SUSTAINABILITY ASSESSMENT OF THE PRODUCTION OF MICROBIAL BIO-BASED SURFACTANTS

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ABSTRACT: Related to the development of production processes for microbial bio-based surfactants like rhamnolipids and mannosylerythritol lipids a sustainability assessment was carried out within the project Bio². Developments at lab-scale and technical scale built the base for an industrial design scenario of different process chains, whereby exemplary co-products of sugar beet processing were used as substrates. Environmental impacts, economic issues and social risks of defined process chains allowed a classification of different microbial surfactant production options by the assessment of the three dimensions of sustainability. The generated results work as an indicator for further development, provide insights to potential hotspots and allow the estimation of future market positions.

Keywords: bio-based products, bioeconomy, fermentation, life cycle assessment (LCA), socio-economic impact, sustainability criteria

1 INTRODUCTION

In the context of increasing importance of sustainability and awareness of consumption [1, 2], as well as enhanced political efforts such as the European Green Deal [3], the development of corresponding products is promoted. To get a clearer understanding on new production processes operating under the umbrella of the so-called bioeconomy, it is important to subject such developments to a critical examination regarding their different aspects of sustainability. Appropriate tools for the realization of such a study that illustrates all three dimensions of sustainability, are the established methods of the environmental Life Cycle Assessment (LCA), the Life Cycle Costing (LCC) and the Social Life Cycle Assessment (S-LCA). This methodical triad basically pursues the idea of Life Cycle Sustainability Assessment (LCSA), which was formulated methodologically by the United Nations Environment Programme (UNEP) back in 2011 [4].

Based on the general idea of sustainability the project Bio² dealt with the production of the microbial bio-based surfactants rhamnolipids (RL) and mannosylerythritol lipids (MEL) as a possible alternative to conventional (petro- and oleochemically produced) surfactants, which dominate today's market. Used substrates in the present study are molasses (MOL) and hydrolyzed sugar beet pulp (SBP) from sugar production industries. The configuration of the process chains studied here are based on a process engineering derived from lab and technical scale experiments and the biotechnological design of the involved modified microorganism *pseudomonas putida* (PP, producing RL) and *ustilago maydis* (UM, producing MEL) [5, 6, 7, 8].

Previous LCAs regarding surfactants can be found for different contexts and with different focusses, whereby products, specific considered scales or system boundaries differ (e.g., [9, 10]). A systematic study and the following provision of datasets of different conventional surfactants was made available by CESIO/ERASM in 2017 based on industry data [11]. Environmental impacts of the technical scale version of the Bio² processes were evaluated and results were presented in Tiso et al. [12].

Starting from a global surfactants market size of approximately 37 bn € in 2017 and assumed market growth rates of nearly 5 % per year, the economic potentials seem promising [13]. The European share in the global market amounted to about 9-10 % with a turnover of ca. 3.4 bn € and production amounts of estimated 4.7 M Mg of different surfactant types in 2017 [14]. The differentiation of the market by application fields shows the mass- and turnover-related domination (market share > 75 %) of surfactant usage for detergents (household & professional), cosmetics & pharmacy, and textiles & fibers [15]. With regard to the type of production and its raw materials, the majority of surfactants (> 95 %) originates from petrochemical and oleochemical processes at the global level [16], while the microbial surfactants addressed here (RL, MEL), have market shares of less than 0.1 % by own calculations. Market and literature research shows a broad variety of prices for microbial surfactants from one digit prices per kg for mass application ([17]) to two digit prices per mg, for example ([18]). The pricing depends on different product characteristics like purity, application field, the number of congeners and other factors [17].

According to our current state of knowledge, regarding social issues there have been no studies on (bio-) surfactants in the sense of the S-LCA-methodology described here or similar methods. Depending on the location of production, the origin of used materials and further activities like manufacturing or recycling, social risks and impacts (positive and negative) of potential stakeholders along the life cycle can be found and assessed [19, 20]. The conventional classification of stakeholders includes workers, local community, society, consumers and value chain actors, which can be considered by specific impact indicators [21]. If a European reference is made to social risks, it becomes visible that existing problems in Europe and specific countries [22, 23] justify a closer look to particular aspects (e.g., decreasing trade union density).

2 GOAL AND SCOPE

The following methodological description and the presented results shall provide first insights related to the three dimensions of sustainability for the production of the bio-based surfactants RL and MEL. On the one hand, the selected results show the general possibilities of a holistic process analysis by specific assessment methods. On the other hand, the results show project-specific critical points by the identification of the most effective process modules and stages as well as impact pathways. This means that besides the identification of more advantageous process designs, specific environmental, economic and social hotspots, as well as conspicuities are detected and open up the possibilities of process optimization. Furthermore, the position within the market can be examined. Limitations of the study can be found in the fact that the results are related to a theoretical scale-up and different uncertainties regarding the economic data, due to the early development level and a currently low significance of microbial biosurfactants in the market.

2.1 System description

An estimated share of totally available substrates, based on the co-product data of German sugar industries and the number of locations [24, 25], enables the development of an overall scenario in which the process chains are embedded. The theoretical yearly production of 15,000 kg of surfactants determines the scale of the assessed four process chains. The four process variants differ by their surfactant product (RL, MEL) and their substrate (MOL, SBP). Considered process chains are

RL_MOL, RL_SBP, MEL_MOL, and MEL_SBP (naming: product_substrate). The scale up was based on data from lab and technical scale (e.g., [5, 12]). The basic principle of the examined process chains is illustrated in in Figure 1. It shows the main stages of each cradle-to-gate system. Technology differences in the upstream and the downstream result from the targeted products and used substrates. Each stage represents summarized single process modules. So the fermentation contains not only the fermentation tank but also a first separation of liquid and solid parts of the fermentation broth by centrifugation as well as the necessary flow infrastructure such as pumps, for example. The assessment and its results are related to all processing activities within the system boundary (grey dotted line, relevant for LCA, LCC, S-LCA). An exemplary more detailed process flow chart of RL production can be found in [12] for the technical scale design of the process (fermentation operation volume of 112.5 L).

Sugar beet production and processing were modelled by the use of data from an already available LCA published by Spoerri et al. in 2014 with a European reference [26]. Though, the first stages of substrate origin, seed fermentation, storage and preparation as well as fermentation are qualitatively the same for each product (RL, MEL), the downstream differs clearly by variously configured stages of precipitation, extraction and final conditioning. Varying substrates such as MOL and SBP led to technical differences of process modules in the upstream before fermentation, due to different substrate-properties (e.g., sugar content or state of aggregation), which results in different requirements related to preparation and storage. The core of each chain is formed by a fermentation of 5,000 L operation volume, which consists of specific amounts of substrate and different added amounts of water and mineral media (depending on product and substrate). Differing yields of the specific modified microorganism (PP, UM) generate process chain specific amounts of product per single volume exchange of fermentation (see section 3).

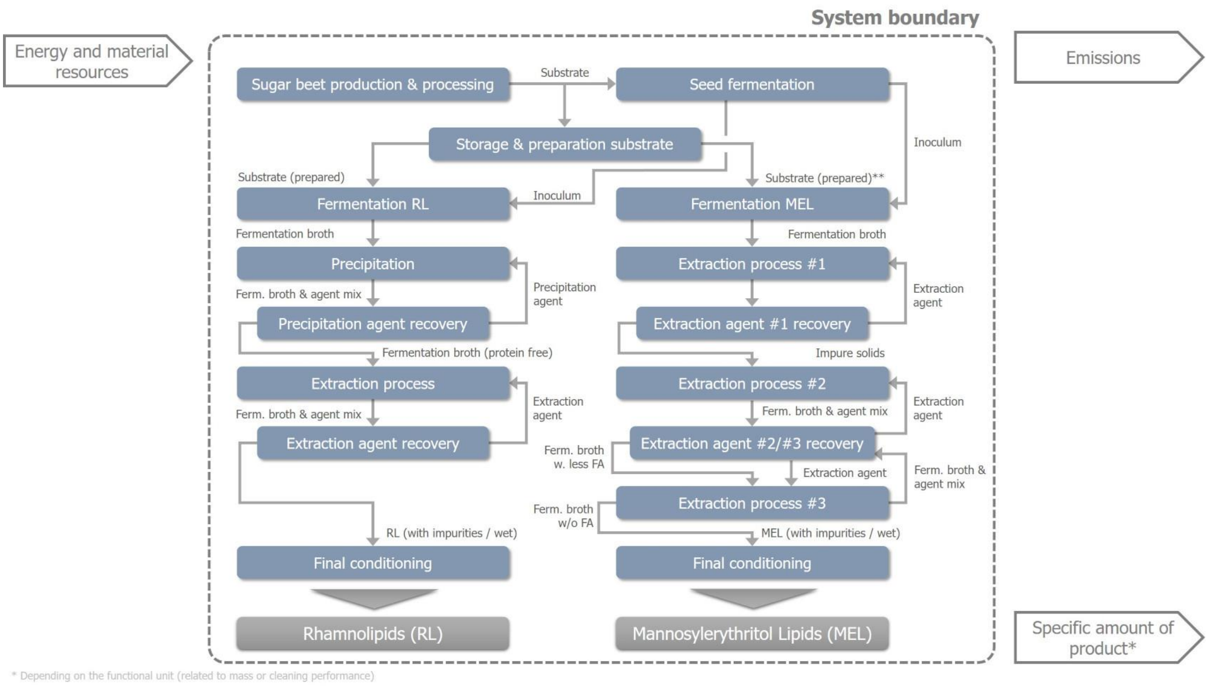

Figure 1: Flow chart of different process chains of the cradle-to-gate systems for the production of RL and MEL by different substrates (MOL, SBP) containing the basic process stages and (recycling) flows; the systems contain all stages from cultivation and production of basic materials up to the surfactant products

In the case of RL production, the fermentation broth (solid biomass separated by centrifuge) is led to a precipitation stage, where precipitation agent acetone is added, to separate process specific proteins. In a following extraction, the agent ethyl acetate is added to further isolate and purify the products (e.g., separation of fatty acids). During the final conditioning further separations of impurities (e.g., agent residues) increase the quality of the powdery product. This stage includes also a storage of the RL.

The downstream chain of MEL production starts with the separation of biomass solids from the fermentation broth by a centrifuge. The following process provides three different extraction stages (1 x agent: ethyl acetate, 2 x agent: n-hexane) to isolate and purify the product. Similar to the RL production the final conditioning stage enables a further purification of the powdery product MEL and includes the storage.

Besides the basic components (e.g., tanks, mixer-settler, etc.) the process chains include components of infrastructure (e.g., pumps, conveyors, etc.). The storage of process-specific materials (e.g., mineral media) and the used space is also included in proportion to their share in the total scenario. The recycling of precipitation and extraction agents is realized by flow-rate specific dimensioned heating and cooling units. In all process chain variants, the recycling of agents is considered with a rate of 80 % and purge flows. Purge flows have to be treated as hazardous waste, while the used processing water is assumed to be discharged as wastewater and the separated biomass as bio-waste. The necessary energy supply (electricity, heating) was considered assuming todays German electricity mix and the use of natural gas. A possible heat recovery or after-use was not taken into account.

2.2. Functional unit and cleaning performance

Initially the functional unit of the LCA, which provides a reference to which the inputs and outputs are related, was set to the production of 1 kg of surfactants (RL, MEL). While the comparison of surfactants of the same type (e.g., RL vs. RL) is possible with mass-based results, the comparison of different product types (e.g., RL vs. MEL) is only possible by using an additional parameter that describes the cleaning performance to ensure a fair comparing. The optimum of cleaning performance can be described by the critical micelle concentration (CMC) of surfactants and can be related to the mass of product [27]. The ratio between the product-individual CMCs reflects the ratio between the necessary amount of product to get the same cleaning performance (necessary requirement: same application field). In the present study, the ratio between RL and MEL can be numbered by the scaling factor 3.6 as it can be derived from the individual CMC values in Table 1. The carried out CMC-scaling of results relates to both, the LCA and S-LCA results. In the case of pricing, the results are fixed to the mass reference, as this is a standard market specification.

2.3 Assessment methods

Based on the ISO 14040/14044 standards [28, 29] the LCA was performed. Calculations of scale-oriented mass and energy flows allowed the implementation of processes in the LCA-Software GaBi 9.0 [30]. Quantitative input data and scale up design for the main (foreground) processes from the lab and technical scale were provided and agreed by project partners or taken from literature. Data for background processes like energy or water supply were implemented by the use of datasets from GaBi and ecoinvent 3.5 databases [31, 32]. Where possible, the non-project data was not older than five years or ideally had a current reference. The German or European level was used as the geographical reference, depending on availability. The results for specific environmental impacts are represented by 16 impact categories recommended by the International Reference Life Cycle Data System (ILCD) [33]. To receive a total impact per process, a normalization was performed with the method of Product Environmental Footprint (PEF Pilot 1.09) which refers to the EU-27 [34].

An LCC in line with SETAC (2011) [35] was conducted regarding economic aspects. Starting from the equipment cost and further other financial issues (e.g., substrate cost) related to the above mentioned scenario it was possible to determine further cost positions by using calculation structures based on Peters et al. (2003) [36]. Equipment costs were estimated by the use of equipment databases and market research for single components. Taking into account resulting and additional proportional costs (e.g., end-of-life costs of manufacturing plant), it was possible to estimate an appropriate pricing for the products. To get an impression of the competitiveness the data was compared to data generated in a market screening.

The implementation of an S-LCA was made in accordance with the established guidelines of UNEP/SETAC [37] to point out specific social risks. Starting from the defined system boundaries and the determined input and output flows the process chains were modelled in the software openLCA [38]. Relevant material and energy flows, as well as further activities were transformed into corresponding financial data and economic sectors in line with NACE [39]. Combining these data with the so-called PSILCA database [40] within the openLCA software enabled the quantification of selected social risks. Addressed social issues and the associated indicators were identified by literature research and the screening of sustainability reports of different companies from the chemical industry sector. The presented indicators are related to the stakeholder group of workers.

3 LIFE CYCLE INVENTORY

The main characteristics and selected flows of each single process chain like described above can be found in Table 1. Presented data indicates that the use of different product-specific microorganism come along with essentially different yield and conversion rates, which influence the product output per volume exchange significantly. Moreover, this fact requires a different dimensioning of process technology in the mentioned 15,000 kg scenario. The yield of RL production is clearly lower than the one of MEL production options (factor 2.4). A further striking parameter is the CMC value, which indicates large differences in relation to the comparison options (see 2.2).

Depending on the substrate choice, its demands are based on particular sugar contents and influence the substrate water ratio in the fermentation process. This fact influences also the following stages due to the different dimensioning. Mineral media shows smaller amounts for RL production but the agent use is clearly lower in MEL production. Besides the lower product mass per fermentation exchange (RL: 12-16 kg/5,000 L; MEL: 55-74 kg/5,000 L), the relative loss of product in RL production (ca. 12 %) is approximately two times higher than in MEL (ca. 6 %). With regard to economic evaluations, it should be kept in mind that the lower yield results in higher expenses, since higher technical expenditures tend to be necessary to achieve the same product quantities.

Table 1: Selected Life Cycle Inventory with characteristics, input and output flows for the four assessed process chains for the production of RL and MEL by the different substrates (MOL, SBP) with reference to one volume exchange (5,000 L)

	unit	RL_MOL	RL_SBP	MEL_MOL	MEL_SBP	source
basic parameter						
product	[-]	RL	RL	MEL	MEL	-
substrate	[-]	MOL	SBP	MOL	SBP	-
yield coefficient	[$kg_{Product}/kg_{Glucose}$]	0.1	0.1	0.235	0.235	data from project Bio²
conversion rate	[%]	10	10	21	21	data from project Bio²
critical micelle concentration (CMC)*	[Nm/m]	121	121	27	27	average value from 10 different literature sources
inputs						
specific substrate demand	[$kg_{Substrate}/kg_{Product}$]	241.0	171.0	43.5	30.9	calculated
substrate demand per 5,000 L fermentation	[$kg_{Substrate}$]	3,396	1,762	3,205	1,686	calculated
mineral medium per 5,000 L fermentation	[$kg_{Mineral\ medium}$]	65	65	287	234	data from project Bio²
Σ agent use during process per 5,000 L fermentation	[kg_{Agent}]	4,357	4,115	1,710	1,610	calculated
intermediate products						
theoretical mass product in fermentation broth	[kg_{RL}] or [kg_{MEL}]	16.0	11.7	74.3	55.4	calculated
product losses	[kg]	1.9	1.4	4.8	3.6	calculated
output						
product	[kg]	14.0	10.3	69.6	51.9	calculated

4 RESULTS & DISCUSSION

The selected results of the assessment of the three dimensions of sustainability are intended to show the main distinctive features of particular assessments and first hints for optimization.

4.1Environmental impacts

The results of the environmental LCA are presented in Figure 2 per process chain variant by summarized relative impact category shares. The process chain RL_SBP (CMC scaled, see section 2.2) generates the highest environmental impact, so it was set to 100 %. The four columns in Figure 2 represent the relative results per process chain scaled by the CMC scaling factor, so all results are comparable to each other, assuming the same cleaning performance. It gets visible that the use of SBP substrate for the fermentation led to approximately 20 % (RL) and 25 % (MEL) higher relative environmental impacts compared to MOL. The results of the process chains RL_MOL and RL_SBP were multiplied with the scaling factor 3.6 to reach the same specific cleaning performance and to enable the comparison. The substrate-indicated differences remain but the significantly larger environmental impact of RL production gets obvious (RL_MOL: 83.3 $\%_{largest\ impact}$, RL_SBP: 100 $\%_{largest\ impact}$). Regardless of the choice of substrate, the environmental impact of RL production is more than 20 times higher than the impact of MEL production.

Furthermore, the marked impact categories on the right side of Figure 2 ("Human toxicity, chancer effects" = HT CE; "Resource depletion, Water" = RD W, "Ecotoxicity, Freshwater" = ET FW) represent the impact categories with the largest influence in all product chains as they are responsible for 62-68 % of the total impacts per studied process chain. The relative share of the specific impact indicator (e.g., HT CE) on the total impact is in the same range for all examined process chains. Mainly responsible process stages for the impacts could be identified with the precipitation and extraction stages (agent production), the agent recovery stages (waste utilization), and the fermentation stage (steel production, compressed air supply).

To generate lower impacts by the production of the microbial surfactants, the identified impact hotspots have to be checked in relation to the possibilities of influencing. Exemplary possible options would be the increase of recycling rates for agents (precipitation, extraction), the change of agents, a more precise design of components or demand-oriented aeration (fermentation). Moreover, also sensitivity analysis of specific parameters such as yield coefficients of microorganism could offer new insights for further planning of the process design.

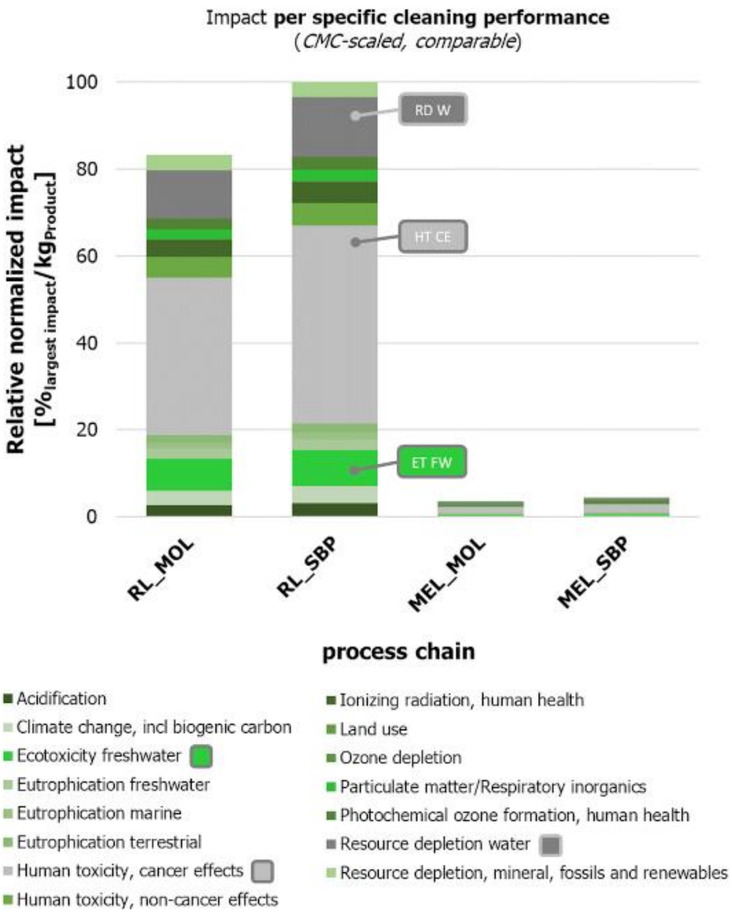

Figure 2: Relative normalized impacts of the assessed process chains for the substrate specific production of RL (RL_MOL, RL_SBP) and MEL (MEL_MOL, MEL_SBP) with the highest absolute impact set to 100 % (RL_SBP, CMC scaled) per cleaning performance, CMC-scaled; largest impact categories highlighted

The following Figure 3 shows the relative shares of environmental impacts per process stage for the production of RL with different substrates. The proportions of shares are relatively similar. Exemplary deviations are given with the share of biomass production and processing, which is larger in the case of MOL use. Furthermore, the share of fermentation and precipitation recovery is slightly lower in the case of MOL use. Both effects can be traced back to the different properties of substrates and the resulting technological efforts. The largest contributions to the impacts are related to the fermentation and the precipitation recovery stage (each more than 30 %). The precipitation recovery stage contains also the production of new added agent, which is the main driver for impacts. The fermentation stage is characterized in terms of environmental impacts by the steel production for the fermentation tank and the air supply during fermentation. The lowest shares can be seen in the stages of seed fermentation as well as the storage and preparation stage.

Although the extent and technological share of the individual process stages differ in this case the decisive sections can be directly identified. An examination of the originating process modules offers the possibility of identifying points for optimization (e.g., precipitation agent use). The following technical delimitation also allows an estimation of the influenceability (in principle and by sensitivity analyses).

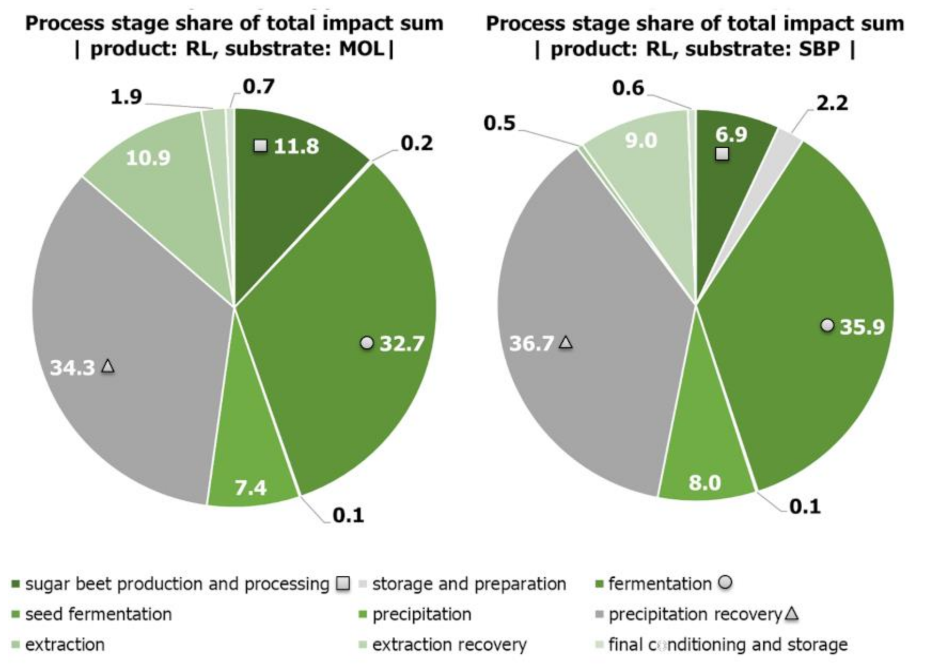

Figure 3: Environmental impact share per process stage for the production of RL by different substrates, MOL and SBP

4.2Economic aspects

Figure 4 shows relative total production cost (TPC) and the costing of the process chains driven by the use of MOL substrate (RL_MOL, MEL_MOL). The comparison of TPC on the left side of Figure 4 shows that the main cost positions are the direct production cost and the fixed charges (RL_MOL: 76.6 %; MEL_MOL: 74.3 %). The share of the five cost positions presented is similar in all cases regardless from the product. The most significant fact is that the TPC of MEL_MOL is 3-4 times lower than for RL_MOL. As a result from this fact the pricing structure comparison leads to identical ratios of 3-4 times higher prices for RL_MOL as it is shown in the two columns on the right side of Figure 4. While the specific price (with margin of 0 % = cost) of MEL_MOL production is located in a lower three digit range per kg (ca. 325 €), the specific minimum price of RL_MOL is situated in a lower four digit range (1,125 €).

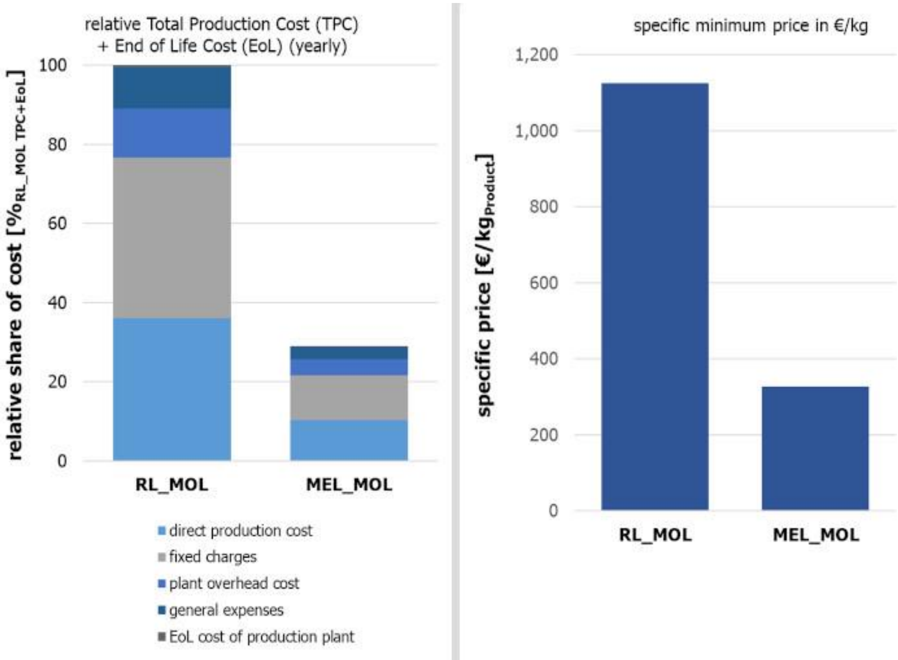

Figure 4: Relative total production costs (TPC, left) and specific minimum pricing (with a margin of 0 % = cost, right) for 1 kg of product; TPC: highest absolute cost set to 100 % (RL_MOL)

Like mentioned before, the pricing depends on different factors like purity or application. Own market research has shown a general relation between purity and price. Mass markets like the application field of detergents are related to lower surfactant purities than niche markets like pharmaceuticals or food applications. Taking into account the reached purities within the project Bio² (> 98 %), it can be assumed that the reachable minimum pricing is located within the market range. Nevertheless, an optimization of economic issues should be checked in further studies by analyzing the cost positions in detail. As the present study represents cost estimations of an early stage development, the pricing has to be checked in a further iterative approach. Influences like the LCA-indicated processing changes or the consideration of future CO_2-pricing could generate advantageous pricing structures.

4.3 Social risks

Results for preselected social indicators can be found in the following Figure 5. The comparison of the results for RL_MOL and MEL_MOL is possible due to the applied scaling of mass specific results by the CMC scaling factor like mentioned in 2.2. Each result is expressed by an indicator specific unit. The production of RL_MOL results in 1,560 "fair salary (FS) medium risk hours", while the MEL_MOL production results in ca. 110 FS medium risk hours, for example. A comparison of the different indicators among each other is not possible because of the different units. It gets visible that the result ratio of the studied indicators is similar, so the social risks of RL_MOL production are approximately 17 times higher than the MEL_MOL production. Strong impact causing process modules could be identified with the production of mineral media (fermentation stage) for MEL production or the production of precipitation agents (precipitation stage) in the case of RL production. In conclusion, it can be observed that the main social risks result from the economic sectors of manufacturing chemical, metal and plastic products (sector mapping not shown here).

Figure 5: Comparison of absolute results for RL_MOL and MEL_MOL production by selected social categories with CMC scaling

Because the assessment of social risks depends mainly on material flows and related financial data the further development may change the future results coming up from an iterative adjustment of the process framework. Keeping in mind the results from LCA and conclusions regarding dimensioning, a qualitative similar result related to the social risks is not surprising. The more the specific material demand is rising, the more specific costs and social risks are to be expected. Nevertheless, the possible increase of recycling rates could lower the social risks in the sector of chemical products in a clear way, for example. Likewise, a more detailed engineering in a later development state could lower the risks by less metal or plastic consumption. However, it gets clear that the more advantageous process can be found in MEL production.

5 CONCLUSIONS

This present study compiles the environmental, economic and social performance of microbial RL and MEL production based on molasses and sugar beet pulp substrates in an industrial scale.

Regarding the environmental impacts the strongest influenced impact categories (e.g., Human toxicity, cancer effects) and their origin of effects (e.g., production of extraction agents) were identified. Furthermore, the comparison of the products' impact results based on their specific cleaning performance has shown clearly that RL production leads to much higher environmental impacts. The analyzing of different choices of substrate has shown that the use of SBP results in moderately higher environmental impacts due to substrate properties and the related increased technology efforts. By an analysis of impact shares for specific process sections and a further examination, optimization starting points were detected and technically narrowed.

The determination of total production costs has shown the starting points for economic optimization that could also be generated by the design changes indicated by the LCA results, for example. A specific pricing for the products has shown that economic competitiveness could be possible in the future, at least for the production of MEL.

Analyzing selected social indicators has shown a clear advantage for MEL production too. The most influencing process modules and economic sectors connected to the social risks could be identified (e.g., manufacturing of chemicals). Based on the identified environmental, economic and social hotspots within the process chains it was possible to formulate starting points for an optimization and needs for further investigations.

Further studies should analyze the results at a more detailed level. In combination with a progressing state of development and an iterative exchange with process developers, the lowering of impacts is possible. Summed up, the production of MEL is related to lower impacts and costs in the current state of process design. Despite the early stage of development, it can be assumed that the qualitative result differences will continue to be valid, so MEL production will also show clear advantages in all three dimensions of sustainability in the future.

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8 ACKNOWLEDGEMENTS

The presented outcomes are related to the project Bio² (2017-2020), as part of the NRW-Strategieprojekt BioSC and funded by the Ministry of Culture and Science of the German State of North Rhine-Westphalia. The used process engineering data was provided and generated by project partners from the institutions RWTH Aachen University, AVT - Chemical Process Engineering, RWTH Aachen and RWTH Aachen University, AVT - Fluid Process Engineering. Underlying basic data for the process design and related to aspects of microorganism and microbiology was provided by the Heinrich-Heine-University Düsseldorf - Institute for Microbiology - Department of biology, the RWTH Aachen University - Institute of Applied Microbiology (iAMB) and the Heinrich-Heine-University Düsseldorf - Institute of Molecular Enzyme Technology (IMET).