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Integrating life cycle assessment in early process development stage: The case of extracting starch from mango kernel

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ABSTRACT

An important issue in the development of new processes is how to perform environmental impact assessments that support decisions at an early stage of process development. In this study, a methodological procedure was applied to insert life cycle assessment (LCA) in early design of two alternative processes (A and B) to extract starch from mango kernel. This procedure allowed to perform LCAs at technology readiness levels (TRL) 4 and 5 considering different functional units, production scales and alternative scenarios. The analysis of process A and B identified the phase of starch purification as one of the most impacting one. After modifications were implemented, the comparison of Process A with B showed that process A, characterized by extracting only starch, performed better in all situations, being recommended for the implementation in a pilot plant, the next level in the technology maturity scale. Process B still requires improvements to reduce the impacts on climate change and human toxicity. This case study showed reductions in energy and water use, and life cycle impacts, when moving production from lab to industrial scale, through simulation. It also showed that crop production should be considered when evaluating processes that use biomass waste as raw material. The lessons learned from this case study allowed the simplification and detail of the applied procedure for inserting LCA at early research stage. This procedure can be applied to perform ex-ante LCA of new processes.

1. Introduction

One of the goals of the circular bioeconomy is to design processes that enable the transformation of food waste into valuable products. Collaboration between technology developers and the environmental team is necessary to ensure that these transformation processes are developed with a reduced environmental impact. However, an important issue in the development of new processes is how to perform environmental impact assessments that would support decisions at an early stage of process development.

Life cycle assessment (LCA) has long been applied to evaluate the environmental impacts of processes and products (Baumann and Tillman, 2004). LCA is a methodological approach for accounting environmental aspects and impacts of a product system from resources extraction, processing, product use and end-of-life. Recently, however, the challenges of applying conventional LCA for evaluating processes and products at early research stage have been discussed (Giesen et al., 2020).

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The main challenges of applying LCA in the study of processes at early research and development stages are poor inventory data, high uncertainties regarding manufacturing and product functionality, adoption of current background processes in the future, and lack of characterization factors in impact methods to account for the toxicity of new products, such as those from nanotechnology. To overcome these challenges, guidelines for performing LCA at early research have been proposed and encompass: the use of primary data for the inventory of foreground processes; simulation of lab processes at industrial scale for comparisons with mature technologies; consideration of multiple functional units, system boundaries and production scenarios, and communication of uncertainties to decision-makers (Arvidsson et al., 2017; Cucurachi et al., 2018; Buyle et al., 2019; Thonemann et al., 2020; Giesen et al., 2020; Moni et al., 2020). Regarding background processes, an approach for improving temporal consistency when comparing incumbent and new technologies was proposed for considering changes in efficiency and market scenarios in processes such as electricity and mobility (Beltran et al., 2018).

Moreover, Buyle et al. (2019) and Bergerson et al. (2020) highlighted the importance of informing the maturity level of new processes and products in development, especially when making comparisons with incumbent ones. These authors proposed to associate a technology readiness level (TRL) when performing a LCA and presenting its results.

TRL follows a scale (1–9) that shows the evolution of a technology from conceptual design, laboratory experimentation, pilot production and final commercialization (Moni et al., 2020). This approach provides clear information about the maturity level of a technology and prevents a comparison between immature and mature technologies, thereby increasing transparency. Furthermore, Bergerson et al. (2020) proposed an approach to consider the TRL of both technology and market to better support the goal and scope definition of an LCA study as well as decisions regarding which tools to apply.

In this context, many new processes for extracting materials from food processing waste have been proposed to foster the bioeconomy and circularity in the food system worldwide. Caldeira et al. (2020) and Campos et al. (2020) found that significant research has been done to investigate valorization pathways for fruit wastes, especially peels and seeds. These researches proposed processes at low TRLs, especially those using tropical fruit wastes, with most processes tested in lab experiments and some modeled at pilot scale. Ex-ante LCA studies of these processes are scarce and devoted to olive and citrus wastes (Caldeira et al., 2020).

Fruit wastes from fruit processing companies are especially important because great amount of this biomass is concentrated especially in pulp, juice and jam companies, facilitating collection and reducing waste degradability, especially when producing facilities are installed close to the waste generation source. Furthermore, fruit processing wastes are important sources of starch, proteins, oil and fibers that can be further processed to obtain diverse value-added products such as bioactive compounds, enzymes, biopolymers, organic acids, polysaccharide, polyphenols and biofuels (Esparza et al., 2020; Caldeira et al., 2020; Campo et al., 2020).

Starch is a complex carbohydrate that can be extracted from some tropical fruit wastes, especially banana peels and avocado, jackfruit and mango seeds (Kringel et al., 2020). Lab scale processes were proposed for extracting starch from green banana peels (approximately 30% of dry matter) with their immersion in ascorbic acid or sodium sulfate (Hernández-Carmona et al., 2017). A pilot scale plant for extracting starch from avocado seeds (represents circa of 25% of the fruit dry weight with 29% of starch) was modeled by Tesfaye et al. (2020) based on a lab scale experiment using sodium sulfate. Jackfruit seeds are responsible for 8–15% of the fruit weight and are reach in starch (around 70% of dry matter) that can be extracted using wet-grinding, alkaline method or enzyme methods (Zhang et al., 2021). Mango seed and peel accounts for 30–50% of the fruit weight and have been send for final treatment in major fruit producing and processing countries, such as Brazil and India (Kringel et al., 2020). However, many products can be extracted from mango peel and seeds (tegument and kernel): i) pectin and bioactive compounds from peel; ii) cellulose from tegument; and iii) starch and oil can be extracted from mango kernel (Zuin et al., 2020).

Mango kernel starch (MKS) is still a poorly explored product with the processes for extracting starch from kernels at laboratory stage. Cordeiro et al. (2014) proposed a technological route for extracting white MKS, whereas Melo et al. (2019), using a biorefinery approach, proposed a route for extracting polyphenols and fat, besides white MKS. The starch extracted from mango kernels in both processes had amylose content higher than 22% with great potential to be used in the production of bioplastics. The fat presented similar characteristics to cocoa butter, whereas the polyphenols had similar antioxidant properties to those extracted from other fruit peels, such as apple peel. These two co-products of MKS extraction have great potential to be used in the food industry (Cordeiro et al., 2014; Melo et al., 2019).

So far, no study has assessed the environmental impacts of extracting starch and other coproducts from mango kernels. Arora et al. (2018) and Tesfaye et al. (2020) evaluated the economic feasibility of processing mango waste, using data from modeled industrial processes, without considering environmental impacts.

In this study, a methodological procedure is applied for inserting LCA in the design of two alternative processes for extracting starch from mango kernel: process A, defined by Cordeiro et al. (2014) and Process B, proposed by Melo et al. (2019). Recommendations for future research with mango kernel and for the simplification of the adopted procedure are provided.

2. Methods

2.1. Procedure used for evaluating the environmental impacts of process at early development stage

The methodological procedure to integrate environmental impact assessment at early development stage was applied in this study and is summarized in Fig. 1. This procedure has been used by the research team at the Biomass Technology Laboratory of the Brazilian Agricultural Research Corporation (Embrapa) for decision making about new processes and products (Silva et al., 2020).

The procedure requires a sequence of activities to analyze new processes and products in TRLs 4 and 5. Two life-cycle based environmental assessments (LCA1 and 2 in Fig. 1) are performed in these TRLs to support research team decisions regarding whether to evolve in the technology maturity level or to modify processes to reduce their environmental impacts. LCA1 and 2 follow the recommendations of ISO 14040 and 14044 (ISO, 2006a and 2006b).

In regular TRL4 research and development activities, experiments are performed at lab scale resulting in processes completely described, with their production phases designed to generate the highest amount of products and coproducts. At this technology maturity level, alternative processes are identified together with the development team.

At TRL 4, the inventories of each process are built performing mass balances at each production phase in the laboratory (Step 1 in LCA1). Initially, production phases that cause the highest potential impacts are identified (Step 2). Modification in these phases are discussed with the production team and scenarios are analyzed to evaluate changes in the environmental impacts (Step 3). Processes are finally compared to identify the best environmentally performing one at the lab scale (Step 4).

In TRL 5, processes defined in TRL4 are simulated at the industrial scale, allowing their assessment at relevant production environment in LCA2 (Steps 1 to 4). The inventories of processes are built from the simulations of production at the industrial scale (Step 1). These processes are evaluated again to identify critical phases (Step 2), possibilities for changes (Step 3) and best performing process (Step 4). Finally, products extracted from up scaled processes are compared to similar ones (Step 5).

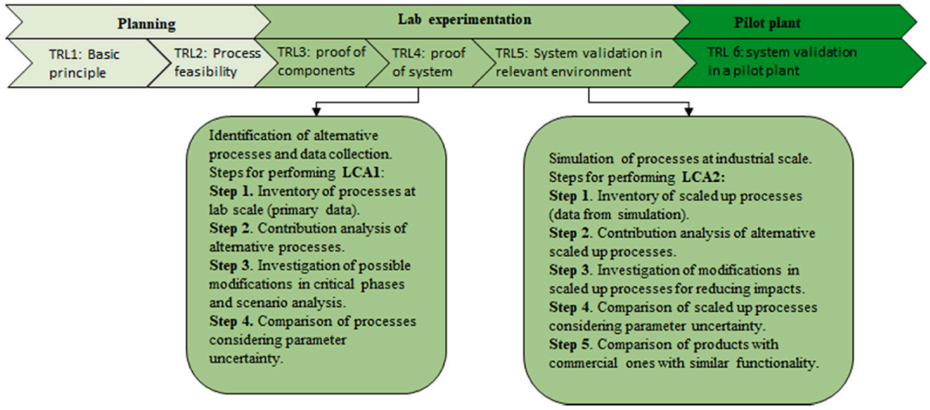

Fig. 1. Procedure adopted to evaluate processes at early development stage.

2.2. Case study: extraction of valuable products from mango kernels

The methodological procedure described in section 2.1 was applied in the study of two alternative processes proposed for extracting valuable products from mango kernels: process A (Cordeiro et al., 2014) and B (Melo et al., 2019). The following subsections detail the aim, scope, data collection and impact methods applied when performing LCA1 and LCA2 in this case study.

2.2.1. Aim and scope of LCAs 1 and 2

Both LCA1 and LCA2 aimed to answer the following questions formulated by the research team at Embrapa Tropical Agroindustry: What are the environmental impacts of each process and, specifically, of MKS? Are processes impacts relevant in the supply chain? Which processes phases most contributes to impacts? Is it possible to reduce impacts of processes? Which process cause less impacts?

To answer these questions, two functional units were applied, considering recommendations from Nemecek et al. (2011), when evaluating multifunctional cropping systems, and Ahlgren et al. (2013), when analyzing biorefinery systems: the monetary and production units. The monetary functional unit allowed to study multifunctional processes, presenting impacts per US$ 1 of revenue, without discriminating products. The revenue obtained in process A and B was calculated multiplying the mass of product (starch) and coproducts (fat and polyphenols), at each production scale, by its average market value in 2020, considering the following values per ton of product: US$ 840/ton of fat, US$ 750/ton of polyphenols and US$ 258/ton of starch. This unit was chosen because it was easy to communicate results to researchers despite the fact that prices fluctuates over time. Other functional units for studying multifunctional process have been used and regards the mass of raw material, the number of plant units and the total mass of products (Ahlgren et al., 2013). The mass of raw material was indicated for determining the best use of land or biomass, for example, when comparing waste management alternatives. Although the number of plant units or the total mass of products may also be used to compare processes, it is harder to communicate results to stockholders.

The production functional unit focused on starch, the main product obtained in both processes, presenting impacts per kg of MKS. This functional unit allowed to answer the research team questions that focused on MKS.

The adoption of the production functional unit (1 kg of MKS) required the allocation of impacts among product and coproducts. Mass and economic allocation criteria were adopted. The allocation percentage, as well as mass and economic values in each process, are presented in Table 1.

Allocation was first required in mango pulping, which produced mango pulp (product), peel and stone (coproducts). Furthermore, in both processes for MKS extraction (A and B), the phase of shell removal required allocation because it separates kernel (product) from shells (coproduct). For mango peel, the price of apple peel was considered.

Table 1
Mass and economic allocation factors.

Process	Mass (ton)	Monetary value (US $/ton)	Revenue (US$)	Mass allocation (%)	Economic allocation (%)
1. Pulping					
Pulp	27042	1000	27041887	55.5	83.3
Peel	10957	250	2739197	22.5	8.4
Stone	10716	250[a]	2679031	22.0	8.3
Total mass	48715	Total revenue	32460114		
2. Process A and B: shell removal phase					
Kernel	5351	150	802651	49.9	59.9
Shell	5365	100	536500	50.1	40.1
Total mass	10716	Total revenue	1339151		
3. Process B					
Fat extraction phase					
Fat	205.4	840	172501	7	8
Puree 1	2809	750[b]	2106720	93	92
Total mass	3014	Total revenue	2279221		
Polyphenols extraction phase					
Polyphenols	274.4	750	205801	10	24
Puree 2	2592	258[c]	668617	90	76
Total mass	2866	Total revenue	874418		

[a] $ Stone = $/ton of kernel (150.0) + $/ton of shell (100.0).
[b] The value of Puree 1 was considered to have the same value as polyphenols.
[c] The value of Puree 2 was considered to have the same value as starch.

The following phases of process B also required allocation: fat extraction and polyphenols extraction. The value of mango stone was obtained by the commercialization of products with similar functionality of kernel and shell. Starch is the major constituent of mango kernel (51%), whereas cellulose (55%) is the main one of shell. In this way, the value of maize, major source of starch, was attributed to kernel and the value of sawdust, source of cellulose, for shell.

Regarding system boundary, at the reference situation (base case, Fig. 2), it encompassed mango crop production, mango pulping, kernel separation, two alternative MKS extraction processes (A and B), the production and transportation of inputs to facilities. As mango kernels are currently regarded as food waste by the mango pulping industry, with no defined economic value, an alternative system boundary was also analyzed, disregarding the impacts from mango cropping and pulping and focusing on kernel separation and the starch extraction processes, production and transportation of inputs to plant facilities (scenario 1).

Both process A and B included mango kernel separation from the

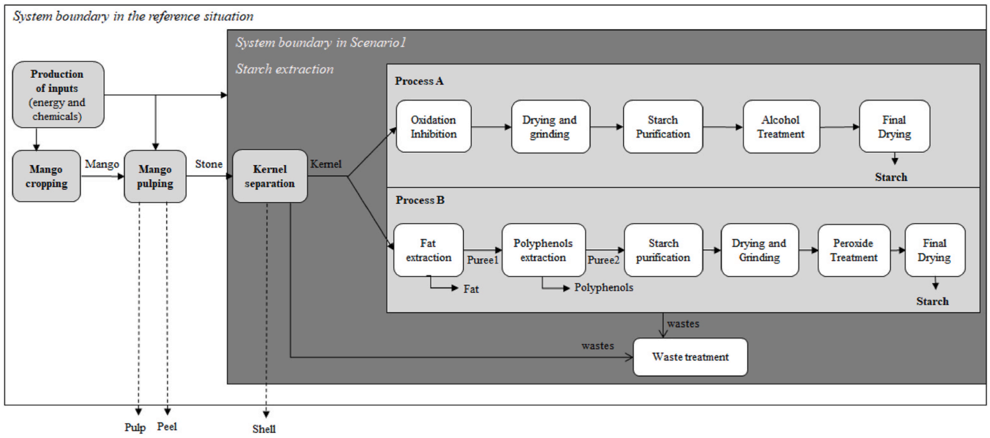

Fig. 2. System boundary for mango kernel starch (MKS) extracted by process A and B in the reference situation and scenario 1.

other parts of the fruit (peel, pulp, and stone shell), as well as the phases necessary for starch extraction. The following phases were considered in process A: shell removal from stone, oxidation inhibition, grinding and drying, starch purification, alcohol treatment, and final drying. In process B, the phases included were shell removal, fat extraction, polyphenols extraction, starch purification, peroxide treatment and final drying.

Waste treatment was considered for liquid effluents and solid bio-waste generated at kernel separation and specific MKS extraction phases, in both reference situation and scenario 1 (Fig. 2): i) oxidation inhibition and starch purification in process A and ii) starch purification and peroxide treatment in process B. A generic treatment was considered for wastewater, whereas composting was considered for treating bio waste.

This study considered that crop production, mango pulp plant and MKS plant were in the same area.

2.2.2. Data collection

Primary lab scale data were collected at the Biomass Technology Laboratory of the Brazilian Agricultural Research Corporation (Embrapa), for mango pulping and process A and B (Fig. 1). Input and outputs of process A and B were collected at each phase. These inventories were used to perform LCA 1 (Fig. 1).

The simulation of process A and B at the industrial scale was implemented in software *SuperPro Designer* version 10. To build this simulation, the following data obtained with the research team and performing the inventory analysis at lab scale were used: composition and amount of inputs and outputs (products and residues), description of process conditions (reaction time, temperature, pressure, sequence of input use) and equipment used. Industrial equipment options from *SuperPro* database were chosen to perform similar to the functions of lab equipment. The proportion between the amount of raw material and chemicals used at the laboratory scale was maintained at industrial scale for process A and B. The description of processes, equipment, and plant flowsheets at the industrial scale are in Annex A (supplementary material).

The inventories of process A and B, used in LCA2 (Fig. 1), were built after simulating MKS extraction at the industrial scale. The final amounts of input and outputs of each process phase, considering the processing capacity and energy efficiency of each chosen machinery, were used to build these inventories.

The cycle duration of process A and B differed at both the lab and modeled industrial scales. To make these processes comparable, inventories were built for one year of production, at both the lab and industrial scales. The inventories of process A and B are in Annex B (supplementary material).

Secondary data were obtained from the LCA inventory database ecoinvent v.3.1 (Frischknecht et al., 2007) for background processes regarding energy and chemicals production and transportation. The chemicals used in process A and B were found in this database, except sodium metabisulfite in process B. In this case we used a generic inorganic chemical inventory. The inventory of mango crop production was obtained from Carneiro et al. (2019). The list of secondary inventories used in this study are found in Annex C (supplementary material).

2.2.3. Impact assessment and interpretation of results

The following environmental impact categories were assessed based on the International Reference Life Cycle Data System (ILCD) handbook (Commission, 2011): climate change, human toxicity/non-cancer effects, human toxicity/cancer effects, acidification, freshwater eutrophication, marine eutrophication, and ecotoxicity. Additionally, AWARE version 1.00 model (Boulay et al., 2018) was used to evaluate the water scarcity impact.

LCA1 and LCA2 were performed in SimaPro 9.0.0.35. The following analysis were made at both production scales (Steps 2, 3 and 4 in LCA1 and 2, Fig. 1): i) contribution analysis to identify critical phases in process A and B (Step 2); ii) scenario analysis to investigate opportunities for reducing impacts (Step 3); i) comparison of processes environmental performance, considering parameter uncertainty through Monte Carlo (Step 4). An alternative production scenario was defined together with the development team after the identification of critical phases in process A and B. For each of these analysis, results from lab (LCA1) and industrial scale (LCA2) are presented together aiming to identify changes related to production scale.

To compare process A and B as well as the coproducts from these processes (starch, polyphenols, and fat) with similar commercial ones, uncertainty analysis of environmental impact results was performed with Monte Carlo, considering 95% confidence (Goedkoop, 2008). The standard deviation of inventory data was obtained from the Pedigree Matrix. All variables were considered to follow a lognormal probability distribution.

The comparison of process A and B was performed in a 1000 runs. For each impact category, it was counted the number of times that the impact value of A-B < zero and this number was divided by the total number of runs (1000). If the percentage of times A-B < zero was equal or higher that 95% for an impact category, the impact of A was considered significantly lower than B in this category. Impact results were obtained for the production (per kg of product) and monetary (per US$ of revenue) functional units (section 2.1).

To compare mango kernel products with similar commercial ones, the mean, minimum, and maximum impact values of starch, polyphenols, and fat were calculated after 1000 runs. Results were obtained for the production functional unit (kg of starch, polyphenols or fat).

MKS was compared with starches extracted from maize and potato, using inventories from ecoinvent v.3.1. MKS was also compared with cassava and sago starch for the impact category of climate change, considering the results obtained by Yusuf et al., 2019 and Usubharatana and Phungrassami (2015), respectively, using IPCC (2007) characterization factors.

For fat, the comparison was made with cocoa butter, considering the impact reported by Ntiamoah and Afrane (2008). For polyphenols, no similar commercial product was found and the comparison was made with polyphenols extracted from pomegranate peels in a biorefinery proposed by Shinde et al. (2020), modeled at the industrial scale.

Ntiamoah and Afrane (2008) and Shinde et al. (2020) calculated impacts using the CML2001 method, but did not report the ranges of impact values. To allow comparisons with these studies, the impacts of polyphenols and fat from process B were also calculated using CML2001. The impact ranges of MKS, polyphenols, and fat were compared with the average impact values of similar products.

3. Results and discussion

3.1. Process A and B at lab and modeled industrial scales

Process A and B presented different batch times, materials use, production, yield, and revenue at the lab and industrial scales (Table 2). The batch time was reduced in both processes with the scale up, whereas production increased.

MKS yield was measured considering two alternative references: mass of raw material (mass of starch/mass of kernels) and batch time (mass of starch/batch hours). In process A, the yield increased with the scale up, independently of the reference used. Process A had a reduced loss of material, mainly because of the filtration phase present at the lab scale, which was considered unnecessary and was removed at the industrial scale.

In process B, the yield measured in relation to the mass of kernels decreased with the scale up, whereas the yield in relation to batch time increased. The main reason for this was the higher complexity and additional phases of process B for extracting polyphenols and fat, in addition to starch, resulting in material loss. The reduction in batch time with the scale up improved the performance of process B, but was not enough to make the yield as high as the yield of process A.

Significant differences in revenue from the commercialization of MKS and coproducts were found. At the lab scale, process A generated higher revenue per year, but at the industrial scale, process B had better results. The best revenue from process B was generated from the commercialization of fat and polyphenols, besides MKS. While the revenue obtained in process A increased 99,971-fold with the scale up, the revenue in B increased 1137-fold.

Table 2
Process A and B parameters at the lab and modeled industrial scales.

Scale	Parameters	Process A	Process B
Laboratory	*Duration*		
	Batch duration (h/batch)	44	325
	Annual operation time (h)	7891	7840
	Number of batches per year (batches/year)	178	24
	Raw materials and products		
	Stone (kg/year)	280.56	3.41
	Kernels (kg/year)	129.14	1.57
	Shell (kg/year)	151.56	1.84
	Starch (kg/year)	8.29	0.48
	Polyphenols (kg/year)		0.25
	Fat (kg/year)		0.14
	Yields		
	Starch (kg/kg of kernel)	0.06	0.31
	Starch (kg/h)	0.0011	0.0001
	Polyphenols (kg/h)		0.03
	Fat (kg/h)		0.02
	Total revenue (US$)	2138.69	433.97
Industry	*Duration*		
	Batch duration (h/batch)	5.25	12.25
	Annual operation time (h)	7891	7840
	Number of batches per year (batches/year)	1503	640
	Raw materials and products		
	Stone (kg/year)	9,702,995.26	9,721,516.80
	Kernels (kg/year)	4,845,294.75	4,854,360.32
	Shell (kg/year)	4,857,777.16	4,867,049.60
	Starch (kg/year)	828,710.61	583,157.76
	Polyphenols (kg/year)	–	248,932.48
	Fat (kg/year)	–	186,298.24
	Yields		
	Starch (kg/kg of kernel)	0.17	0.12
	Starch (kg/h)	105.02	74.38
	Polyphenols (kg/h)	–	31.75
	Fat (kg/h)	–	23.76
	Total revenue (US$)	213,807,337.38	493,644,583.68

3.2. Process A: Contribution analysis

In this section, the environmental impacts of background (mango farming and pulping) and foreground processes (starch extraction) are presented for the extraction of MKS through process A, at the lab (LCA1 in Fig. 1) and modeled industrial scales (LCA2).

3.2.1. Contribution of foreground and background processes

The analysis of potential impacts of mango crop production, pulping, and starch extraction showed that the contribution of the foreground process (starch extraction) was reduced when production moved from the lab to industrial scale (Fig. 3a and b). This pattern was also observed in previous studies of nanoscale products (Piccinno et al., 2018; Tan et al., 2018; Bartolozzi et al., 2020) and bacterial cellulose (Silva et al., 2020) that compared lab and pilot modeled environmental impact results.

The contribution of MKS extraction was higher when economic allocation was used. This occurred because the estimated economic value of kernels (raw material for MKS) was higher than the value of shells, increasing the impact when the economic criterion was adopted (Table 1).

Mango crop production at both scales was important mainly for marine eutrophication (Fig. 3a and b). The impacts of mango cropping were mostly due to the production and use of nitrogen fertilizers.

The contribution of mango pulping became more relevant at the industrial scale because there was a reduction in the impacts (all categories) caused by the starch extraction process A (Fig. 3b). The production of sodium hypochlorite, used as disinfectant for surfaces, water, and fresh product, was responsible for the majority of these impacts. The contribution of pulping was higher when using mass allocation because the monetary value of mango stones was four-fold lower than pulp (Table 1).

3.2.2. Contribution of phases in process A

Analyzing the contribution of the phases in process A, they were similar in a production scale, independently of the functional unit used (Fig. 4a and b). This was expected because process A only produced starch. The only change was the reference used for calculating the impacts ($ or kg of starch), but the phases kept the same impact proportionality.

When scaling up, the importance of the different phases changed. At the lab scale, the phases of oxidation inhibition, alcohol treatment and starch purification were the most important ones for all impact categories. At the industrial scale, starch purification lost importance and the most important phases were oxidation inhibition, alcohol treatment, and grinding and drying.

Impacts from the oxidation phase at both scales were mainly due to the production of sodium metabisulfite, used to inhibit kernel darkening. The contribution of the alcohol treatment phase was more important for water scarcity (93%), due to the water consumed in the

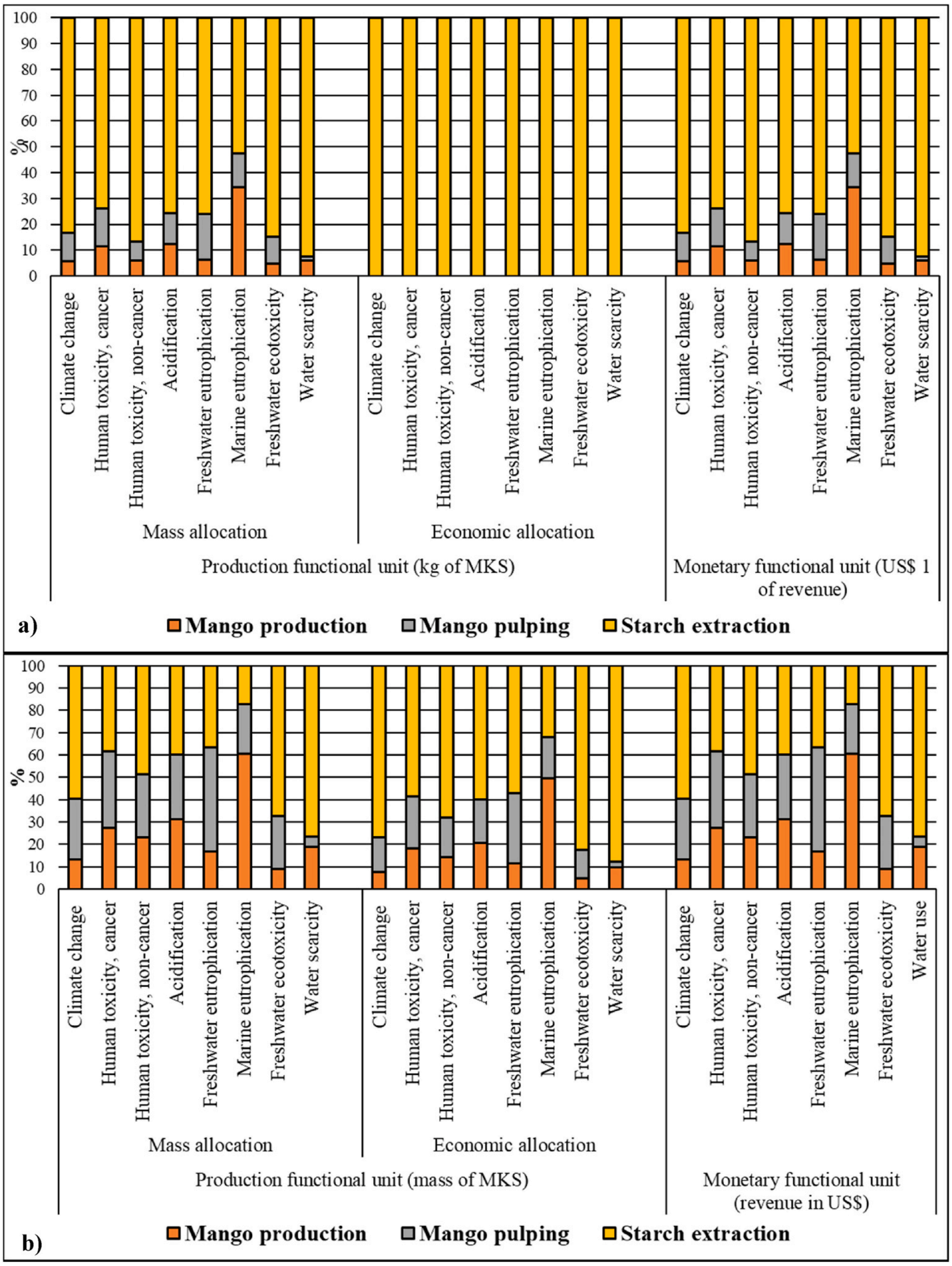

Fig. 3. Contribution of foreground and background processes, when process A was used for starch extraction at the a) lab and b) industrial scales, applying the production and monetary functional units.

production of ethanol, and to human toxicity, non-cancer (77%), due to the use of agrochemicals in sugar-cane production.

The grinding and drying phase became relevant at the industrial scale for four impact categories (climate change, acidification, marine eutrophication, and water scarcity), mainly due to steam production chain. Steam was produced from burning natural gas and oil.

Another aspect that changed with the scale up was the use of energy and water in each phase. There were high decreases in total energy (68%) and water (66%) usage with the scale up of process A (Tables 3 and 4).

Although the total energy and water use decreased with the scale up, some phases increased their energy and water usage. Regarding energy, some phases (shell removal and oxidation inhibition) were manually performed at the lab scale, not requiring energy. Furthermore, at the lab scale, electricity was the sole power used for generating mechanical work and heating. At the industrial scale, all phases made use of electricity for mechanical power, but some of them (especially alcohol treatment and grinding and drying) used natural gas and oil to generate steam applied in heating procedures, increasing energy use per kg of MKS or per US$ (Table 3).

The use of steam and the clean-in-place (CIP) of equipment required the use of water at the industrial scale for the shell removal and alcohol treatment and drying (Table 4). Water for CIP was not accounted at lab scale.

3.3. Contribution analysis: Process B

In this section, the environmental assessment of background and foreground processes as well as the main phases of process B are presented, considering the lab (LCA1 in Fig. 1) and modeled production

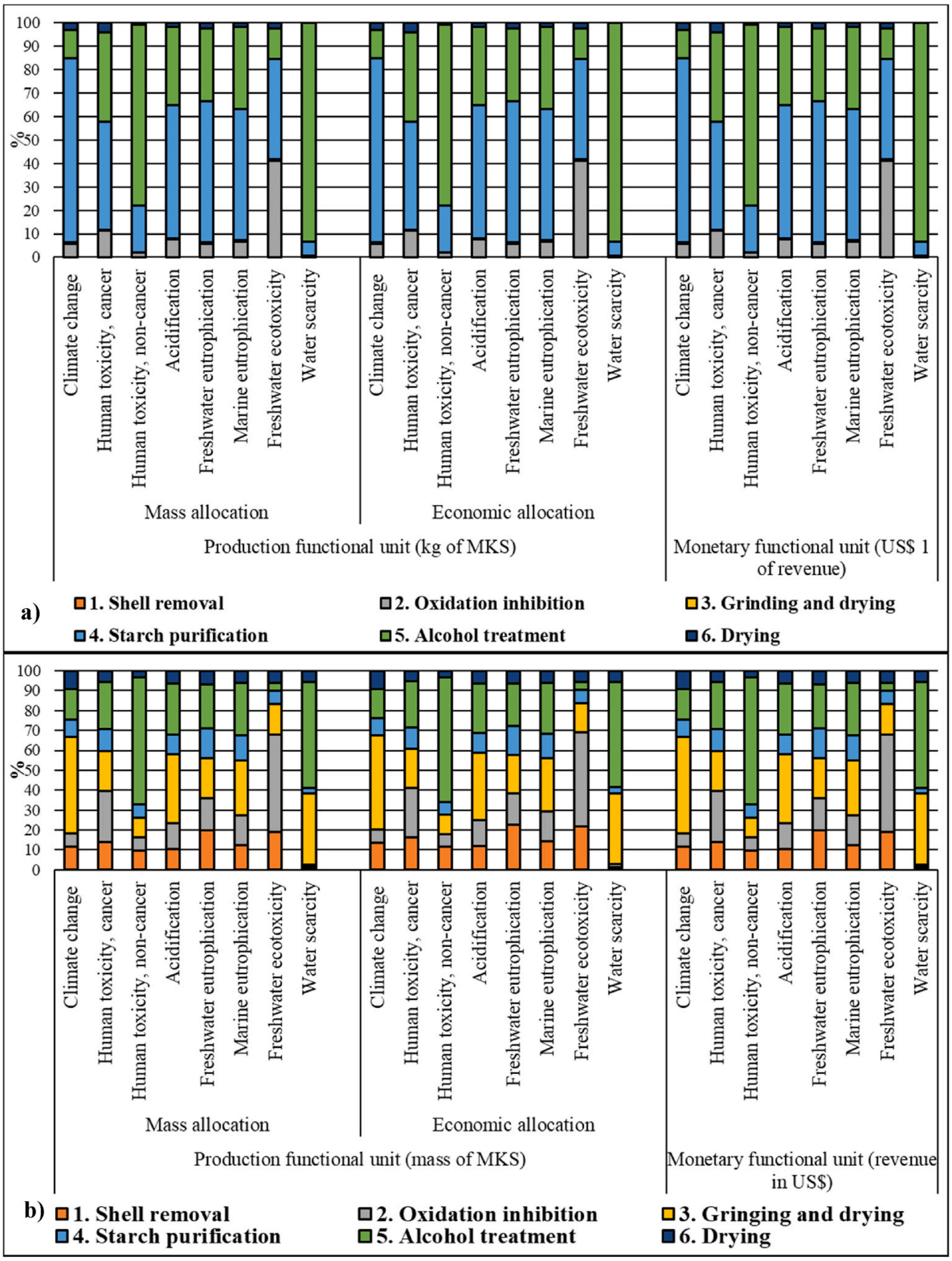

Fig. 4. Contribution of starch extraction phases in process A at the a) lab and b) industrial scales, applying the production and monetary functional units.

scales (LCA2).

3.3.1. *Foreground and background processes*

The contribution of starch extraction also decreased with the scale up of process B (Fig. 5a and b). However, process B still generated most of the impacts in all categories at the industrial scale (Fig. 5b). This happened despite the significant reduction in total energy (97% in Table D1 in Annex D, supplementary material) and water use (88% in Table D2 in Annex D, supplementary material) with the scale up and the high increase in the production of MKS, polyphenols and fat (Table 1). The higher contribution of process B in relation to process A (Figs. 3b and 5b) was mainly due to the higher amount of energy at both scales (70% higher at the lab and 66% at the industrial scale, from Tables D2 and D2, Annex D, supplementary material).

3.3.2. *Contribution of phases in process B*

The analysis of process B shows that the relative importance of its phases to impacts changed when moving from lab to modeled industrial scale (Fig. 6a and b), as occurred in process A (Fig. 4a and b). However, differently from process A, the contribution analysis changed with the choice of functional unit at the same production scale.

At the lab scale, the most important phases when the monetary unit ($ of revenue) was adopted were the more energy-intensive ones (drying and grinding, fat and polyphenols extraction, and peroxide treatment in Table D1 in Annex D, supplementary material). When the contribution analysis was performed per kg of starch (production functional unit), the phases fully related to starch prevailed (peroxide treatment and, drying and grinding). This happened because only part of the impacts from the phases of polyphenol and fats extraction was allocated to starch (Table 1).

At the industrial scale, the use of energy was significantly reduced by

Table 3
Energy use in process A at lab and modeled industrial scales.

Extraction phases	Lab scale			Industrial scale			Reduction or Increase* with the scale up (%)	
	Energy use (KWh/year)	Energy use (kWh/kg of MKS)	Energy use (kWh/US$)	Energy use (kWh/year)	Energy use (KWh/kg of MKS)	Energy use (kWh/US$)	Energy use per kg of MKS	Energy use per US$
1. Shell removal	–	–	–	2,23E+06	2,69E+00	1,04E-02	100%*	100%*
2. Oxidation inhibition	–	–	–	9,83E+03	1,19E-02	4,60E-05	100%*	100%*
3. Grinding and drying	3.41E+00	4.11E-01	1.59E-03	4,72E+06	5,70E+00	2,21E-02	93%*	93%*
4. Starch purification	2.75E+02	3.32E+01	1.29E-01	3,51E+05	4,23E-01	1,64E-03	99%	99%
5. Alcohol treatment	2.98E+00	3.59E-01	1.39E-03	1,10E+06	1,33E+00	5,14E-03	73%*	73%*
6. Drying	1.30E+01	1.56E+00	6.07E-03	9,37E+05	1,13E+00	4,38E-03	28%	28%
Total	2.95E+02	3.55E+01	1.38E-01	9,34E+06	1,13E+01	4,37E-02	68%	68%

Table 4
Water use in process A at lab and modeled industrial scales.

Extraction phases	Laboratory scale			Modeled at industrial scale			Reduction or Increase* with the scale up (%)	
	Water use (m^3/year)	Water use (m^3/kg of MKS)	Water use (m^3/US$)	Water use (m^3/year)	Water use (m^3/kg of MKS)	Water use (m^3/US$)	Water use per kg of MKS	Water use per US$
1. Shell removal	–	–	–	3,08E+02	3,72E-04	1,44E-06	100%*	100%*
2. Oxidation inhibition	3,87E-01	4,67E-02	1,81E-04	1,74E+04	2,10E-02	8,15E-05	55%	55%
3. Grinding and drying	1,20E-01	1,45E-02	5,61E-05	3,01E+02	3,63E-04	1,41E-06	97%	97%
4. Starch purification	8,25E-01	9,95E-02	3,86E-04	2,38E+04	2,87E-02	1,11E-04	71%	71%
5. Alcohol treatment	–	–	–	2,80E+03	3,38E-03	1,31E-05	100%*	100%*
6. Drying	–	–	–	7,52E+01	9,07E-05	3,51E-07	100%*	100%*
Total	1,33E+00	**1,61E-01**	**6,23E-04**	4,47E+04	**5,39E-02**	**2,09E-04**	66%	66%

97% (Table D1 in Annex D, supplementary material), except at the shell removal phase that became mechanical, demanding a measurable amount of energy. In this way, other sources of impacts appeared when both functional units were used. The production of hydrogen peroxide, used at the peroxide treatment phase, was the main source of impacts at this scale for almost all categories, except water scarcity. The high-water demand by the steam production chain of the polyphenols extraction phase results in a great contribution to water scarcity.

3.4. Scenario analysis

Scenarios were built reducing system boundary (scenario 1) and changing critical production phases (scenario 2). It has been a common practice in LCA of recyclable materials to disregard all processes before recycling, fostering the use of secondary and low-valued materials in a circular economy (Commission, 2011). Considering that mango kernels are currently considered as waste in the food industry, scenario 1 was built, reducing the system boundary to encompass only the extraction process and the production of inputs (Fig. 2). In this case, the highest impact reduction occurred in process A because it used more mango kernels per year than B (Figs. E1 and E2 in Annex E, supplementary material).

The contribution analysis of process A and B showed that one important source of impact was the phase that inhibited starch darkening: oxidation inhibition in process A and peroxide treatment in process B. An expert meeting revealed that removing these procedures would not change the amylose content of starch (around 25%), which is the most important starch property for its use in bioplastics. Only the starch color would change, becoming darker and making films rather translucent than transparent and light brownish.

In this way, a scenario 2 was built removing the oxidation inhibition phase in process A and the peroxide treatment in process B. This change reduced the impacts at industrial scale, per kg of starch, 1–35% (according to the category) in process A, and 21–87% in B (Figs. E1 and E2 in Annex E, supplementary material).

3.5. Comparison of process A and B

The comparison of environmental impacts of process A and B was performed applying the production (kg of MKS) and monetary ($ of revenue) functional units at the reference situation and in scenarios 1 and 2 (Table 5). In the reference situation, Process A performed better than B at both production scales, independent of the adopted functional unit. Furthermore, the impact values were reduced at least 56% in process A and 68% in process B when moving from lab to industrial scales.

The comparison of processes considering the uncertainty analysis showed that Process A performed significantly better than B, at both production scales (Fig. 7a and b). When the production functional unit was used, process A generated significant lower impacts in four categories at lab scale and in six, at industrial scale (Fig. 7a and b). However, when adopting the monetary functional unit at the industrial scale, only one category (human toxicity, cancer) produced a significant difference. The performance of process B per US$ improved at the industrial scale because this process resulted in two additional co-products (polyphenols and fat). The total revenue obtained from process B (US$ 493 million/year, Table 1) was twice as high as the revenue from process A (US$ 213 million/year, Table 1) that commercialized MKS, only.

The comparisons of process A and B in scenarios 1 and 2 at lab and industrial scales showed that process A performed better than B at lab scale (Fig. F1, Annex F, supplementary material). However, at industrial scale there was no significant difference between them for most of the

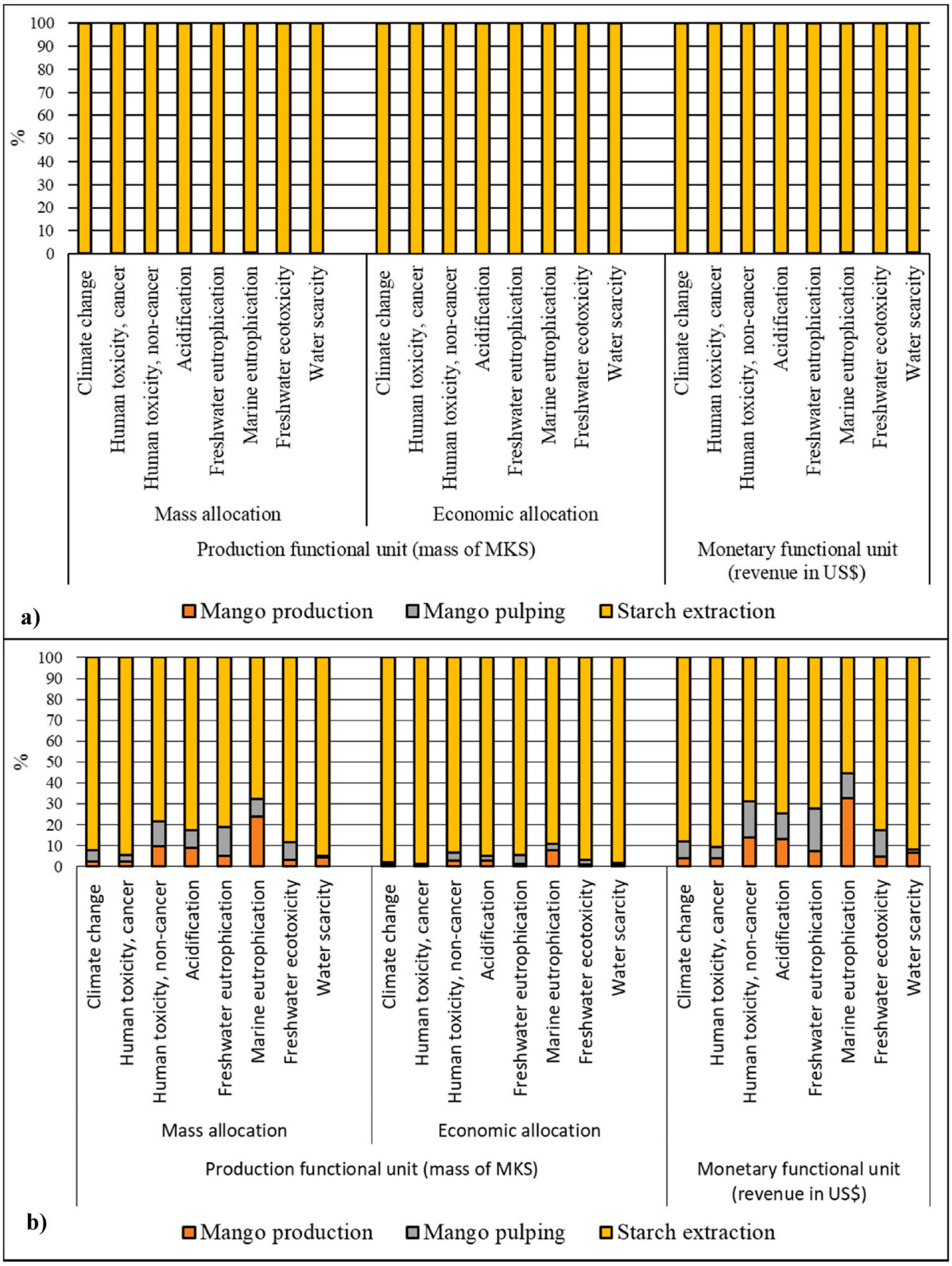

Fig. 5. Contribution of foreground and background processes, when process B was used at the a) lab and b) industrial scales, applying the production and monetary functional units.

impact categories, except climate change (Fig. F2, Annex F, supplementary material).

3.6. Recommendations for future research with MKS

A short-term recommendation is to invest in process A for white starch extraction and higher revenue. Process A performed better than B for white starch, considering the investigated functional units and system boundaries.

A long-term recommendation regards process B and mango cropping. It is important to evaluate the market for off white starch in bioplastics and for polyphenols and fat in the food industry. In the case of market demand for these products, process B should be reanalyzed and new alternatives be investigated to reduce the impacts on climate change and human toxicity, cancer.

Furthermore, it is important to foster mango crop systems with reduced use of fertilizers. These systems will reduce impacts in mango-derived products, in this case, starch, polyphenols, and fat.

These recommendations are based on the results from this study and the comparison of mango kernel products with similar market products. At first glance, they reveal how difficult it is to develop environmentally sound biorefinery systems, such as process B. Although generating more products, the cascading extraction of many substances turned process B more complex, resulting in more losses of materials when transferred among machineries in the modeled industrial plant.

The analysis of process A and B per production unit (kg of starch), showed that process A performed significantly better than B for at least climate change in the reference and scenario situations, at the lab and industrial scales. According to IPCC scenarios, climate change is and will continue to be a very important impact category for society as a whole

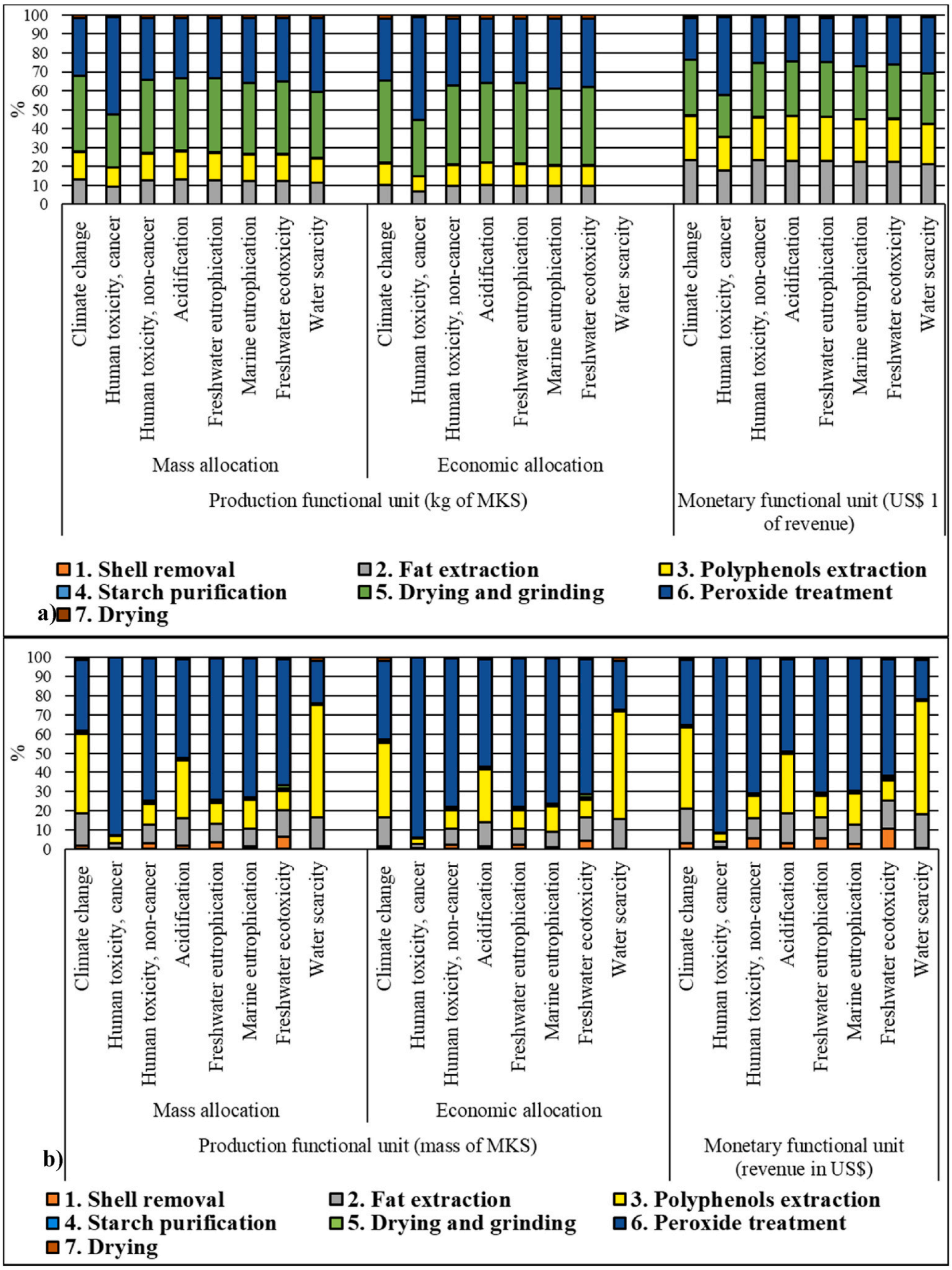

Fig. 6. Contribution of starch extraction phases when process B was used at the a) lab and b) industrial scales, applying production and monetary functional units, with impacts calculated per 1 kg of starch and US$ 1 of revenue.

(IPCC, 2019). Moreover, food retailers have valued the carbon footprint certification, increasing the demand for low carbon technologies over the food production chains (International Trade Center, 2012).

The analysis of processes per US$, also indicated that process A performed better than B, in this case for human toxicity, cancer. Toxicity related to the extraction process B (Fig. 5b) was mainly due to the use of hydrogen peroxide for starch bleaching.

The impact on human toxicity has increased its importance among consumers and food producers with the increase demand for sustainable bio-based products, with less toxicity impacts (FAO, 2016). Thus, it is important to reduce the use of chemicals whose production or use cause impact in human health, such as hydrogen peroxide in process B.

Regarding mango cropping, impacts from agricultural practices became relevant at the industrial scale for products from mango kernel, when impacts were calculated per kg of starch or per US$, especially for the marine eutrophication (Figs. 4b and 6b). This means that attention should be given to reduce the use of nitrogen fertilizers in mango cropping. Dias et al. (2020) showed that integrated cropping systems of mango trees with plant mixtures, used as cover crops and natural source of nutrients, reduced the environmental impacts of mangoes, while increasing yield and revenue. Thus, the adoption of alternative mango cultivation systems that make use of cover crops should be fostered among producers.

The comparison of MKS with starches from maize and potato (inventories from ecoinvent) showed that white MKS from process A resulted in similar impacts. The white MKS from process B caused higher impacts for climate change and acidification, whereas the off-white MKS from this process caused similar impacts to MKS from A, potato, and

Table 5
Average environmental impacts of MKS from process A and B at lab and modeled industrial scales.

Production functional unit (kg of MKS) – Mass allocation							
Impact categories	Unit	Lab scale		Industrial scale		Reduction with the scale up (%)	
		Process A	Process B	Process A	Process B	Process A	Process B
Climate change	kg CO2 eq	1,58E+01	4.00E+02	4,92E+00	2.10E+01	69%	95%
Human toxicity. cancer	CTUh	7,71E-07	1.00E-05	2,38E-07	2.10E-06	69%	79%
Human toxicity. non-cancer	CTUh	1,05E-05	8.00E-05	2,03E-06	3.90E-06	81%	95%
Acidification	molc H+ eq	1,21E-01	1.70E+00	3,54E-02	1.01E-01	71%	94%
Freshwater eutrophication	kg P eq	4,37E-03	1.00E-01	1,20E-03	3.00E-03	73%	97%
Marine eutrophication	kg N eq	3,35E-02	4.00E-01	1,41E-02	2.90E-02	58%	93%
Freshwater ecotoxicity	CTUe	2,27E+02	3.66E+03	9,04E+01	2.09E+02	60%	94%
Water scarcity	m3	1,18E+02	3.12E+02	2,75E+01	1.00E+02	77%	68%
Production functional unit (kg of MKS) – Economic allocation							
Impact categories	**Unit**	**Lab scale**		**Industrial scale**		**Reduction with the scale up (%)**	
		Process A	**Process B**	**Process A**	**Process B**	**Process A**	**Process B**
Climate change	kg CO2 eq	1,31E+01	3.69E+02	3,90E+00	1.80E+01	70%	95%
Human toxicity. cancer	CTUh	5,71E-07	1.00E-05	1,60E-07	2.00E-06	72%	80%
Human toxicity. non-cancer	CTUh	9,14E-06	7.00E-05	1,48E-06	3.20E-06	84%	95%
Acidification	molc H+ eq	9,16E-02	1.55E+00	2,39E-02	8.20E-02	74%	95%
Freshwater eutrophication	kg P eq	3,33E-03	8.00E-02	8,01E-04	3.00E-03	76%	96%
Marine eutrophication	kg N eq	1,75E-02	3.30E-01	7,74E-03	2.10E-02	56%	94%
Freshwater ecotoxicity	CTUe	1,93E+02	3.39E+03	7,66E+01	1.79E+02	60%	95%
Water scarcity	m3	1,09E+02	2.90E+02	2,40E+01	8.50E+01	78%	71%
Monetary functional unit (US$ of revenue)							
Impact categories	**Unit**	**Lab scale**		**Industrial scale**		**Reduction with the scale up (%)**	
		Process A	**Process B**	**Process A**	**Process B**	**Process A**	**Process B**
Climate change	kg CO2 eq	6,11E-02	6.00E-01	1,91E-02	3.00E-02	69%	95%
Human toxicity. cancer	CTUh	2,99E-09	2.00E-08	9,23E-10	3.00E-09	69%	85%
Human toxicity. non-cancer	CTUh	4,09E-08	1.20E-07	7,86E-09	6.00E-09	81%	95%
Acidification	molc H+ eq	4,68E-04	3.00E-03	1,37E-04	1.00E-04	71%	97%
Freshwater eutrophication	kg P eq	1,69E-05	1.00E-04	4,65E-06	5.00E-06	73%	95%
Marine eutrophication	kg N eq	1,30E-04	1.00E-03	5,46E-05	4.00E-05	58%	96%
Freshwater ecotoxicity	CTUe	8,81E-01	5.46E+00	3,50E-01	2.90E-01	60%	95%
Water scarcity	m3	4,57E-01	4.60E-01	1,07E-01	1.30E-01	77%	72%

maize (Fig. G1, Annex G, supplementary material). Nevertheless, the comparison of white MKS starch with sago and cassava starches showed that white MKS caused higher impact on climate change. The sago starch extracted from sago stems collected in Indonesian forest and traditionally processed by local communities caused an impact of 0.017 kg CO_2 eq/kg of starch (Yusuf et al., 2019), while the cassava starch produced in Thailand companies, an impact of 0.6 kg CO_2 eq/kg of starch (Usubharatana and Phungrassami, 2015).

The comparisons of polyphenols and fat from process B with similar products analyzed in previous studies (Ntiamoah and Afrane, 2008; Shinde et al., 2020) revealed similar environmental impacts only when the system boundary of process B was reduced, disregarding the processes of mango cropping and pulping (Figs. G2 and G3, Annex G, supplementary material). In the reference situation for process B, the minimum impact values of mango kernel fat were higher than the average values of cocoa butter (Ntiamoah and Afrane, 2008) in five out of the eight categories. For polyphenols in the reference situation, the minimum impact values of mango kernel polyphenols from process B were higher than the average impact values of pomegranate peel polyphenols (Shinde et al., 2020) in two out of the five categories. It is highlighted that pomegranate cropping was not considered in the impact assessment of polyphenols performed by Shinde et al. (2020).

3.7. Recommendations for improving the procedure used for evaluating the environmental performance of processes at early development stage

Applying the methodological procedure described in section 2.1 (summarized in Fig. 1) to study alternative MKS processes allowed its simplification and detailing some activities that will reduce time and human resources in future studies of new processes and products. From the lessons we learned, a new procedure is suggested that encompasses a sequence of three steps (Fig. 8): 1) data collection at TRL 4; 2) process scale up at TRL5; and 3) LCA at TRL5.

In Step 1, alternative processes shall be defined and data collected for building processes inventories and basing processes scale up. For each process phase, it is indicated to perform a mass balance of inputs and outputs, determining the composition of raw material (mango kernels in this study), and of intermediate and final coproducts. These data allow building inventories per phase and guide the selection of industrial machinery, their size, and efficiency for modeling process flows at the industrial scale. Gathering good quality data at the lab scale reduces parameter uncertainties in LCA. Many studies rely only on lab processes descriptions done by researchers in the development team, not performing mass balances, and intermediate product characterization at the lab scale. It is necessary to invest time in collecting detail data at the lab scale to reduce uncertainties in the scale up process and for future products comparison with similar available ones.

A good way to make this data collection is to first interview developers for gathering detailed data already available and then to perform mass and energy balances per process phase. The best time to do this lab work is after the parameters of temperature, pressure, and amount of chemicals were defined by developers, usually at TRL 4.

In Step 2, processes need to be modeled at the industrial scale. This is of foremost importance before identifying critical phases, defining production scenarios, and comparing new products with current similar ones. Together with other studies (Piccinno et al., 2018; Bartolozzi et al., 2020; Silva et al., 2020), it was found in this study a reduction in energy and water usage, an increase in yield and a reduction in environmental impacts when moving from the lab to the industrial production. Furthermore, results from this study showed the need to model processes at the industrial scale to identify critical points, define and investigate opportunities for improvement. At the lab scale, results are dominated

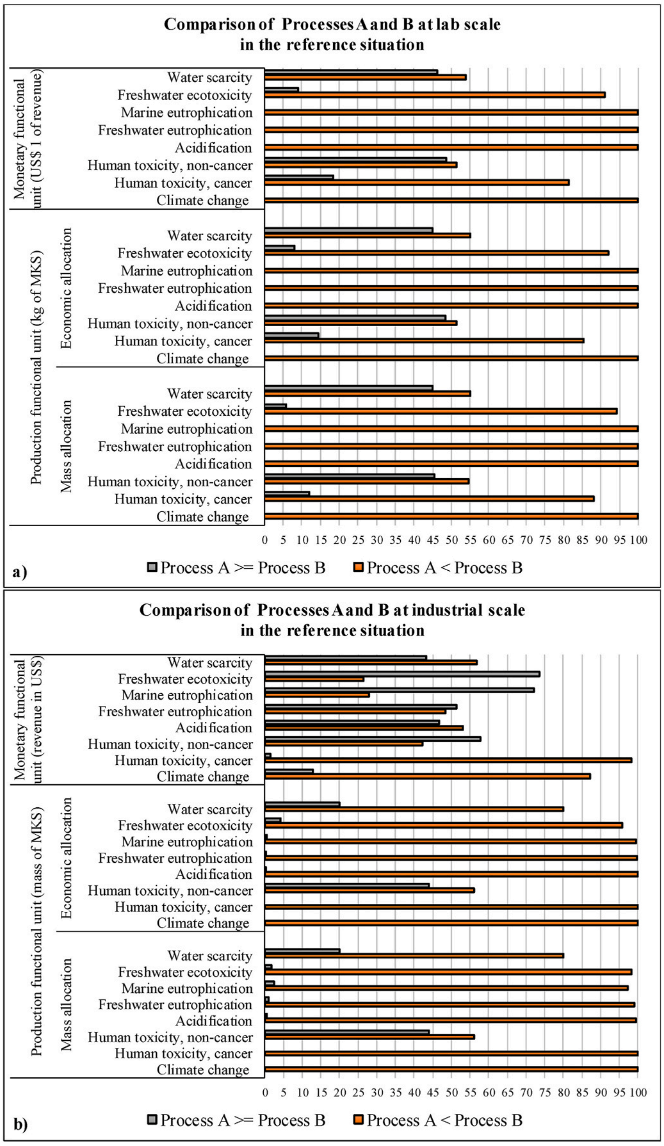

Fig. 7. Monte Carlo results for the comparison of process A and B at a) lab and b) industrial scales, applying the monetary functional unit.

by energy associated impacts in all production phases, making it hard to identify which phases are more relevant. Silva et al. (2020) suggested removing energy use in TRL4 to identify critical aspects and define alternatives for scenario analysis in a LCA performed at this scale. Although this is feasible, it seems more practical to scale up both alternatives for identifying critical process phases and then perform LCA.

Modeling processes at the industrial scale requires the definition of plant production capacity, besides data gathering at the lab scale. This definition requires the analysis of raw material availability in a region to set a common ground for plant processing capacity. This is important when alternative processes are compared in terms of total revenue. Alternative processes shall be modeled at the industrial scale for attending a specific plant processing capacity.

Furthermore, alternative machineries shall be compared for choosing the equipment that leads to higher yields, less energy and water usage, and lower price. The knowledge about product composition improves the identification of similar products for future comparisons.

In Step 3, appropriate data will be available for performing LCA. Contribution analyses should be performed to identify critical phases in each evaluated process and define modification opportunities whose environmental performances are accessed through scenario analysis. The comparison of processes, considering parameter uncertainty, allows the identification of environmentally sound processes and formulation of recommendations for the development team.

Regarding the decision about functional unit, it is important to consider the production and the monetary functional units when comparing processes with multi-functionality. The production unit (kg of product) focus in specific products, allowing the comparison of in-development products with similar ones after the process scale up. On the other hand, the monetary unit accounts for the whole process, encompassing all phases and generated products. This unit allows the comparison of production systems using an important aspect for business, the total revenue from products commercialization.

The use of the monetary functional unit has hardly been done at the industrial scale. Most of the studies of biorefinery systems have used the amount of raw material processed as functional unit (Cherubini and Ulgiati, 2010; Shinde et al., 2020), maybe to reduce uncertainties regarding changes in products value in the marketplace though time. However, focusing on raw material processing instead of production may favor processes with low batch time and great processing capacity but that result in low total production and revenue. To account for variations in product prices, it is important to perform a sensitivity analysis considering the standard variations observed.

Regarding system boundaries, it is relevant to consider upstream and disregard downstream processes at early research of biomaterials. Currently, there is no consensus guideline established for disregarding upstream processes of recycled materials, although the Product Environmental Footprint (PEF) handbook advised that when recycled materials are used as the raw material input, only the conversion of recycled materials should be included in the inventory (Ahlgren et al., 2013). Disregarding the crop production of agroindustrial waste is a good incentive for adding value to these materials. However, at an early stage, it is important to consider prospective utilizations for materials, especially when they are currently acknowledged as biomass waste. With the growing efforts to convert biomass into new materials, today bio-waste will become a regular tomorrow raw material, with bio-waste having an important role in the future food chain economy.

Furthermore, little information is available regarding how production chains will incorporate the biomaterials as inputs in the production of bioproducts, being hard to include downstream processes in LCA studies of biomaterials at early research stage. Information regarding recyclability or disposal options for these materials are also scarce at this stage. In this study, process A and B were developed to extract starch as the most important product and at TRL 4. At this maturity level, the available characterization of obtained starch, polyphenols, and fat was enough to confirm their similar functionality to other products. Information on how MKS will be incorporated in bioplastics production or any other bioproduct was hardly available. Nevertheless, in early stages of bioproduct development, it is important to evaluate its biodegradation and alternatives for its end of life in a circular economy perspective.

4. Conclusions

This study applied, simplified and detailed a procedure for evaluating the environmental impacts of processes at early development stage. The simplified procedure can be applied in the evaluation of new processes at TRL 4. This case study showed the importance of integrating the environmental and research teams for collecting appropriate lab data, scaling up processes with reduced uncertainties and assessing the environmental impacts of processes to formulate valuable recommendations.

Regarding the MKS case study, we recommend process A to advance to pilot plant implementation level. Process B requires improvements to reduce the impacts on climate change and human toxicity. This case study showed that crop production needs to be considered when evaluating processes that use biomass waste as raw material. Crop

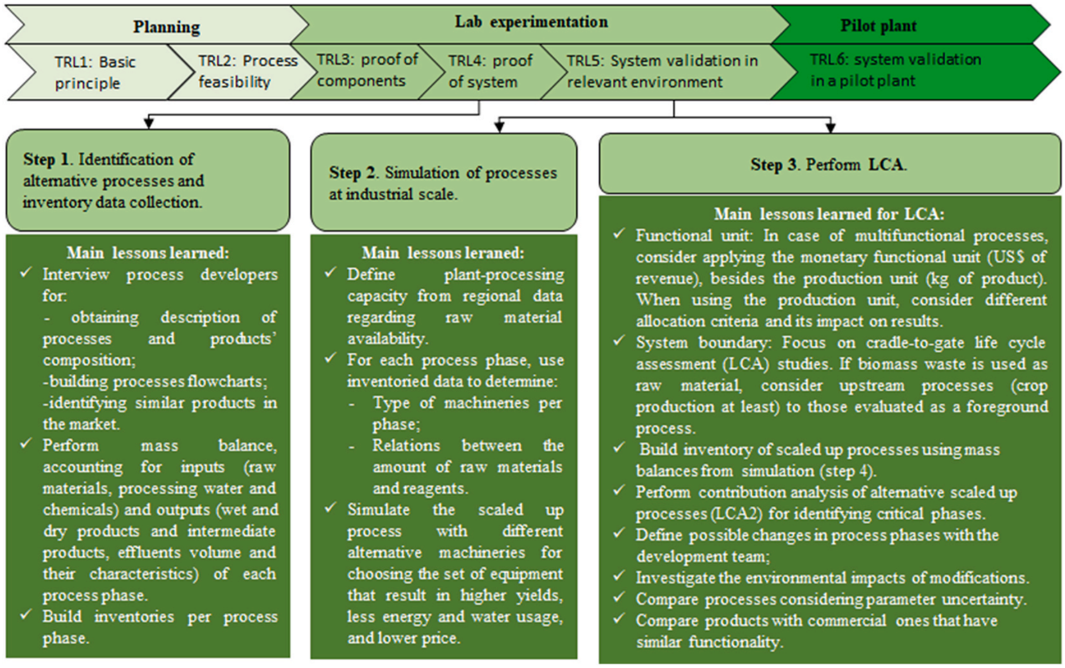

Fig. 8. Simplified procedure for inserting LCA in early process development stage.

production became relevant when processes were modeled at the industrial scale, revealing the need to seek for alternatives that reduce impacts in both foreground and background processes. This study also showed reductions in energy and water use, and in life cycle impacts, whereas critical phases changed when moving from lab to industrial scale production. These results highlighted that a scale up simulation become important when performing LCA at early research stage.

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CRediT authorship contribution statement

Anne Karolyne Pereira da Silva: Data curation, Writing – original draft, preparation. **Alexandre Cardoso:** Investigation, Verification. **Ednaldo Benício de Sá Filho:** Software, ValidationValidadtion. **Henriette Monteiro Cordeiro de Azeredo:** Investigation, Verification. **Fausto Freire:** Investigation, Verification. **Francisco Casimiro Filho:** Investigation, Verification. **Maria Cléa Brito de Figueirêdo:** Conceptualization, Methodology, Supervision, Writing – review & editing.

Declaration of competing interest

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

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jclepro.2021.128981.

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