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Does enzymatic catalysis lead to more sustainable chemicals production? A life cycle sustainability assessment of isopropyl palmitate†

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In this work, a comprehensive Life Cycle Sustainability Assessment (LCSA) is performed assessing environmental, economic and social impacts of switching from chemical to enzymatic catalysis for the esterification of Isopropyl palmitate (IPP). A dedicated LCSA methodology with a common goal, system boundary and life cycle inventory is presented. A 7 to 13% reduction in environmental impacts was found due to less hazardous waste formation, lower feedstock consumption and reduced steam usage. The social medium risk hours increase by 9% due to a longer production time, however, certain social benefits which were identified by stakeholder interviews, such as improved safety for workers, are not properly captured by the social impacts database used. Despite reductions in utility and feedstock costs, the total operating costs are higher (+40%) due to the immobilized enzyme cost and higher labour costs. Nevertheless, profitability indicators show that switching to enzymatic production is likely to be profitable. To reduce costs, optimization efforts should focus on reducing the batch time and increasing enzyme reuse. From a social and environmental perspective, upstream impacts linked to palmitic acid and isopropyl alcohol production should be addressed.

Introduction

Today's economy – from food, mobility, health to electronics – depends on the products of the chemical industry. Chemicals are also important building blocks in low-carbon, zero pollution and energy- and resource-efficient technologies, vital in finding new solutions for the green transition of our economy and society.[1] However, the sector also stands as the leading industrial energy consumer, and is associated with chemical pollution of soils, air and water.[2] In the past decades, the chemical industry has been actively seeking more environmentally sustainable production methods. Enzymes, for example, are promising biocatalysts that can increase energy efficiency, improve chemical safety, reduce chemical waste production, and even reduce the chemical production costs.[3] Enzymes are proteins that act as selective biological catalysts. Today, they are already used in various industrial sectors such as pharmaceuticals, cosmetics and food.[4,5] While enzymatic applications in the chemical industry have increased in recent years, this has not yet led to a major commercial breakthrough, and the number of products remains limited.[6–9]

Esters are an important class of chemicals with a wide range of applications such as emollients, surfactants, and emulsifiers in food, cosmetic, and pharmaceutical products.[9] Esterification reactions in industry typically use chemical catalysts, like strong acids, *e.g.*, *p*-toluene sulfonic acid, or metals, *e.g.*, tin or zinc salts, which lack selectivity and require harsh reaction conditions and complex downstream product purification.[7,9] Alternatively, lipases can be used for catalysing esterification reactions.[8] In previous studies, lipases were used to synthesize various esters and were found to be promising due to mild reaction conditions and reduced hazardous waste formation.[9–11] The main drawbacks, however, are the high enzyme cost and the difficulty of reusing lipases due to irreversible enzyme inactivation.[6] Immobilization of lipases, by attaching them to a solid phase or support, has been an important step to enabling multiple reuses of lipases.[12,13]

Isopropyl palmitate (IPP) is an oleochemical ester, commercially used as an emollient in cosmetics, healthcare products and lubricants due to its good absorption characteristics.[14] IPP is typically synthesized by the esterification of palmitic acid (PA) and isopropyl alcohol (IPA) using a chemical acid catalyst such as sulfonic acid.[15] Various studies have successfully used lipases for

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the production of IPP in a lab-scale batch configuration.[8,14] Furthermore, kinetic models have been studied and the optimum reaction conditions have been proposed.[16,17] However, to the authors' knowledge, enzymatic IPP production at pilot or industrial scale has not been reported.

Although switching from chemical to enzymatic catalysis is largely perceived as sustainable, it is essential to measure the environmental, economic and social impacts before implementation on an industrial scale.[8] Life Cycle Sustainability Assessment (LCSA) is a comprehensive framework for evaluating the three pillars of sustainability for a product, process, or service throughout its life cycle.[18] While TEA studies for the enzymatic production of other oleochemical esters, such as isopropyl myristate, have been reported, environmental and socioeconomic implications were not accounted for, primarily due to lacking data and since SLCA is still under development.[14,19–21] To the authors' best knowledge, only one study has been published assessing the three pillars of sustainability for an enzymatic process, namely by Singh *et al.* (2021) for the esterase based polyester recycling of poly(ethylene terephthalate) into terephthalic acid and ethylene glycol using process model data.[22] Singh *et al.* (2022) used Environmental Life Cycle Assessment (LCA) and Techno-Economic Assessment (TEA), with value added and job creation as indicators for quantifying the socioeconomic impact. However, no full Social Life Cycle Assessment (SLCA) was performed. The study found favourable long-term socioeconomic benefits and a reduction of total supply chain energy use by 69–83% and greenhouse gas emissions by 17–43% per kg of terephthalic acid.[22] However, to the authors' best knowledge, no environmental and social sustainability assessment for enzymatic IPP production, and no comprehensive LCSA comparing enzymatic and chemical production in general, has been reported in the literature.

In this study, a comprehensive LCSA is presented assessing and comparing the environmental (LCA), economic (TEA) and social (SLCA) performance of enzymatic and chemical catalysis for the esterification of IPP. This study presents for the first time a sustainability assessment of IPP production based on pilot-scale data. In addition, it presents the first detailed TEA, LCA and SLCA of this process. A contribution analysis was performed to identify the main social, environmental and economic sustainability hotspots in the enzymatic process. A sensitivity analysis was conducted to investigate the importance of reusing enzymes and sustainable feedstock sourcing.

Materials & methods

The applied LCSA methodology (Fig. 1) for comparing chemical and enzymatic IPP production followed the four phases of the ISO14040s framework for Environmental LCA: (i) Goal and Scope definition, (ii) Life Cycle Inventory (LCI) (iii) Life Cycle Impact Assessment (LCIA) and (iv) Interpretation.[23] In this study, a common goal and scope definition was defined and a common LCI was collected to streamline the environmental,

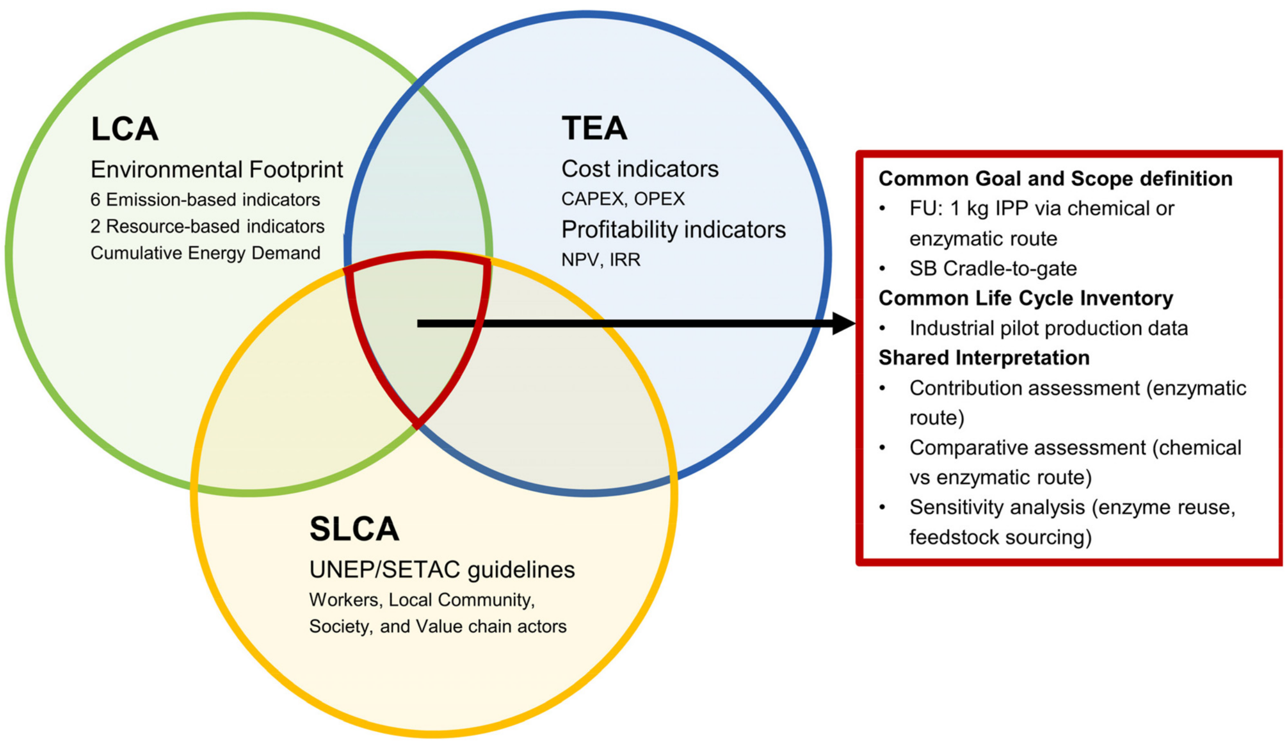

Fig. 1 Life cycle sustainability assessment methodology for comparing enzymatic and chemical production of IPP. FU = functional unit. SB = system boundaries. NPV = net present value. IRR = internal-rate-of-return. OPEX = operational expenditures. CAPEX = capital expenditures.

social and techno-economic assessments. The LCA in this study has been conducted in accordance with ISO 14040 and ISO 14044 standards.[23,24] The social LCA was performed in accordance with the UNEP/SETAC guidelines.[25] For the economic assessment, both TEA and life cycle costing (LCC) are methodological frameworks that provide systematic approaches for assessing the economic viability of a technology. In this study, TEA was chosen as the scope of the economic assessment is limited to an investor-perspective with cradle-to-gate system boundaries.[26] The TEA was guided by the framework of Van Dael *et al.* (2013).[27]

Goal and scope definition

The goal of this study was to assess the environmental, social, and economic life cycle sustainability of the production of Isopropyl Palmitate (IPP) *via* enzymatic esterification and identify relevant hotspots that can affect its sustainability performance. In addition, the study aimed to compare the sustainability of enzymatically produced IPP to conventional chemically produced IPP. For all assessments, the functional unit was defined as one kilogram of IPP produced *via* chemical or enzymatic production with the same functionality and a cradle-to-gate system boundary was used, meaning that the processes from resource extraction to the factory gate were considered as presented in Fig. 2.

In the enzymatic route, IPP is produced *via* a lipase-catalysed, solvent-free process. The lipase-catalysed esterification process includes vessel preparation, esterification, enzyme recycling, and post-treatment (deodorization and filtration). The esterification process requires PA, IPA and enzymes (lipases) and takes place at 60 °C. PA is derived from crude palm oil through a series of steps including hydrolysis, distillation, and fractionation. Isopropyl alcohol is a fossil-based chemical, and it is typically produced by hydration of propene or by gas fermentation technology using steel mill off-gas. Enzymes used in the analysis, Novozym® 435, are an immobilized form of *Candida Antarctica* lipase B, and produced by Novozymes A/S.[28] The immobilized enzyme catalyst is isolated/fixed in a separate column in the installation. Since the enzyme column is only used for esterification, multiple use of enzymes is possible without the need for harsh cleaning between batches. Based on pilot testing, it is assumed that these enzymes are reused 20 times. Aside from these materials, the enzymatic route also includes the consumption of utilities (electricity, steam, and nitrogen), for esterification and post-treatment, and filter aids for filtration. The removed isopropyl alcohol, waste filter aids and spent enzymes are incinerated as chemical waste.

The chemical route takes place in a stirred reactor tank at the same location. The route includes esterification, isopropyl alcohol removal and post-treatment (distillation, neutralization and washing, deodorization). In the chemical route,

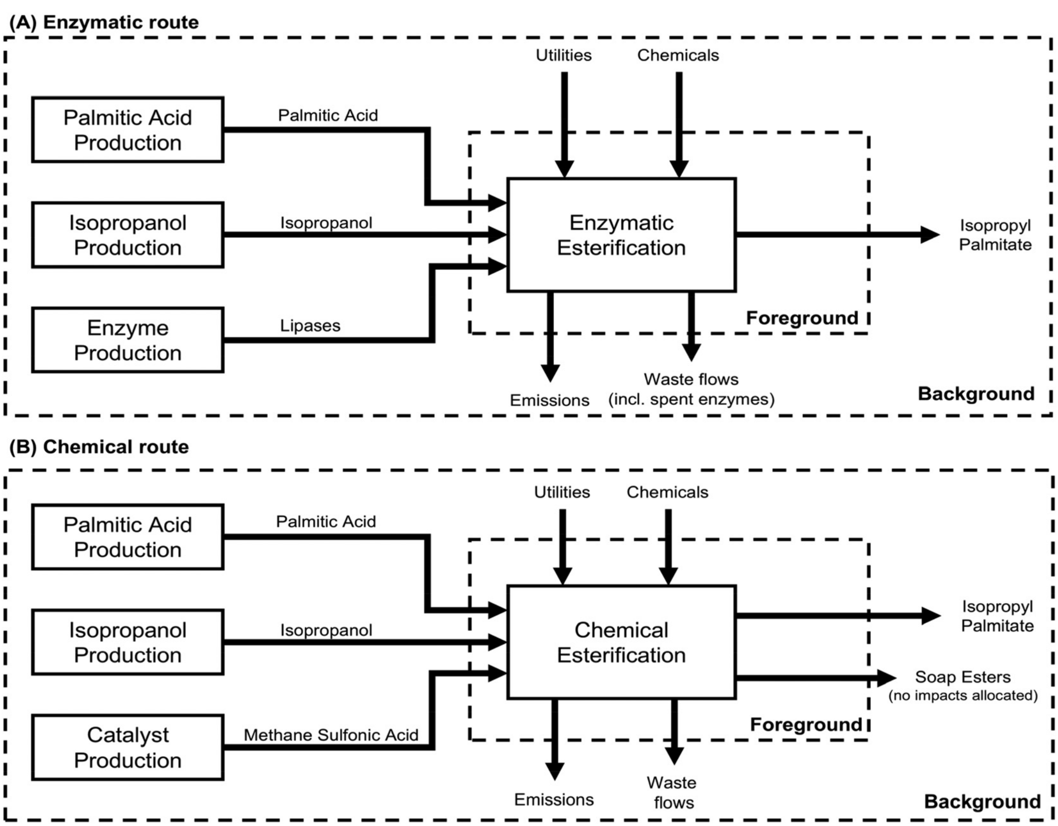

Fig. 2 Simplified flow diagrams of the production of IPP *via* (A) enzymatic route and (B) chemical route.

methane sulfonic acid (MSA) was used as an acid catalyst in the esterification, along with PA, IPA and auxiliary chemicals (*e.g.* NaOH). Esterification takes place at 130 °C. A neutralization step produces soap esters as a by-product. Because of the limited amount and low value, no impact is allocated to this by-product. The relative batch time of enzymatic esterification compared to chemical esterification is 4 : 1.

Life cycle inventory

Primary data for the enzymatic and chemical route was collected from respectively Oleon's pilot facility and the industrial batch process at their production site in Oelegem, Belgium. The aggregated LCI is available in ESI S2.† Due to confidentiality of Oleon's industrial process data, the detailed LCI, giving the mass and energy balance of the chemical and enzymatic process, is not included. However, basic process information is shared in Table 1.

Fig. 2 illustrates the differentiation between the foreground and background systems. For the background data, ecoinvent database version 3.9.1[29] was utilized. 'Market for' activities were selected if available to ensure the inclusion of transportation to the production site. For the PA production, palm oil produced in Malaysia was considered as feedstock. Additionally, the transportation of palm oil from Malaysia to the plant in Belgium was included. The conversion of palm oil to PA was modelled using internal Oleon data for fatty acid hydrogenation and fractionation processes, as described in Nachtergaele *et al.* (2019).[30] A life cycle inventory on lipase production was provided by the supplier company Novozymes A/S. The LCI of enzyme production is included in the aggregated LCI in ESI (S2),† however, the detailed LCI cannot be made available due to industry confidentiality.

Environmental life cycle impact assessment

The LCA in this study has been conducted in accordance with ISO 14040 and ISO 14044 standards.[23,24] For LCA, the maintenance and infrastructure aspects were excluded. In the impact assessment phase of this study, the Environmental Footprint (EF) v3.1 method[31] was used. From the 16 impact categories included in this method, six emission-based impact categories were selected according to the recommendations of the Life Cycle Metrics for Chemicals Products.[32] In addition, two resource-based impact categories were evaluated, namely land use and water use. Furthermore, primary energy consumption was analysed by assessing the Cumulative Energy Demand (CED).[33] SimaPro® software version 9.5[34] was used for conducting the LCIA.

Table 1 Operational conditions of enzymatic and chemical routes

	Enzymatic route	Chemical route
Catalyst	Novozym® 435	Methane sulfonic acid
Temperature (°C)	60	130
Pressure (atm)	1	1
Post-treatment	Deodorization, filtration	Distillation, neutralisation and washing, deodorisation
Relative batch time	4	1

Social life cycle impact assessment

This UNEP/SETAC methodology for social LCA categorizes social impacts by stakeholder categories, recognizing that social sustainability involves identifying and managing both positive and negative impacts on people (stakeholders).[25] In the methodology six stakeholder groups are identified, including workers, local communities, society, value chain actors, consumers and children. For each of these stakeholder categories, socially significant themes are defined and considered as impact categories. For Workers, for example, these impact categories include "freedom of association", "health and safety", and "discrimination", among others. Each of the impact categories are assessed by several social and socio-economic indicators. For instance, for the subcategory "health and safety", the indicators were the "adequate general, occupational measures", "number of fatal accidents" and "number of non-fatal accidents". The stakeholders' categories considered in this assessment were workers, local community, society, and value chain actors. Stakeholder consumers and children were not included given they fall outside of the system boundaries of the study. The identification of relevant impact categories was conducted *via* a sectorial social risk analysis based on: (1) literature review, (2) stakeholder consultation for the identification and prioritization of impact categories and (3) a sectorial hotspots exercise using an S-LCA database, *i.e.* the Product Social Impact Assessment (PSILCA) database.

Modelling for the foreground–background system was based on the same primary data collected for LCA. The background activities include energy and materials required to produce the IPP, which were further modelled using the PSILCA database v3.

To facilitate this inventory, a tool based on the UN Global Compact Self-Assessment Methodology[35] was developed. The tool consisted of an Excel sheet containing questions corresponding to the stakeholder categories and impact categories in UNEP/SETAC's Social-LCA methodology. Each question included a list of indicators used to characterize the risk of the impact categories. For each selected social indicator, a risk level using the PSILCA risk framework is assigned, which is based on international conventions and standards.[36] There are typically 6 different levels: no risk, very low risk, low risk, medium risk, high risk, and very high risk. Similarly, if the positive scale is taken, the "risk" is replaced by "opportunity". In PSILCA, risk/opportunity levels are scored based on the level of risk or opportunity: no risk = 0, very low risk = 0.01, low risk = 0.1, medium risk = 1, high risk = 10, and very high risk = 100.[36] The overall social impacts of each impact category were calculated by aggregating all the social risks involved in the life cycle of each process, using the PSILCA "Social Impacts Weighting Method".[25] Next to performing the S-LCA, stakeholder interviews using semi-structured questionnaires were performed to evaluate stakeholder perceptions. A sampling was designed to include a diverse group of interviewees varying in distance to the factory, gender, and age. Several key assumptions underpinned this approach: participants were assumed to be truthful in their responses, the sample was considered to reflect the broader population affected by the industrial site accurately, and it was expected that participants were informed and unbiased by the interviewer's presence, and that they provided consistent and reliable insights. The results of stakeholder interviews were discussed only in a qualitative manner. The questionnaire and details of the demographics of the stakeholder interviews are available as ESI† (S3 Social LCA questionnaire).

Techno-economic assessment

Contributions of different costs to the total variable operating cost were determined for both production routes, considering raw materials (PA, IPA), utilities (steam, electricity) and catalyst (enzyme or MSA). All cost data for the TEA were provided by Oleon. The operational expenditures (OPEX) of the enzymatic route, including labour, energy & waste, material and other costs (maintenance, logistics), were compared to the OPEX of the conventional chemical route. In addition, for the enzymatic route, the total capital expenditures (CAPEX), and the profitability indicators net present value (NPV) and internal-rate-of-return (IRR) were quantified.[27] Due to confidentiality of the industrial data, the costs were only presented relative to each other, while profitability indicators were only discussed in a qualitative way.

Interpretation

Within the scope of this study, a comparative assessment of the environmental impacts, social benefits and risks and economic costs of the enzymatic and chemical routes was performed. Furthermore, a contribution analysis was carried out to identify sustainability hotspots in the enzymatic process. For LCA, an uncertainty analysis was included to assess the robustness of the results to uncertainty in the background data. The uncertainty assessment was performed by a Monte Carlo analysis of 10 000 runs. Finally, sensitivity analyses were performed to investigate the effect of enzyme reuse on environmental and economic sustainability and feedstock sourcing on environmental and social sustainability of enzymatic IPP.

Results and discussion

Environmental impact of IPP production

The results of the contribution analysis for the enzymatic production route are listed in Table 2. PA production is the main contributor to all impact categories. For climate change, the contribution of this feedstock amounts to 81%, primarily due to land-use change from deforestation, high energy consumption and waste generation during palm oil cultivation. Deforestation and related biodiversity loss are also reflected in the high contribution of palm oil within the land use impact category (99%).[37] The other feedstock, IPA, also has a significant contribution for most assessed impact categories, particularly water use (25%), cumulative energy demand (17%), acidification (13%) and climate change (9%). The primary raw material for IPA production is propylene, which is typically derived from fossil resources through energy-intensive processes.[38] Producing IPA from alternative feedstocks is a promising route to reduce the environmental impact of this input.[39] For example, a recent study on the production of IPA from industrial waste gas feedstocks through fermentation reported a negative cradle-to-gate carbon footprint of −1.17 kg CO_2 eq. per kg of produced IPA. The negative value is acquired by considering the avoided off-gas emissions.[40] In contrast to both feedstocks, enzyme production has only a minor contribution on the total environmental impact of IPP production for all examined impact categories. It is important to note that in the base case, the assumption is made that enzymes are reused 20 times. Notably, for water use, enzymes contribute 8% to the total impact, primarily attributed to the fermentation and purification stages in enzyme production.[41,42] Utilities such as electricity, steam, and nitrogen have relatively low contributions across all analysed categories. While waste treatment shows a low impact in categories such as acidification (3%) and cumulative energy demand (2%), its relative impacts are higher in the ecotoxicity (10%) and human toxicity (12%) categories. It is important to note that in this study, the wastewater is classified as hazardous waste due to the presence of isopropanol. In a full-scale industrial plant, it is expected that improvements in liquid waste treatment will reduce this impact.

Fig. 3 presents the relative environmental impacts for IPP production for the enzymatic route (ER) and chemical route

Table 2 Environmental impacts of 1 kg IPP production *via* enzymatic route for the selected impact categories

Impact category	Unit	Feedstock supply		Catalyst supply	Esterification			Total
		PA	IPA	Enzyme	Chemicals	Utilities	Waste	
Acidification	mol H+ eq	1.4×10^{-2}	1.7×10^{-3}	1.90×10^{-4}	7.2×10^{-5}	1.6×10^{-4}	4.2×10^{-4}	1.6×10^{-2}
Climate change	kg CO_2 eq.	3.9×10	4.3×10^{-1}	3.00×10^{-2}	2.0×10^{-2}	1.0×10^{-1}	3.6×10^{-1}	4.8×10
Ecotoxicity, freshwater	CTUe	4.5×10^{1}	2.7×10^{-1}	1.30×10^{-1}	2.3×10^{-1}	8.0×10^{-2}	5.3×10	5.1×10^{1}
Eutrophication, freshwater	kg P eq	1.6×10^{-4}	3.5×10^{-6}	1.00×10^{-6}	2.6×10^{-7}	1.6×10^{-6}	7.4×10^{-6}	1.8×10^{-4}
Human toxicity, cancer	CTUh	1.4×10^{-9}	3.4×10^{-11}	1.70×10^{-11}	4.6×10^{-11}	6.8×10^{-12}	2.0×10^{-10}	1.7×10^{-9}
Land use	Pt	8.8×10^{1}	1.2×10^{-1}	3.30×10^{-1}	3.0×10^{-2}	3.3×10^{-1}	8.0×10^{-2}	8.9×10^{1}
Photochemical ozone formation	kg NMVOC eq	8.5×10^{-3}	1.8×10^{-3}	8.50×10^{-5}	4.9×10^{-5}	1.7×10^{-4}	3.8×10^{-4}	1.1×10^{-2}
Water use	m^3 depriv.	2.8×10^{-1}	1.4×10^{-1}	4.00×10^{-2}	0.0×10	4.0×10^{-2}	4.0×10^{-2}	5.5×10^{-1}
Cumulative Energy Demand	MJ	8.2×10^{1}	1.4×10^{1}	4.70×10^{-1}	1.5×10^{-1}	3.5×10	1.8×10	1.0×10^{2}

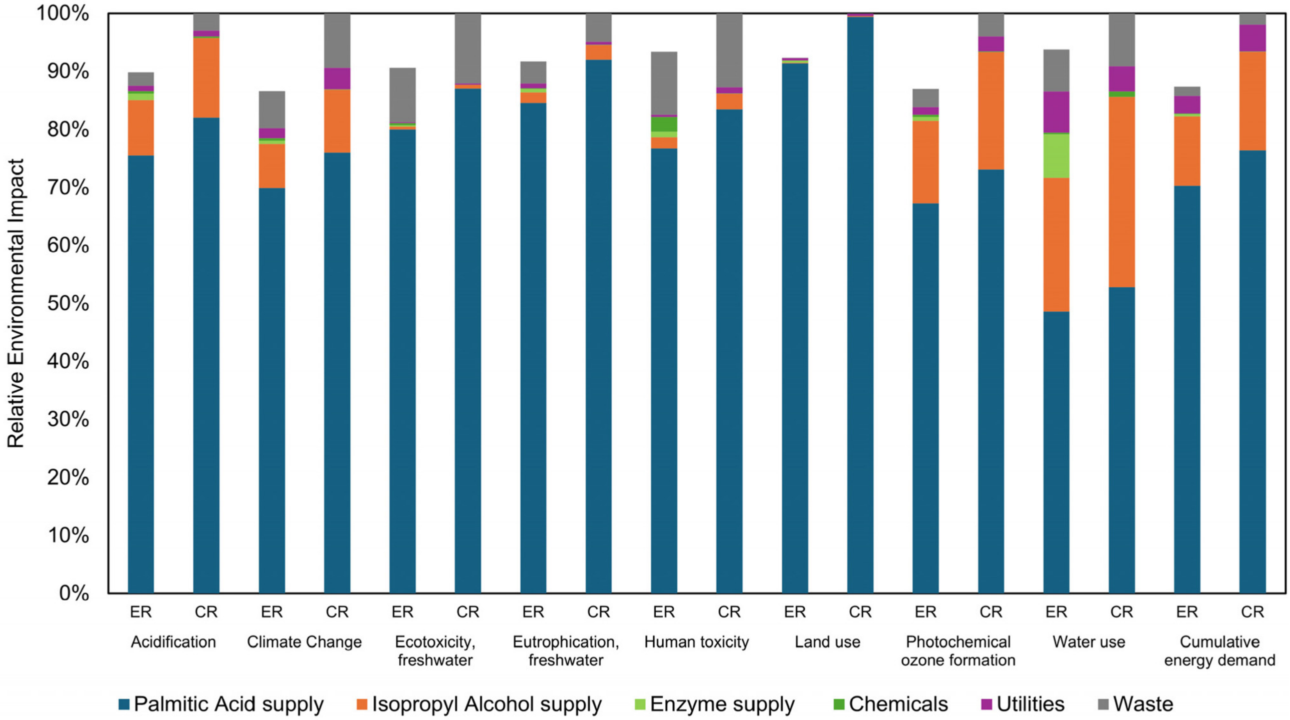

Fig. 3 Comparative life cycle impact assessment of the enzymatic route (ER) and chemical route (CR).

(CR). The enzymatic route shows a reduction between 7 and 13% compared to the chemical route, depending on the considered impact category. The reduction is most prominent for climate change and photochemical ozone formation, with reductions of 13%. It is possible to attribute this reduction to the triple advantage observed for the enzymatic route, namely (1) reduced chemical waste (2) higher yield, which results in a lower impact from the feedstocks PA and IPA, and (3) reduced steam consumption (part of utilities) due to the lower process temperature and easier downstream processing. The uncertainty analysis (see ESI S1†) showed that the enzymatic route consistently (100%) scores better than the chemical route for the indicators acidification, climate change, eutrophication (freshwater), land use, photochemical ozone formation and water use, while the uncertainty in the background data may result in reversed results for ecotoxicity (freshwater), human toxicity (cancer) and land use.

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Social risks and benefits of IPP production

Table 3 lists the results comparing the social risks for producing IPP *via* the chemical and enzymatic route. The total medium risks hours for producing 1 kg IPP enzymatically (70.6 medium risk hours per kg IPP) are higher than for the chemical route (64.8 medium risk hours per kg IPP). This is primarily due to the longer batch time for the enzymatic process, resulting in higher direct (on-site) social risks. A high share of social risks are identified upstream (96–100%), especially in palm oil production. In Malaysia, low levels of mechanization in oil palm cultivation mean this crop is labour intensive, while its production has been associated with negative social impacts on rural communities, indigenous people, and labourers.[43,44] It is therefore crucial to use raw materials originating from areas where forests and peatlands are not destroyed, and where the rights of local farmers and communities are respected according to the NDPE (No Deforestation, no Peat, no Exploitation) principles. The share of direct impacts of on-site chemical production is higher for general chemical production (15%) than for IPP production (<1%). While the results in Table 3, provided by coupling the LCI to the PSILCA database, are valuable to identify potential risks upstream or on-site, they fail to capture many social benefits linked to enzymatic production. For example, during the stakeholder interviews, workers indicated that switching to enzymatic production has resulted in greater skills and improved communication across units. In addition, increased safety in the process and increased pride in working within the company are important social benefits. For the local community, local employment and reduction of nuisance (odour) are indicated as important benefits, while increased transport in the area is a risk. For society, potential social benefits are linked to increased GDP and reduced environmental impact.

Table 3 Medium risk hours associated with producing 1 kg of IPP *via* the enzymatic route and the conventional chemical route and chemicals (general) in Belgium

	IPP – enzymatic route			IPP – chemical route			General chemicals (Belgium)	
Impact category	Social impact (med risk hours)	Share direct (%)	Share upstream (%)	Social impact (med risk hours)	Share direct (%)	Share upstream (%)	Share direct (%)	Share upstream (%)
Fair salary	11.5	3.6	96.4	9.9	1.2	98.8	21.1%	78.9%
Biomass consumption	9.0	0.0	100.0	8.4	0.0	100.0	14.9%	85.1%
Industrial water depletion	8.2	0.0	100.0	7.6	0.0	100.0	27.6%	72.4%
Public sector corruption	7.5	0.0	100.0	7.3	0.0	100.0	0.0%	100.0%
Trade unionism	7.2	0.0	100.0	6.9	0.0	100.0	0.5%	99.5%
Social security expenditures	6.7	0.0	100.0	6.6	0.0	100.0	0.1%	99.9%
Promoting social responsibility	1.5	2.8	97.2	1.1	1.1	98.9	30.1%	69.9%
Other risks	19.0	0.3	99.7	16.9	0.1	99.9	7.6%	92.4%
Total	70.6	0.7	99.3	64.8	0.2	99.8	15.2%	84.8%

For the value chain, customers indicated that they value sustainable innovations, with respect for people and the environment.

Techno-economic impact of IPP production

Fig. 4 shows the results of the cost assessment. In both enzymatic and chemical routes, the variable operating costs are dominated by the feedstocks PA and IPA, highlighting the importance of increased yield. In the enzymatic route, the share of the catalyst (24%) is significantly higher compared to the chemical route (<1%), confirming the importance of reusing enzymes for multiple production batches. In the case of the chemical route, utilities account for a higher share of total variable operating costs (10%) than for the enzymatic route (6%), showing the economic benefit of reduced steam consumption. Despite lower feedstock costs (−13%), the enzymatic route has a higher OPEX (+40%) than the chemical route. The reason for this is primarily the higher catalyst and labour costs. An improved scenario considering 30 enzymes reuse cycles, 35% reaction time reduction and 2% increased batch volume, would result in only a 20% higher OPEX than the chemical route.

Regarding the profitability indicators, a positive NPV was found, even when considering an interest rate of 8%. The IRR was below 25% but likely higher than the return rate that can be generated in lower risk markets or investments, *e.g.*, saving the investment money in a bank.[45] According to these results, even though operational costs are higher for enzymatic IPP production, the investment in enzymatic production was still found to be profitable.

The effect of enzyme reuse

The importance of reusing enzymes for multiple batches was examined through a sensitivity analysis. Based on pilot testing, the base case was to use the enzyme column for 20 batches before reloading. The climate change impacts of IPP when using enzymes for 1, 10, and 25 batches are also presented in Fig. 5(A). In the base case the contribution of enzymes to the

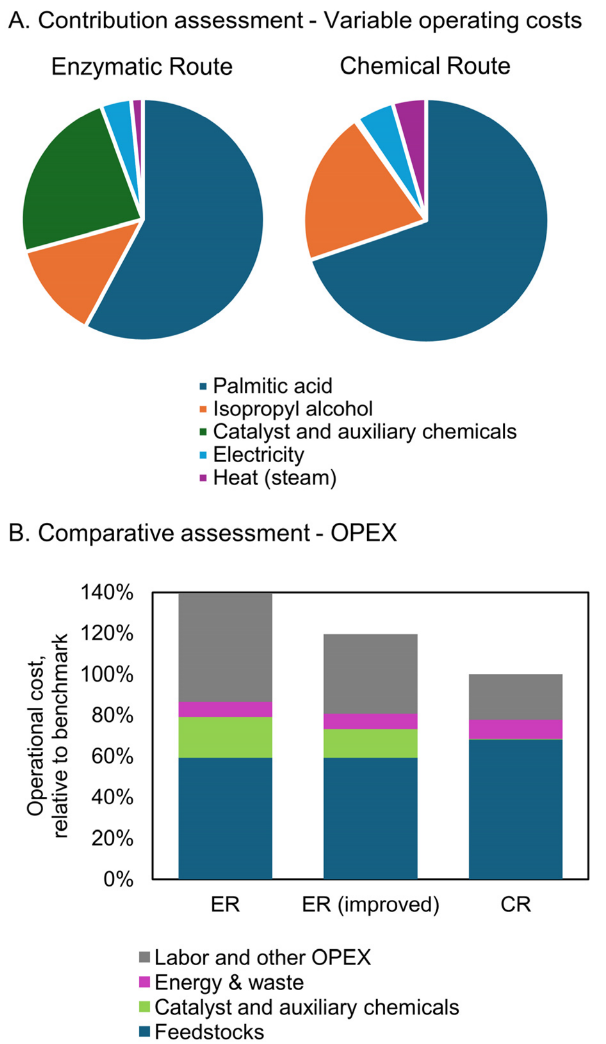

Fig. 4 Cost assessment comparing (A) contributions to the variable operating cost and (B) total operational cost for the enzymatic and chemical production of IPP.

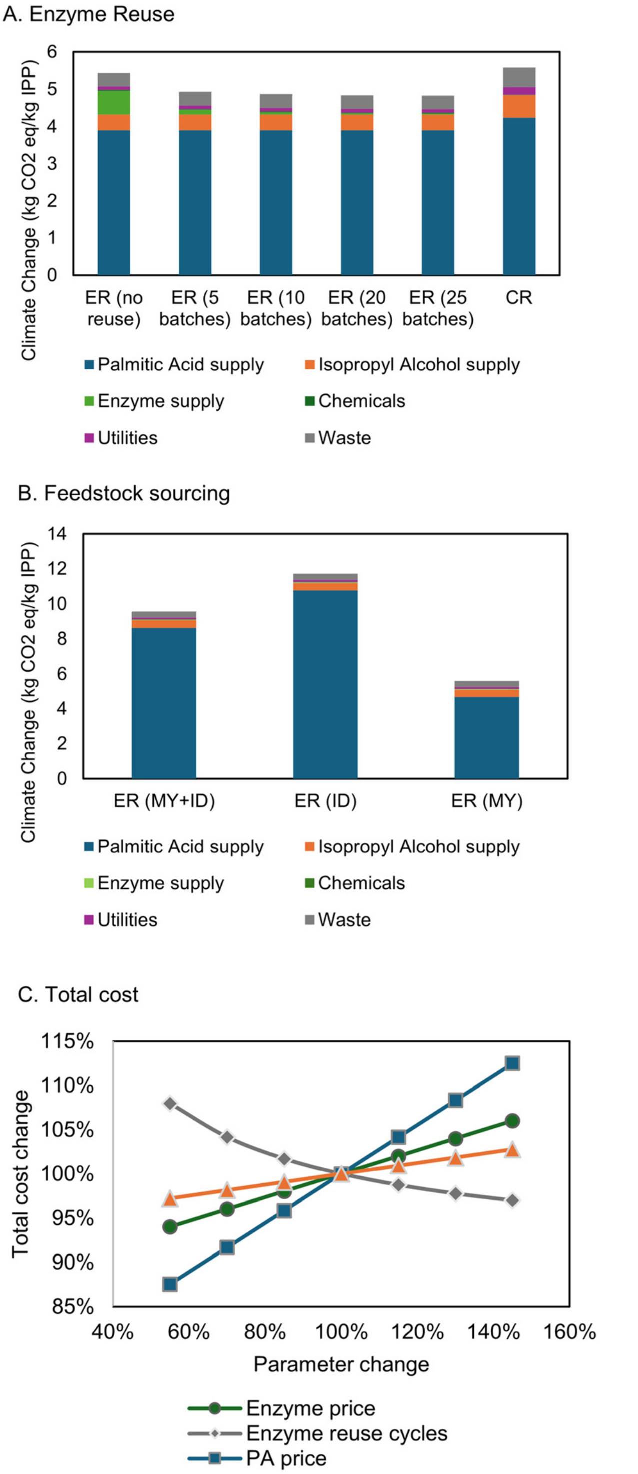

Fig. 5 Sensitivity analysis of the different scenarios to investigate the impact on climate change for (A) enzyme recycling and (B) different sourcing of palmitic acid and (C) to investigate the effect of key parameters on total cost. ER = enzymatic route, CR = chemical route. ER = enzymatic route, CR = chemical route. MY = Malaysia. ID = Indonesia.

climate impact category was below 1%. In case of no reuse, the contribution increased to 12%, resulting in a climate change impact for the enzymatic route close to the chemical route. These results show the importance of reusing enzymes for multiple batches to achieve environmental sustainability gains. Using enzymes for 25 batches does not lead to a significant change compared to 20 batches in terms of environmental sustainability.

The effects of varying the number of batches on the total cost (OPEX + capital depreciation) are shown in Fig. 5(C). Compared to the base case, reusing enzymes 15 times or 25 times would result in respectively a 4% increase and 2% reduction in total cost, indicating the importance of further optimising enzyme reuse from an economic perspective. It should be noted that the cost of downtime for catalyst change is currently not accounted for, indicating that the actual effect on total cost is expected to be even higher.

The effect of feedstock sourcing

The results of the hotspot assessment in Fig. 3 show the high contribution of palmitic acid, and more specifically palm oil cultivation, for all environmental impact indicators. The base case considered crude palm oil produced in Malaysia. The effects of changing the supply from Malaysia to Indonesia or a mix from both Malaysia and Indonesia were analysed. In the case of the mixed supply from both countries, the assumption was that 68.84% of palm oil was supplied from Indonesia and 31.16% from Malaysia. For this assessment, the Agri-footprint database was used for palm oil from both Malaysia and Indonesia, as palm oil from Indonesia was not available in ecoinvent at the time of the assessment. Fig. 5(B) shows that sourcing palm oil from Indonesia rather than Malaysia would more than double the overall climate change impact. This demonstrates that the sourcing of palm oil has a significant impact on the environmental sustainability of IPP production. In both countries, conventional methods of palm oil production cause the destruction of carbon-rich forests and peatlands, contributing to global warming.[46] However, less deforestation occurred in Malaysia, both in absolute and relative terms, in previous decades.[47]

The International Sustainability & Carbon Certification (ISCC) is an international certification system that covers various bio-based feedstocks and renewables, including palm oil. This certification ensures that the feedstock was not cultivated on land with high biodiversity or high carbon, thereby protecting against deforestation and indirect land-use.[48] To account for ISCC certification, the crude palm oil data used were modified by excluding the burdens of "land-use transformation" and "CO_2 emission due to land transformation".[30] Using ISCC certified palm oil as feedstock reduced the climate change impact for the enzymatic and chemical route to 1.54 and 2.00 kg CO_2 eq. per kg IPP, a reduction of respectively 68% and 64%. Due to the smaller overall impact of IPP production, the relative reduction of the enzymatic route on the climate change impact compared to the chemical route increased from 13 to 23%.

For SLCA, palm oil from Indonesia was not available in the PSILCA database. Therefore, in order to investigate the potential effect of alternative sourcing, palm oil from Thailand was considered, as it was the only other South-East Asian country for which palm oil was listed in the PSILCA database. When changing the sourcing to Thailand, the overall medium risk hours reduce (−21%) from 70.6 to 55.21 medium risk hours per kg IPP. Large reductions are also observed for the categories industrial water depletion (−83%) and social security expenditures (−89%). The PSILCA database uses indicators for industrial water depletion related to water resources and total withdrawal. The Thai model assumes a "very low" risk in both cases. In Malaysia, the indicator "level of industrial water depletion (based on total withdrawals)" carries a very high level of risk. However, according to Silalertruksa *et al.* (2016), water issues are a high concern in Thailand as well.[49] In Malaysia, the lack of an integrated water management strategy, high water loss rates, changing weather patterns, destruction or deterioration of water catchments, and a lack of efficient agricultural water use are some of the issues reported. Initiatives such as the National Water Resources Policy, launched by the Malaysian government in 2012, provides holistic strategies for water resource management in Malaysia going forward.[50]

Conclusions

The sustainability of producing 1 kg IPP *via* enzymatic catalysis was compared to conventional chemical catalysis. It was found that the feedstocks, and specifically PA, were the main contributors to the environmental and social impact and economic cost of IPP. Developments toward more sustainable palm oil cultivation and the production of bio-based IPA could therefore result in a significant reduction of the environmental impact of IPP. The comparative assessment showed that switching to enzymatic catalysis for IPP production reduced the environmental impacts between 7 and 13%, depending on the considered impact category. This was due to a triple benefit, being the production of less hazardous waste, lower feedstock consumption due to higher yield, and a lower steam consumption. The social risks associated with chemical and enzymatic IPP production were similar, with an overall increase in medium risk hours of 9% when switching to enzymatic production due to the longer production time. However, many social benefits, such as improved safety for workers, an increase in skills and employability and local employment, were not properly captured by this assessment. A cost comparison showed a higher operational cost (+40%) for enzymatic compared to chemical production of IPP, primarily due to the enzyme cost and higher labour cost. The performed sensitivity analysis underscores the crucial role of enzyme reuse for environmental and economic sustainability.

The proposed LCSA methodology provided clear guidance and insights on assessing and improving the life cycle sustainability of enzymatic catalysis for chemicals production. Using an LCSA methodology with a common goal and scope definition and life cycle inventory reduced the overall time for data collection and streamlined the interpretation. However, several limitations to the current methodology should be noted. Firstly, the methodology currently does not account for differences in scale when comparing enzymatic and chemical catalysis. Comparing technologies at low technology readiness levels (TRLs) with mature processes, which benefit from high levels of process integration and decades of optimization, may lead to an underestimation of sustainability gains.[51] Existing prospective sustainability assessment frameworks, *e.g.*, Thonemann *et al.* (2020),[51] should be tailored for predicting the industrial scale LCI of enzymatic catalysis when still at lab or pilot scale (TRL 3–5). Besides scale, other dimensions of uncertainty require further investigation, such as the uncertainty on social and economic input data. Secondly, the PSILCA database is currently suggested for the SLCA. However, this database provides only sector and country specific data, lacking detailed information about the system under study.[36] Thirdly, the results of the three assessments lead to ambiguous results, favouring either chemical or enzymatic catalysis. If a decision between both technologies needs to be made, a method accounting for those trade-offs, such as multi-criteria decision analysis, should be included.[52]

Author contributions

Pieter Nachtergaele: conceptualization, formal analysis, investigation, methodology, project administration, supervision, visualization, writing – original draft. Ozan Kocak: investigation, formal analysis, methodology, writing – original draft. Yblin Roman Escobar: investigation, formal analysis, methodology, writing – original draft. Jordy Motte: methodology, writing – review & editing. Dries Gabriels: resources, formal analysis, writing – review & editing. Leopold Mottet: methodology, writing – review & editing. Jo Dewulf: project administration, funding acquisition, writing – review & editing.

Data availability

The data supporting this article have been included as part of the ESI,† including the aggregated LCI. The detailed LCI of the enzymatic and chemical production cannot be made available due to industry confidentiality.

Conflicts of interest

There are no conflicts to declare.

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