario code	Description	Surfactant	Lipophilic component	Amount of surfactant [% w/w]	End-of-life packaging
1 2 3 4a 4b	B7.4-P C7.4-P B10-P-no credit B7.4-S B5-S	Base case Reference conventional surfactant  ↑ dosage + no credit Bio-based oil phase  ↓ dosage + bio-based oil phase	MEL <sup>21</sup> Reference formulation <sup>29</sup> MEL <sup>21</sup> MEL <sup>21</sup> MEL <sup>21</sup>	Paraffin oil Paraffin oil Paraffin oil Sunflower oil Sunflower oil	7.4 7.4 10.0 7.4 5.0	Credit Credit No credit Credit Credit

lack of a specific formulation tailored to MEL at the current stage of development.

#### Impact assessment

The impact assessment was conducted using the EF 3.1 impact assessment method.<sup>15</sup> The following indicators were selected due to their robustness and particular relevance for the studied product systems:

- Acidification.
- Climate change, total.
- Eutrophication, freshwater.
- Eutrophication, marine ecosystems.
- Eutrophication, terrestrial.
- Photochemical ozone formation, human health.
- Resource use, fossil.
- Resource use, mineral and metals.

At the end-of-life, the conversion of carbon from fossil formulation components and its release as fossil  $CO_2$  is considered. In contrast, the uptake and release of carbon from biogenic formulation components as  $CO_2$  are not characterized according to the EF 3.1 impact assessment method ("0–0-approach").

#### Scenario analysis

A scenario analysis was carried out to identify relevant variables and potentials for process optimizations in the product systems under consideration. Due to the current state of research, no data from application trials is yet available. Therefore, the scenarios use hypothetical assumptions for possible parameter variations to better understand their influence on the product systems.

Tables 1 and 2 provide an overview of the scenarios analysed for the LLD and cosmetic cream respectively. The parameters that vary from the base case scenario are shown in bold.

Except for the surfactant used (conventionally or biotechnologically produced), all the parameter variations assumed in the LLD product system refer to the use phase. The following parameters were considered: the washing temperature (30 °C, 40 °C and 60 °C), which results in the washing machine requiring different amounts of energy; the energy source (renewable and non-renewable) for operating the washing machine; and the LLD-dosage per wash cycle (90 g, 75 g, 50 g und 37.5 g). These parameters are intended to indirectly reflect hypothetical variations in the cleaning

performance of the formulation, which could be counterbalanced by the dosage or the washing temperature to understand potential offsets. In addition, scenario 5 presents the differences of the revised FU from the PEFCR Guidance.<sup>8</sup>

The defined parameters for the considered facial cream product system are predominantly established during the production phase of the cream. Similar to the LLD product system, this includes the surfactant used and the required amount of surfactant depending on the assumed performance (7.4% w/w, 10% w/w, 5% w/w percentage by mass). Regarding the potential replacement of the fossil components of the reference formulation with bio-based substances, sunflower oil is analysed as a lipophilic component instead of paraffin oil. The parameter for the credit allocation is defined at the end-of-life of the packaging. A scenario in which a renewable energy source to produce the emulsion was evaluated is excluded from further analysis, as the impact is negligible and also not adjustable in the upstream chains.

#### Results and discussion

#### LCIA results for laundry detergent

Fig. 3 illustrates the results of the LLD scenarios analysed in the impact category climate change, total (CC), according to EF 3.1. Scenario groups 1, 3 and 4 are based on the assumption that the biosurfactant-containing LLD formulation results in an increase or decrease in product performance. Consequently, it is assumed, that for a comparable washing efficiency, the dosage and washing temperature, need to be adjusted accordingly. In this context, scenario 1a represents the base case scenario with the use of 75 g detergent at a washing temperature of 40 °C per FU. It shows that approximately 49% of the contribution to climate change can be attributed to the electricity consumption of the washing machine during the use phase. Accordingly, it can be concluded that the greatest potential for reducing the environmental impact through process-regulating measures is to be found here. The second main contribution with approx. 33% is the production of the biosurfactant-containing LLD. A high share of this is attributed to the production of the biosurfactant MEL, which is still at laboratory to pilot scale. Additionally, the use of biosurfactants likely requires an adjustment of the formulation, which was not possible to include in the analysis due to the limitations of the available data. The packaging considered has only a very minor impact on the total result, with 2% over its lifecycle. The

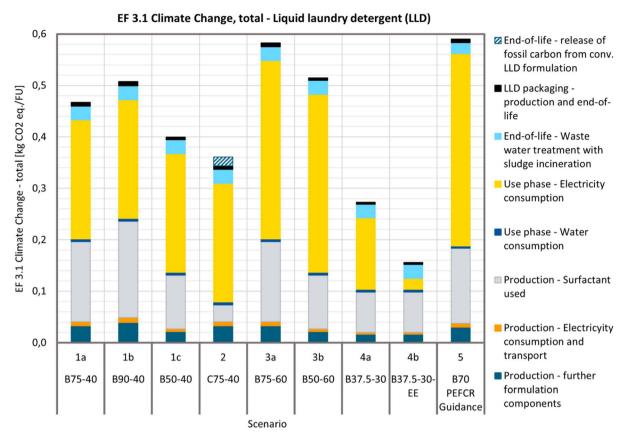


Fig. 3 Results of EF 3.1 climate change, total per FU – LLD – all scenarios, FU = wash of 4.5 kg dry normally soiled fabric with medium water hardness in a 6 kg capacity machine wash (75% loading).

assumed national transport by truck has with 0.62% a negligible effect and the contribution of the required wastewater treatment for the disposal of the washing water is approx. 6%. In scenarios 1b and 1c, the impact of LLD dosage at constant temperature is analysed. The results from scenario 1c shown that a reduction in dosage by 33% decreases the environmental impact in CC by 15% compared to the base case scenario.

In the reference scenario, scenario 2, with conventional surfactants, the LLD production has a lower impact, despite the fossil carbon considered in the EF methodology approach at the end-of-life. This includes distinguishing between biogenic and fossil carbon. Two surfactants in the reference formulation are of fossil origin, releasing about 20 g of fossil CO2 at the end-oflife, which must be added accordingly. The biogenic carbon cycle is already closed and is not considered further regarding anthropogenic climate change in the EF method. Therefore, scenario 2, using conventional surfactants, results in a contribution of 0.36 kg CO<sub>2</sub> eq. per FU. To not exceed the contribution of the reference product, the environmental impact regarding the impact category CC of the base case scenario would need to be reduced by 23%. While the production of conventional surfactants has reached near-optimal process efficiency over decades, biosurfactant production at lab to pilot scale is still evolving. Thus, this highlights the opportunity to further reduce the environmental impacts significantly through process and formulation improvements. However, the comparison between

bio- and conventional surfactants currently has limited significance and is intended as a preliminary approximation in this study.

In scenario group 3, the assumption is made that a higher washing temperature is necessary to achieve a comparable washing result. Therefore, a washing temperature of 60 °C is investigated. The results of the scenario 3a shown an increase in environmental impact in the category CC by around 25% compared to the base case scenario. Therefore, a 33% reduction in dosage is insufficient to offset the increased impact due to the energy demand of the washing machine (Sc. 3b).

A combination of optimization approaches is investigated in scenario group 4. The results shown a major reduction of  $CO_2$  eq. per FU in relation to the base case scenario with a 50% decrease in the LLD dosage and a washing temperature of 30 °C. The impact is reduced by about 42% with a conventional energy supply during the use phase (Sc. 4a) and by 67% when renewable energy sources are considered (Sc. 4b).

The results of the scenarios 1, 3 and 4 aim to identify optimization strategies for the further research of biosurfactants that should be pursued to achieve comparable or reduced environmental impacts relative to conventional formulations. For enhanced comparability with conventional products, the definition of the functional unit (FU) is based on the comprehensive PEFCR study conducted by AISE. To accurately reflect the state of the art, scenario 5 presents results based on the

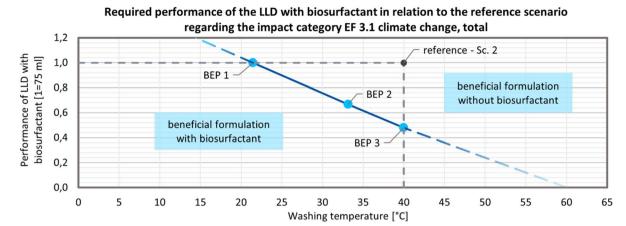


Fig. 4 Results of the required performance of the LLD with biosurfactant in relation to the reference scenario regarding the impact category EF 3.1 climate change, total. Scenarios used for calculating the break-even-points BEP i, = 1-3: 1a & 3a  $\rightarrow$  BEP 1; 1c & 3b  $\rightarrow$  BEP 2; 1a & 1c  $\rightarrow$  BEP 3.

updated FU. The PEFCR Guidelines suggest that, with increased energy input and reduced wash water consumption, approximately twice the amount of laundry can be washed. Nevertheless, it becomes evident that electricity demand during washing, accounting for 63%, has the most significant impact on

environmental performance. This underlines the critical importance of detergent efficiency at low washing temperatures.

In conclusion, the results of the scenario analyses have shown that decreasing the LLD dosage and washing

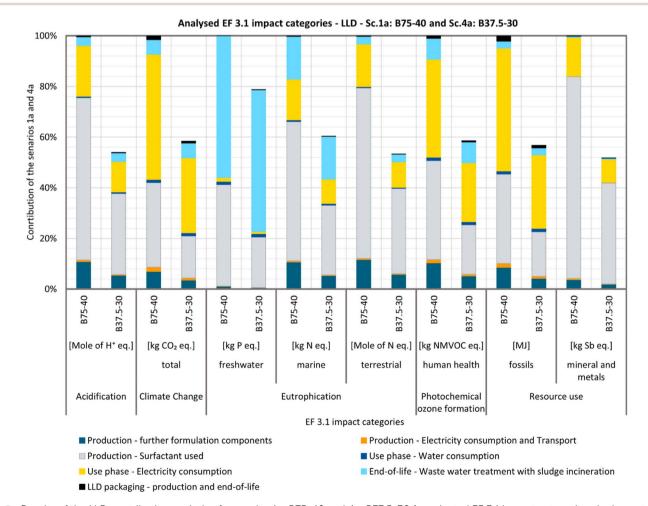


Fig. 5 Results of the LLD contribution analysis of scenarios 1a: B75-40 and 4a: B37.5-30 for selected EF 3.1 impact categories, the impacts are normalized to the base case scenario 1a.

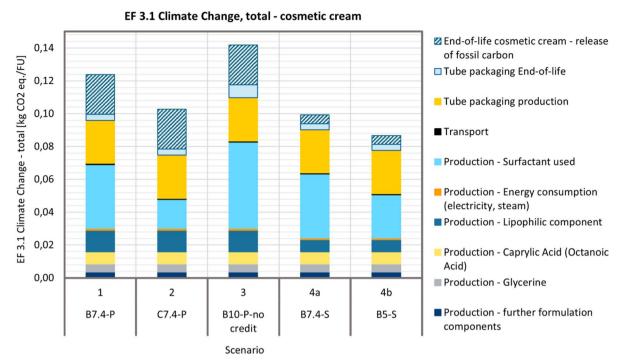


Fig. 6 Results of EF 3.1 climate change, total per FU – cosmetic cream – all scenarios, FU = "moisturize facial skin by applying 50 g cosmetic cream" with the corresponding reference flow of one tube with a volume of 50 mL ( $\approx$ 50 g), comprising the packaging.

temperature are two significant parameters for process optimizing approaches to reduce the environmental impact in the category CC. The impacts could be reduced significantly and could additionally outweigh the increased contribution of the considered biosurfactant given the current state of research if the performance of the formulation can be improved. These findings are visualized in Fig. 4. It illustrates the required performance increase of the biosurfactant-containing LLD based on the current state of research compared to the established and optimized reference product. The calculations are performed according to the break-even-point (BEP) approach representing the comparison of two scenarios with the reference product.

The results indicate that, to achieve a break-even point with the reference for a conventional formulation (scenario 2) at the same dosage of the LLD, a reduced washing temperature of approx. 21 °C would be necessary. Conversely, at the same washing temperature, the formulation dosage would need to be reduced by 50%. By combining these parameters, a comparable environmental performance of a biosurfactant formulation to the conventional formulation reference (scenario 2) could be achieved with a 33% reduction in LLD dosage and a washing temperature of approximately 33 °C (7 °C reduction). This underlines the importance of the formulation's performance, given that washing temperature significantly influences the results

Additionally, the results of the contribution analysis regarding the application example LLD for the selected EF 3.1 impact categories are presented in Fig. 5. The scenarios considered are scenario 1a, which represents the base case scenario and is accordingly scaled to 100%. In comparison,

scenario 4a with the optimistic washing performance assumptions indicates that the use of biosurfactants in combination with enhanced washing performance significantly improves the environmental performance of LLD. This improvement is characterized by a 50% reduction in dosage and a washing temperature of 30 °C to achieve comparable washing efficiency. It is shown that the relative impacts of the different process steps vary depending on the impact category. The production of the biosurfactant considered is one of the main contributing processes in all impact categories investigated. Given the current state of research, it is expected that continued research on technical and process develoments, as well as scale effects of future production at an industrial scale will lead to a reduction of these shares. In the impact categories CC, photochemical ozone formation (human health) and resource use (fossils), energy consumption during the use phase of LLD is the primary contributing process. This impact can be reduced by integrating renewable energy sources and reducing energy comsumption of the washing machine, mainly determined by the washing temperature and closely related to the washing performance of the product formulation. The categories Eutrophication (EP), freshwater is mainly influenced by the wastewater treatment at the end-of-life of the LLD. The considered optimization approaches in scenario 4a result in a reduction of potential environmental impacts for all investigated impact categories. In the case of EP, freshwater the reduction is approx. 20%, for all other seven analysed impact categories the reduction potential is found to be between 40% and 50% in reference to the base case (scenario 1). The investigated measures can thus be considered effective for the eco-design of LLD.

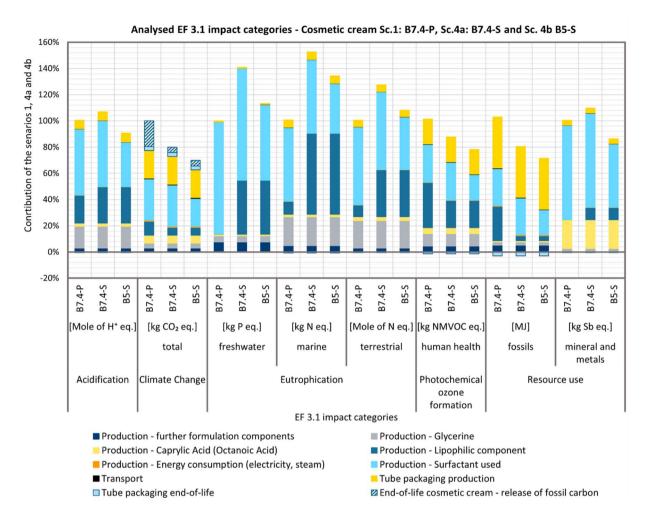


Fig. 7 Results of the cosmetic cream contribution analysis of scenarios 1: B7.4-P, 4a: B7.4-S and 4b: B7.4-S for selected EF 3.1 impact categories, the impacts are normalized to the base case scenario 1.

#### LCIA results for cosmetic cream

The results of the cosmetic cream scenarios analysed regarding the impact category climate change (total), according to EF 3.1 are illustrated in Fig. 6. Scenario 1 represents the base case scenario with 7.4% w/w biosurfactant in a formulation and paraffin oil as lipophilic component. The results shown that the production of the cream is the main contributing process and offers the greatest potential for optimization approaches. In addition to the contribution of the biosurfactant production, the choice of the lipophilic component has a significant contribution to the overall results. This affects both the production and the end-of-life of the cream. For the end-of-life of the fossil lipophilic component, the CO<sub>2</sub> emissions from its degradation are taken into account. On the other hand, in the case of biogenic vegetable oil as lipophilic component, the biogenic CO<sub>2</sub> from its degradation is not characterized in the selected LCIA method. This approach for the carbon balance is mentioned in the previous subchapter. Approximately 20% of the released carbon at the end-of-life is attributed to the degradation of fossil-based formulation components in scenario 1, with 78% of this originating from paraffin oi, 17% from vaseline and 5% from benzoic acid as a preservative. A

purely bio-based formulation would reduce this share to zero and is therefore recommended regarding the development of modern formulations. Furthermore, the examined packaging accounts for approx. 24% of the product system, it is therefore one of the main contributors. As assumed in scenario 3, if there is no credit for thermal and electrical energy from the incineration of the packaging at end-of-life, the impacts in the category CC result in a higher contribution of the tube packaging lifecycle compared to the packaging lifecycle in the base case scenario. Potential reduction measures could include choosing a low impact packaging system and increasing the recycling rate of the packaging if possible. The contribution of the assumed national transport shows to be negligibly low in all scenarios in this case. In addition, in this application example, the use phase includes only the application of the cosmetic cream to the skin. Assuming this process does not have an environmental impact in any of the impact categories analysed, it is therefore excluded from the visual representation of the results.

The reference case (scenario 2) has a 17% lower environmental impact compared to the base case scenario (scenario 1). Considering the different development stages of the surfactants used such optimization of biosurfactant production is within

realistic reach. Nevertheless, the comparison between bio- and conventional surfactants is currently of limited significance and is intended as a preliminary approximation in this study. To offset the higher environmental impact of biosurfactants, the lipophilic component can be replaced with a biobased oil. This is demonstrated by scenario 4a, which, by using sunflower oil, shows a 20% lower environmental impact compared to the base case. Additionally, in scenario 4b the assumption is made that the use of biosurfactants provides a performance-enhancing property, and accordingly, 5.0% w/w of biosurfactant is assumed be sufficient for the formulation to achieve a stable emulsion. The combination of these optimization approaches leads to a reduction of the potential environmental impact by 30% compared to the base case.

The results of the contribution analysis regarding the application example cosmic cream for the further analysed EF 3.1 impact categories are presented in Fig. 7. The scenarios considered are scenario 1, which represents the base case scenario and is accordingly scaled to 100%. In comparison, scenario 4a, which uses sunflower oil as a biobased lipophilic component, and scenario 4b consider potential formulation improvement approaches as mentioned in the previous section. In these cases, the relative impacts of the different process steps vary depending on the impact category. In this application example, given the current state of research, the biosurfactant considered is, as with LLD, one of the main contributing processes in all impact categories analysed.

The production of packaging is one of the main contributing processes in the impact categories CC, photochemical ozone formation (human health) and resource use (fossils). This is due to the release of CO<sub>2</sub>, nitrogen oxides, as well as the use of crude oil and natural gas associated with the production of the packaging material. Glycerine, as a formulation ingredient in the cream, is especially relevant in impact categories AP and EP, marine and terrestrial. This results from ammonia and nitrate emission in the upstream processes in the background system of glycerine production. Furthermore, caprylic acid contributes significantly to impact category resource use, mineral and metals, due to the demand of elementary resources in the upstream processes in the background system. The biobased lipophilic component, sunflower oil, shows a lower potential environmental impact in the analysed impact categories CC, photochemical ozone formation (human health) and resource use (fossils). In the remaining impact categories does sunflower oil have a significantly higher contribution due to the necessary land use and the emissions of agricultural soil contaminants, such as pesticides and fertilizers during the oil's production. However, the combination of the formulation and process optimization approaches in scenario 4b results in a reduction of the potential environmental impact in reference to the base case in all analysed impact categories, except for EP.

#### Discussion

#### LCA as a tool in biotechnological process development

Since for both use cases of the biosurfactants, a laundry detergent and a cosmetic cream, no formulation tailored to the

properties of biosurfactants is currently available, the analyses of this study have a prospective and explorative nature. In general, the adaptability of biosurfactants, such as influencing the side chains and thus their substance properties, allows for functional optimization for according to their application. Research on tailoring both biosurfactants and application formulation is currently under development. However, supporting this development work by including environmental aspects from an early stage guides sustainable development of biosurfactants. Therefore, in the current early stage, where that information is not available yet, literature-based generic formulations are used, as this data is publicly available, and at the same time representative for the respective applications. It provides insight into hotspots and key influencing factors for potential biosurfactant applications. The results of the LCA and scenario analysis highlight the potential impact reductions that increased product performance through tailored biosurfactants could have. Therefore, these aspects need to be addressed in product development with the new and functionalized biosurfactants and their respective product formulations. Thus, this analysis identifies targets that need to be pursued in formulation development to achieve significant environmental benefits.

#### Data quality and uncertainties

Conducting prospective LCA in an early development stage allows for increased understanding of future biosurfactant application scenarios. However, it involves making assumptions that have not yet been tested or confirmed in laboratory studies or been upscaled. This approach is applied for the case studies of biosurfactant applications analysed in this work. These projections and assumptions are discussed in this section.

First, the 1:1 replacement by mass of all surfactants with the biosurfactant MEL was assumed. In contrast, it is expected that the mass-specific performance of the surfactant will be different from the surfactants it replaces. Further, surfactants are typically applied as a system consisting of several surfactant types to realize advantages of the combination with co-surfactants. The effects to create efficient multi-surfactant systems tailored to the use of microbial biosurfactants has not yet been sufficiently researched (or made publicly available). However, the approach presented in this work and model developed serve as a basis for further investigations and can be expanded to further biosurfactant-based formulations as soon as further insights become available.

For the production of MEL, a prospective LCA on production process optimization was presented in detail in a previous study, both demonstrating reductions of impacts during the development phase to date, as well as discussing further potentials for optimization.<sup>21</sup> However, uncertainties due to the upscaling of laboratory processes compared LCI datasets representing the long established and optimized industrial processes for conventional surfactants apply. For this reason, the aim of the study is not to compare the surfactants directly, but to gain a better understanding of how to improve the

biosurfactant containing products regarding the current state of their development compared to the application of conventional surfactant systems. The data quality of the background system is considered to be high in terms of technical, temporal and geographical representativeness.

For the end-of-life modelling, the disposal of the biosurfactant component via an average municipal wastewater treatment and the complete aerobic biodegradation with an oxidation of the carbon bound in the molecule to CO2 was assumed in this analysis. Although biosurfactants are frequently considered to be highly biodegradable, only few studies on this characteristic can be found in literature. Additionally, biosurfactants are also often attributed with antimicrobial properties, which could, however, in general be associated with an inhibitory effect at higher concentrations.8 In the case of incomplete degradation, substances may remain in sewage sludge or treated wastewater, which would be relevant for impact categories such as climate change in case of methane as degradation product, or ecotoxicity, which was not within the scope of this study. These impacts would strongly depend on fate, e.g. the compartment it is released to, and ecotoxic properties, for which at the moment to data is available yet. Therefore, the degradation for biosurfactants in the considered applications remains an uncertainty that has not yet been fully addressed in LCA. The results of aerobic and anaerobic degradation tests (e.g. according to OECD guidelines) could provide additional insights into the fate of biosurfactants when disposed via wastewater and help to better characterize the potential impacts.

# Identified fields of action for optimization for biosurfactants and comparison with findings of other biosurfactant LCA studies

Biosurfactants production is still at research status, so that the absolute results can only be compared to a limited extend with LCAs of established processes, such as with the research conducted for ERASM, <sup>30,31</sup> for which life cycle inventories were obtained from industrial data collected at companies of the association. Therefore, the LCI of the ERASM study is representative for mature technology development levels as used in the industry.

In previous studies, optimization potentials to produce MEL and cellobiose lipids (CL) were analysed with LCA based on upscaled process models of laboratory experiments and process simulations.<sup>21,32</sup> Hotspots in the fermentation of both MEL and CL are the provision of substrates and energy use for the operation of the bioreactor, especially for aeration. Due to the high contribution of substrates used, several LCA studies therefore investigate the use of alternative feedstocks, such as agro-industrial side and waste streams, for instance, the studies conducted by Lokesh *et al.* 2017,<sup>33</sup> Brière *et al.* 2018,<sup>34</sup> Kopsahelis *et al.* 2018 <sup>35</sup> and more which are summarized in the review paper by Briem *et al.* 2022,<sup>8</sup> as well as newer studies such as those by Bippus *et al.* 2024,<sup>21</sup> Oraby *et al.* 2024 (ref. 36) and Schonhoff *et al.* 2022 and 2023.<sup>20,37</sup> In addition, the downstream

purification of the culture broth contributes significantly because of solvent use and energy consumption of equipment.

In this study, the findings of hotspots and optimization potentials for biosurfactant production are now complemented by an assessment of how the performance of the surfactants influences the environmental impact in the use phase. The results highlight the relevance of performance in consideration of the currently higher impacts associated with the production of the biosurfactant MEL compared to conventional surfactants. The break-even-curves demonstrate that the higher impacts from production in CC can be offset by the formulation quantity. However, this is not observed in the impact categories EP and AP. To avoid such a burden shift, alternative raw materials from 2nd and 3rd generation feedstocks must be utilized in the future.

For liquid laundry detergent, the International Association for Soaps, Detergents and Maintenance Products (AISE) applied the environmental footprint (EF) method with the goal to develop product category rules for these products. The LLD investigated by AISE has a carbon footprint of 0.52 kg CO<sub>2</sub> eq. per FU.24 This is slightly higher but of comparable magnitude to the results of the reference product in this study. The deviation can be explained, for example, by different datasets in the supply chains. However, the formulation considered by AISE does not include biosurfactants.24 Nevertheless, the confirmation of AISE aligns with this study's findings indicating that the use phase of the LLD is the process with the most significant environmental impact during the product's lifecycle. 16,24 For cosmetic cream, Guilbot et al. conducted an LCA of a cosmetic cream containing alkyl glycolipids as surfactants.18 The study identified the oil of the emulsion and the packaging of the cream as well as its purchasing as the main contributing processes. 18 This is partially consistent with the findings of this study, which also recognized the emulsion and packaging of the cream, in addition to the surfactant used and the release of fossil carbon dioxide, as significant contributing processes. The result in the impact category CC is significantly lower in Guilbot et al. with 5.6 kg  $CO_2$  eq. for the use of 584.0 g of a moisturizing cream.18 The deviation can be explained by the varying scope established for the investigation. For example, Guilbot et al. identifies the purchase of the cream as one of the main contributions, which is excluded in this analysis. However, for the other processes, it was not possible to determine the specific differences, as the representation of the results by Guilbot et al. is aggregated.

The environmental impacts of the surfactant used primarily depend on its performance, as it may influence other parameters, such as the quantity necessary in the formulation or variables during the use phase, such as washing temperature and dosage. These can be set as targets so that for example the washing effect is comparable to formulations with other surfactants. The physiochemical properties are largely influenced by the chemical structure which can be influenced in the production process. As discussed above, to date these are not fully understood and researched. Other studies use the critical micelle formation concentration (CMC) to relate the potential performance of biosurfactants to each other for an unspecific

application.<sup>37</sup> Beyond that, with this LCA, the foundation for an understanding of the influence of the environmental aspects for two possible applications of biosurfactants are formed during the product development process. Overall, this study not only provides valuable insights into environmental aspects for two biosurfactant applications but also highlights focus areas for the development of environmentally sustainable biosurfactant-containing products from a life cycle perspective.

#### Conclusions

Prospective life cycle assessment of biosurfactant application provides valuable insights into hotspots and optimization potentials at the early stage of research. For liquid laundry detergents, key hotspots include electricity usage during the use phase and surfactant production, while for the cosmetic cream the critical areas are the provision of the oil component and surfactant, and packaging. A limitation of the study is that there are no commercial formulations tailored to MEL yet and the formulation performance has not yet been finally quantified in full-scale trials. Another major challenge is that although the manufacturing of the biosurfactant is based on upscaled experimental data, not all scale effects such as integrated processes and energy recovery could be considered and thus offers further potential in terms of mass and energy efficiency. Consequently, the technical representativeness of this snapshot in the development process is limited when compared to conventional manufacturing routes of conventional references. It is important to note that, even at the current experimental stage of development, environmental impacts are already in a comparable range to conventional surfactants and therefore has the potential to surpass them in future developments and upscaling. This highlights the need for further investigation in alternative feedstock sources. These have to potential to reduce the impacts which derive from substrate provision. With the expected reduction in potential environmental impact through upscaling, the increasing the significance of tailored formulations to the specific properties of biosurfactant and their application becomes increasingly important. Future work should therefore incorporate further insights and developments in both biosurfactant production and application specific formulations.

All in all, this work contributes significantly to further understanding and transparency in this field and thus offers important insights into biosurfactant-containing products from an environmental perspective. Ongoing process development promises additional efficiency gains, with the potential to be more than just an alternative.

#### **Author contributions**

LG: formal analysis, investigation, methodology, software, visualization, writing-original draft. LB: conceptualization, formal analysis, methodology, project administration, writing-original draft, AKB: conceptualization, funding acquisition, supervision, writing-original draft. AB: funding acquisition, resources, supervision, writing-review and editing.

#### Conflicts of interest

There are no conflicts to declare.

### Data availability

Background data includes secondary data from commercial LCA databases utilized to set up the life cycle inventory like extraction of raw materials, transportation, material production, and electricity generation; the publication of these datasets is restricted according to the terms and conditions. The manuscript includes a clear and comprehensive description of all methods applied, methodological choices made and calculations performed, as well as the material inputs and outputs of the product system, ensuring transparency in the research process. This approach ensures that the reproducibility of results is given while adhering to confidentiality requirements and provides sufficient detail to enable a skilled researcher to reproduce the results.

Supplementary information (SI): formulas of the products under consideration and modelling assumptions. See DOI: https://doi.org/10.1039/d5su00168d.

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