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An Environmental techno-economic assessment for fatty acid removal from fatty acid ester production with a membrane contactor

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Abstract

Fatty acid removal is challenging in esterification processes due to the similar structures between fatty acids and their esters. Traditional methods have high product loss, energy consumption, and waste generation. This study introduces a novel ceramic TiO membrane contactor combination with a propylamine extractant, facilitating selective fatty acid extraction under mild, low-pressure conditions with minimal oil loss. A membrane flux of 700 $g/m^2 \cdot h$ was obtained experimentally. To assess the viability of integrating this technology into a complete production system, we conducted an environmental techno-economic assessment (ETEA) benchmarking against activated carbon-based removal. The results demonstrated, for an annual production scale of 2,000 m^3 isopropyl palmitate (IPP), the membrane process showed a significantly lower fatty acid removal cost (€31/ton IPP) compared to activated carbon (€81/ton IPP). Despite higher environmental impacts associated with titanium dioxide and amine usage, this membrane technology overall offers an energy-efficient, product-conserving approach suitable for green bioprocessing.

1. Introduction

An estimated 250,000 - 300,000 metric tonnes per year of natural fatty acids are utilized globally in the synthesis of fatty acid esters (FAEs), which reached a global market size of 1.8 million tons in 2024, driven by demand in cosmetics, food emulsifiers, lubricants, paper treatment, and water purification sectors.[1, 2] Isopropyl palmitate (IPP) is one of the most versatile FAEs and plays a significant role in personal products such as skin creams, shampoo, conditioner, bath, and shower gels, because of its good compatibility with the skin and high oil content of the products, and no greasy feeling after use. Given IPP has its primary application in the cosmetic sector, high product purities are required, using lipase enzymes for catalyzing an esterification reaction with a lower reaction temperature has been proposed and widely studied for FAEs.[3-6] The immobilized Candida antarctica lipase (Novozym 435) are used to reaction time to 3-8 hours, which further brings a lower personnel cost and a high yield.[7, 8] Novozyme 435 is more expensive than crude lipases, it is highly reusable. It was reported to retain activity over 10 to 50 reuse cycles, compared to crude or free lipases, which often lose activity after 2 - 3 uses.[9, 10] This reusability significantly reduces the cost per cycle, making it suitable for industrial processes despite its higher initial cost.

However, when the reaction time is shortened, the conversion rate is typically reduced, which subsequently increases the challenge of removing unreacted fatty acids from the final product. Traditionally, unreacted fatty acids are removed using one of the two approaches: reactive distillation or alkali neutralization But the distillation process is energy-intensive and costly, especially for large-scale operations.[11] The neutralization method involves additional steps to purify the final product, such as a washing step for the soap removal, which generates a large amount of wastewater and soap stocks.[12] More recently proposed approaches for the removal of free fatty acids from oils are the use of adsorbents such as activated carbon, silica gel, potassium oxide/dolomite, composite adsorbents.[12-14] However, these alternatives raised an issue of waste treatment from the used adsorbents.

Meanwhile, membrane-based separation has been investigated for removing fatty acids from esters, owing to the high surface area and tunable properties of membrane materials. This particularly benefits the production of IPP, a compound widely used in personal care products, which requires mild processing conditions (for example lower temperatures and neutral pH). Compared to chemical catalysis, enzymatic reactions typically occur under milder conditions as well, which reduces membrane fouling and thermal degradation. These conditions are more compatible with membrane contactors, which are sensitive to high temperature and harsh solvents.[15] Furthermore, enzymatic systems produce fewer inorganic byproducts (e.g., soap from alkali catalysis), minimizing the risk of pore blockage or membrane deactivation.[16] Therefore, enzyme-based processes are generally more suitable for integration with membrane-based separations. This compatibility supports the development of greener, more integrated biocatalytic processes. The membranes combined with solvent extraction were proposed as alternatives to traditional deacidification methods for extracting free fatty acids from soybean and rice bran oils.[17, 18] However, these processes required large membrane surface areas to recover the extractant solvents due to the use of three to four stages of membrane filtration to achieve low free fatty acids concentrations in the recycled solvents. As a result, their economic viability remained uncertain. Subsequent studies explored the direct separation of free fatty acids from various vegetable oils, such as palm oil, sunflower oil, and soybean oil, using nanofiltration membranes.[19, 20] For example, Ismail et al. (2018) used organic solvent nanofiltration to separate free fatty acids from palm oil, achieving 45% fatty acid removal and 13% co-extraction of palm oil at an initial fatty acid concentration of 3.6 g/L.[19] A similar study reported 58% fatty acid removal and 80% oil retention using composite nanofiltration membranes.[20] Thurs, they are generally unable to reduce the fatty acid concentration in the product oil to low levels without incurring significant product losses. Recently, membrane-based technologies have been investigated for the recovery of short- and medium-chain fatty acids and volatile fatty acids from fermentation broths and other waste-derived sources.[21-24] Although recovery rates exceeding 84% have been reported, the membrane selectivity remains relatively low, which compromises the purity of the target product.

Despite the efforts reported in these studies, membrane-based processes for fatty acid removal have shown limited economic feasibility, low selectivity, and significant product losses, making it difficult to achieve high product purity. Although recent studies report high recovery rates, membrane selectivity remains a key challenge. Moreover, membrane-based separation following an esterification step has not been reported in the literature. The technical and economic feasibility of implementing membrane technology as part of a complete production process, along with its environmental sustainability, also remains unclear. It is still unknown whether fatty acid removal via membrane contactors can be economically competitive and environmentally advantageous, or under what conditions it could surpass alternative processes. Therefore, it is essential to quantify it within the context of the entire production process, and to benchmark its performance against that of alternative methods.

In this context, this study presents two key innovations. First, we develop a novel membrane contactor-based extraction system employing a ceramic TiO membrane that enhance the selective removal of fatty acid without significant product loss, an advancement over conventional deacidification techniques. Second, we introduce an integrated environmental techno-economic assessment (ETEA) framework to evaluate the feasibility and sustainability of incorporating this membrane technology into a complete industrial production process. To the best of our knowledge, this is the first study to combine selective membrane-based extraction with a full-process ETEA for fatty acid removal in green chemical manufacturing. As a benchmark, a process using activated carbon for FFA removal from esters is selected. Activated carbon is widely used for fatty acid removal in industries such as biodiesel production,[25-28] edible oil refining,[9, 29] oleochemicals and cosmetics,[27, 30] and wastewater treatment.[31] Its natural origin also makes it a cleaner alternative for removing impurities from environmentally friendly chemical products.

In this study, the ETEA methodology includes the process flow diagrams for both membrane-based and benchmark processes, as well as the key input data for the model. A membrane extraction experiment is also conducted to quantify the palmitic acid (PA) mass transfer coefficient as a proof-of-concept. The experimental membrane flux, the production and fatty acid removal costs are discussed, as well as the environmental impact assessment based on 13 midpoint indicators using the ReCiPe 2016 method. Additionally, global and local sensitivity analyses are performed to identify the most influential parameters affecting fatty acid removal cost, and the contribution of each production step to various environmental impact categories is examined for both processes.

2. Method

2.1 The ETEA method

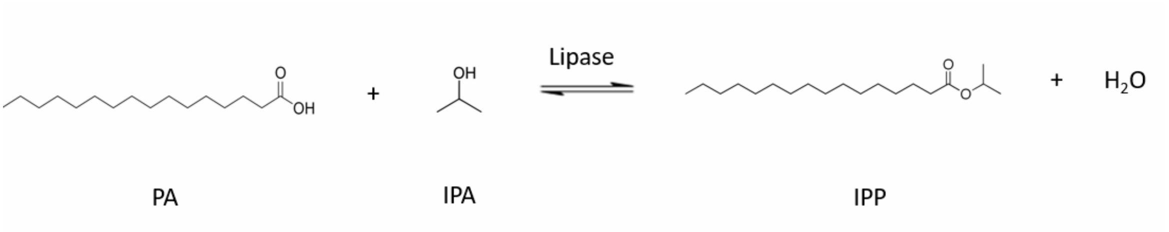
An ETEA is an integrated evaluation of the technological performance, the economic feasibility and the potential environmental impact of a technology.[32-35] It results in separate economic and environmental indicators that are derived from the same underlying technological performance data and aligned system boundaries. Decision makers can therefore use these models to select and direct research and development activities and the related investments. As ETEAs are typically prospective in nature, they serve to derive advice on how to build a stronger business case for an alternative, less mature technology.

In this study, the system boundaries comprise the two full production processes, as shown in Figures 2 and 3. The costs and environmental impacts of the upstream processes are represented by the costs and impacts of the feedstocks mentioned in Figures 2 and 3. The costs and environmental impacts of all waste sources are considered by the addition of costs and impacts for the waste treatment. The costs and environmental impacts of the following product life cycle stages are not included for the two processes: storage, distribution, product use, end-of-life and disposal.

The ETEA framework is structured into five sequential steps: (1) market analysis, (2) process design and development, (3) economic evaluation, (4) environmental assessment, and (5) sensitivity analysis. This methodology is consistent with our previous studies.[32, 33, 36, 37] In Step 1 we investigate the market of FAEs, and select a typical FAE, IPP, as the model product for ETEA study. The IPP production process with activated carbon for PA removal is chosen as the benchmark, which is compared with the alterative process with a membrane contactor. In Step 2 we develop the process flow diagrams for these two processes. This involves specifying the equipment to be used at the desired scale. Consequently, the mass and energy balances of the two processes are drafted, based on the same product quality (99% purity) and annual yield requirement. The annual yield is set at 2,000 m^3 (1,880 tons) per year, which is similar with the production capacity of a small-scale isopropyl myristate manufacturing plant.[6, 38] Given these flows, the process equipment is sized. In Step 3, as demonstrated in Eqs.1 and 2, the economic feasibility is evaluated by calculating the net present value (NPV) and the PA removal cost. The project lifetime is 20 years with a discount rate of 6% for the two cases in this study. The PA removal cost is a part of the overall production cost, which includes annualized capital expenditure (CapEx) and operational expenditure (OpEx), that are calculated based on the mass and energy balances in Step 2. The CapEx includes the equipment costs of reactors, distillation columns, PA filter and membrane modules. The OpEx covers the costs of raw materials, labor, energy, waste disposal, insurance, repair and maintenance. The estimation methods of the dimensions, purchase costs, and energy consumptions of these equipment are described in S.I. Section S1. In step 4 the environmental impact of the two processes is quantified, using the midpoint indicators of the ReCiPe 2016 method. The characterization factors for each of the inputs and resulting emissions, needed to quantify these indicators, are drawn from the Ecoinvent 3.9 database. The characterization factors are directly linked to the mass and energy balance outcomes, similar to how the costs are calculated in economic analysis. Until now, the input parameter values are based on default assumptions. It has an uncertainty due to the early-stage development of alternative technology. To address this uncertainty, Step 5 begins with a global sensitivity analysis to identify the most influential parameters affecting the membrane separation cost for the alternative technology. This analysis is conducted by performing Monte Carlo simulations with Oracle Crystal Ball software. 10,000 observations are generated from the input parameters' distributions (ranging from −10% to +10% of the default values), and the indicators are recalculated accordingly. Subsequently, local sensitivity analyses are performed to analyze the effects of the key parameters, while keeping all other parameters constant.

2.2 Process flow diagrams

The two processes have the same production steps, except for the PA removal step. The product esterification is shown in Eq. 3. The full process flow diagrams are shown in Figures 1 and 2. The TEA takes the whole IPP production process into account, including the product esterification and downstream processing to separate the product and recover the solvents.



2.2.1 Benchmark process

The process is operated in semi-batch. As shown in Figure 1, an excess of isopropyl alcohol (IPA), PA and Novozym 435 lipase are added to the reactor to synthesize the product IPP by means of esterification. Since the esterification is an equilibrium reaction, the reaction water has to be removed continuously to obtain a high ester yield. During the reaction at 65°C, some water and IPA are evaporated. The mixture of the evaporated water and IPA are sent to the IPA rectification tower to separate the IPA from the water. The removed IPA is reused for IPP esterification. The left water from the bottom of the rectification tower is sent to the wastewater treatment plant. When the esterification reaction is finished (40 hours of reaction time), the reaction mixture is filtered to recover the lipase. Afterwards, the mixture is transferred to the distillation tower to remove the remaining IPA and water. The removed IPA and water are sent to the rectification tower to recycle IPA. The IPP and unreacted PA (2 wt%) from the bottom of the distillation tower are sent to the PA filter using activated carbon as adsorbent. The used activated carbon with PA is collected by filtration,[39] and sent to the waste treatment plant. The product IPP is obtained with a high purity above 99%. The IPA recovery rate is above 98%.[40]

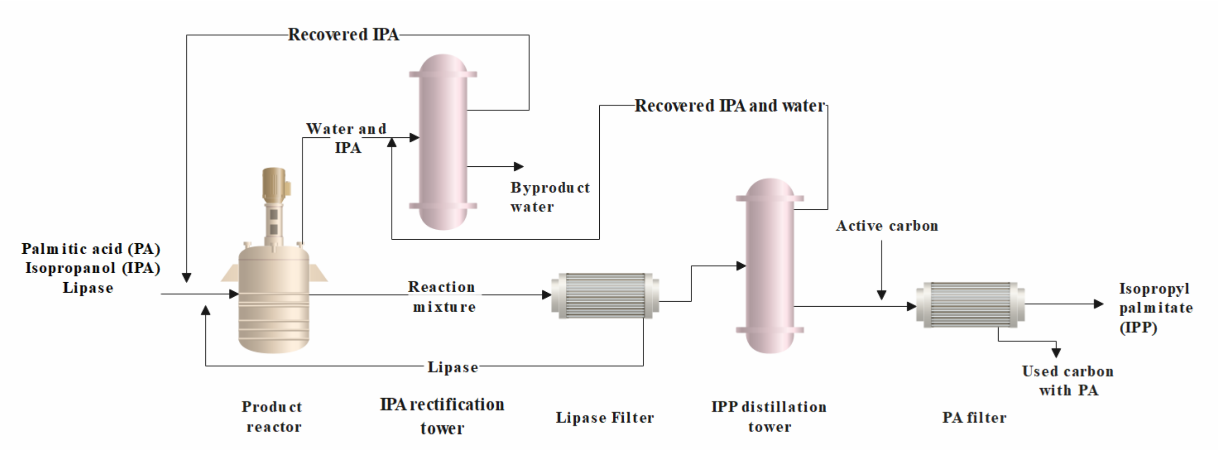


Figure 1. IPP production process with activated carbon

2.2.2 Alternative process with a membrane contactor

The membrane process operates in a semi-batch mode as well. The product synthesis, IPA and water separation steps are the same as the activated carbon process. The only difference is coming from the PA removal step. As shown in Figure 2, PA filter is replaced by a ceramic TiO_2 membrane contactor with aqueous amine (propylamine) solution as extractant. The alkali amine solution extracts the PA following an acid–base reaction. After the PA removal, the extract containing the alkali salt, which is formed from the amine and PA reaction, is sent to a waste treatment plant. The product IPP is obtained as raffinate with a purity above 99% as well.

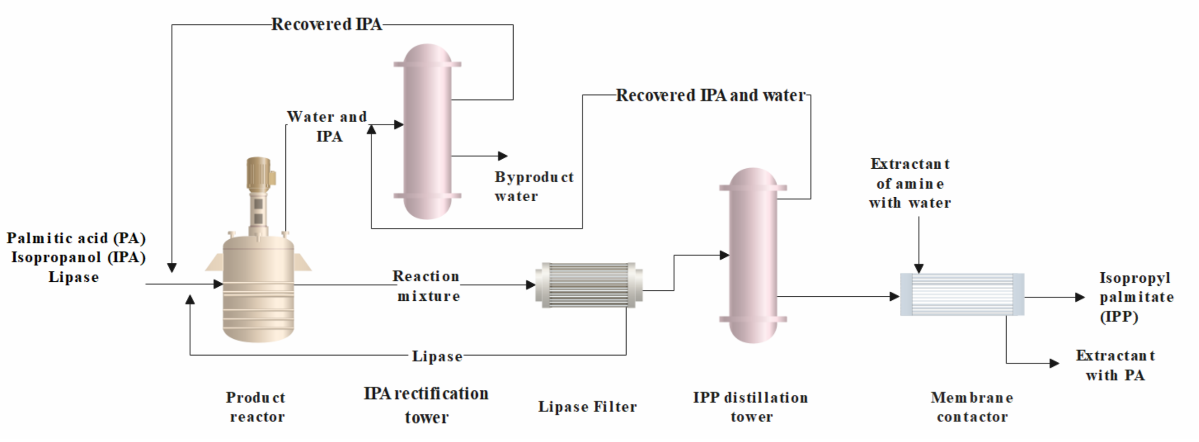


Figure 2. IPP production process with a membrane contactor

2.3 Membrane extraction experiment

An PA extraction experiment with a membrane contactor was performed, which mimicked the PA removal step in Figure 2. The experimental setup is illustrated in Figure 3. The feed solution has the same concentrations as the mixture, being IPP (98 wt%) and PA (2 wt%), coming out of the IPP distillation tower in Figure 2. 50 wt% propylamine and 50 wt% water are mixed as extractant in the amine tank. All chemicals were purchased from Sigma–Aldrich. A native TiO_2 membrane with a pore size of 0.9 nm was applied. A tubular membrane contactor with a surface area of 50 cm^2 was provided by Inopor GmbH (DE). Two pumps (Iwaki) were used to circulate the two phases. The feed solution was pumped from the shell side of the membrane contactor and the extractant phase was pumped through the lumen side of the membrane. The flow rates on both sides were 20 L/h at temperature 30°C. Concentrations of PA, IPP and amine propylamine were determined by gas chromatography - flame ionization detector (GC-FID) (Agilent Technologies).

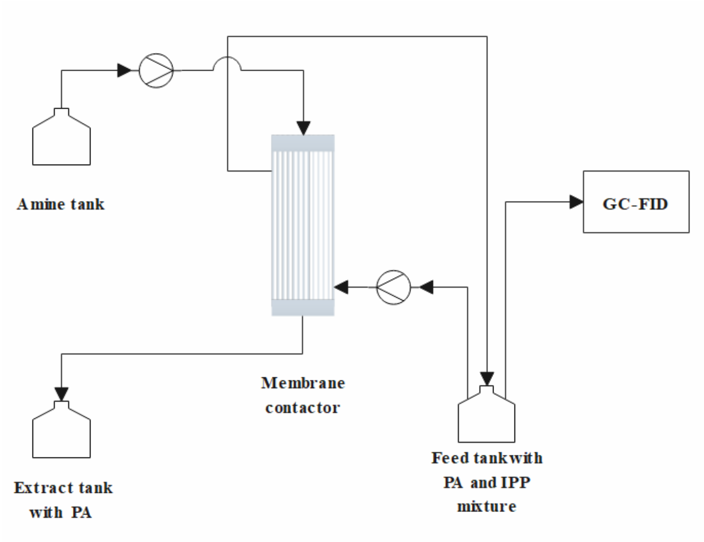


Figure 3. Experimental setup for PA removal using a membrane contactor

2.4 Technological input parameters

To compare the two processes, the same amount of targeted product IPP is produced for each process of 2,000 m^3 per year. The mass and energy balance are calculated based on the processes data in Table 1. The processes are semi-batch. The time per batch is 68 hours, it includes 40 hours of reaction time and 28 hours of cleaning and recharging time of all the equipment (1.5 days). A reaction time of 40 hours is taken to achieve a high PA conversion rate of 98%, which is longer than the reported reaction times of 6-24 hours with conversion rates ranging from 50% to 90%.[7] The reaction times can vary significantly depending on several factors, including the type of lipase used, the reaction medium, temperature, and substrate concentrations. The reaction requires an IPA:PA molar ratio of 2:1. However, during the process, IPA is continuously lost, because it evaporates and is carried to the rectification tower along with the water produced during the reaction. To maintain the necessary 2:1 molar ratio of IPA to PA, additional IPA is periodically added to the reactor. By the end of the process, the total moles of palmitic acid (PA) consumed in the reactor are approximately 3.5 times the moles of IPA initially introduced. 90% of the generated water during the reaction is evaporated to the rectification tower. There are 118 batches per year with a batch yield of 17 m^3 per year in a reactor of 20 m^3. The other equipment, including rectification and distillation towers, filter and the membrane contactor, are sized up based on the batch yield, as described in S.I. Section S1. In the following we explain how we determine the membrane's size based on the PA flux through the membrane.

The membrane contactor purchase cost is estimated by Eqs. 4 and 5. PA flux through the membrane, f_{PA}, is obtained by a membrane separation experiment performed in this study, described in Section 2.3.1.

Table 1. Process parameters

Section	Parameter	Unit	Value	Other papers [3, 7, 41]
Reaction conditions	IPA to PA mole ratio	mol/mol	3.5	3-15:1
	PA conversion rate	%	98	50-90
	PA concentration before PA removal	wt%	2	Experiments in Section 2.3
	IPA recovery rate	%	98	-
	Reaction time	h/batch	40	6-24
	Process cleaning and recharging time	day/batch	1.5	-
Catalyst use	Lipase loading (Novozym 435)	wt%	1	0.3-0.4; 1-4
	Lipases recycle times	-	50	15
Membrane extractant	amine to PA molar ratio	-	1.5	Experiments in Section 2.3
	Amine concentration	wt%	50	Experiments in Section 2.3
	Water concentration	wt%	50	Experiments in Section 2.3
Membrane performance	PA flux	g/hm^2	700	Experiments in Section 2.3
	IPP flux	g/hm^2	0	Experiments in Section 2.3
Activated carbon process	Activated carbon loading	wt% of IPP	1.5	0.5-2

2.5 Economic input parameters

This study focuses on the PA removal cost as part of the overall production cost. It includes capital expenditure (CapEx) for process equipment and operating expenditure (OpEx) for raw materials, utilities, waste management, and labor, which are estimated for the two processes. The economic input parameters required for estimating the production cost are listed in Table 2. The capital expenditure for the equipment in the two processes is estimated by multiplying the equipment purchase cost with a Lang factor.[42] The Lang factor is considered 5.0 for the two processes in this study.[42] The Chemical Engineering Plant Cost Index (CEPCI), 800 for 2024 from CHEMICAL ENGINEERING, is applied to incorporate the effect of time on the cost estimates for equipment.[43] The CEPCI covers values for overall plants on the basis of various types of equipment, building, construction labor, and engineering fees.[44] A regression function approach, based on the purchase cost data from Matche Inc. (www.matche.com), and the formulas from Seider et al. (2016), is used to estimate the equipment purchase cost on a process required scale.[37, 45] The equations to compute the cost and energy consumption of each equipment are described in S.I. Section S1.

Table 2. Economic parameters

Item	Unit	Value	Range
Lifetime	year	20	10-30
Operating time	h/year	8,000	8,760 in total
IPP	€/kg	20	2-100
IPA	€/kg	1.5	1.2-1.9
PA	€/kg	2	1-3
Lipase (Novozym 435)	€/kg	2,500	700-5,000
Activated carbon	€/kg	2.5	1-3
Propylamine	€/kg	5	Vendors
Solid waste treatment	€/kg	0.3	0.036-1
Wastewater treatment	€/m^3	12.25	0.47-20

2.6 Environmental assessment: goal, scope, functional unit and impact categories

The goal of environmental assessment, the Step 4 of the ETEA framework, is to compare the environmental impact of the two processes and to identify hotspots. A gate-to-gate system boundary is used. The scope of environmental analysis is consistent with the whole ETEA, as described in Section 2.1. The environmental impacts of the following life cycle stages are not included as they are assumed to be the same for the two processes: storage, distribution, product use, end-of-life and disposal. Environmental impacts from transportation and labor are excluded as well. The functional unit used in this study is one ton product IPP. The environmental assessment inventory is consistent with the mass & energy balance in Step 2 of the ETEA framework. The midpoint indicators of the ReCiPe 2016 method are used for environmental impact assessment. According to the guideline of Life Cycle Metrics for Chemical Products by the World Business Council for Sustainable Development (WBCSD), ten emission related categories of global warming (GW); fine particulate matter formation (FPMF); terrestrial acidification (TA); freshwater eutrophication (FEU); marine eutrophication (MEU); terrestrial ecotoxicity (TE); freshwater ecotoxicity (FEC); marine ecotoxicity (MEC); human carcinogenic toxicity (HCT); human non-carcinogenic toxicity (HNCT) and three resource-based categories of land use (LU), fossil resource scarcity (FRS) and water consumption (WC) are selected.[46, 47]

3. Results and discussion

3.1 Mass and energy balance

The mass and energy balance including the feedstock, waste discharged, and energy consumed are calculated based on the annual yield of 2,000 m^3 IPP (1,880 ton). 98% of generated water and the unreacted IPA from the esterification reaction are recovered by the distillation. The mass and energy inputs and outputs, per ton product IPP, are listed in Table 3. The calculation equations are listed in S.I Section S2 with Eqs. S11-S20. These two processes consume the same amount of the feedstocks of IPA, PA and the lipase enzyme. The membrane process uses amine and water for PA removal, and the membrane cleaning solvents of NaOH, HCl, NaOCl and water. The wastewater from the membrane process is bigger than the activated process, because the extraction solution with the removed PA is treated as wastewater. The two processes have the same amount of wastewater from the residue of distillation. The activated process uses the activated carbon in a filter to remove the PA. Accordingly, it generates more solid waste of the used activated carbon than the membrane process. The two processes have similar energy consumption.

Based on the mass and energy balance, the equipment sizes and costs are estimated, as shown in Table 4. A PA flux of 700 g/m^2h in the membrane contactor is obtained from the experiment. The experimental results show that only PA was extracted in the membrane contactor. The product IPP stays at the feed phase. The membrane area needed is estimated by Eq. 5 with the PA flux of 700 g/m^2h (0.82 L/m^2h). One study employed nanofiltration membranes under 30-40 bar, achieving higher fluxes of 10-40 $L/m^2 \cdot h$, but observed 55% FFA rejection and 87% oil retention, indicating poor selectivity.[19] Similarly, another nanofiltration study reported higher fluxes of 4-20 L/m^2h under 10-20 bar, but still with substantial oil retention and limited fatty acid removal, again reflecting low specificity for fatty acid extraction.[20] In contrast, Lee et al. (2022) reported lower fluxes (0–0.02 L/m^2h) using a supported liquid membrane system designed for selective extraction. Although highly selective, the low flux limits scalability.[21] While our flux value is lower than those reported for nanofiltration, the key advantage of our approach lies in its selectivity and oil integrity. The use of a ceramic TiO membrane in our system enabled exclusive extraction of free fatty acids with no oil loss, a performance not achieved by the pressure-driven nanofiltration systems reviewed. This highlights the trade-off between permeate flux and selectivity, and demonstrates the potential of membrane contactor technology in applications where purity and product conservation are critical.

Table 3. Raw material inputs, waste outputs and energy consumption of the two processes to produce 1 ton IPP.

Item	Unit	IPP-activated carbon	IPP-membrane	Resource
IPA	kg	722.88	722.88	S.I. Eq. S12
PA	kg	885.60	885.60	S.I. Eq. S11
Lipase	kg	0.32	0.32	S.I. Eq. S13
Extractant amine	kg	-	9.19	S.I. Eq. S14
Extractant water	kg	-	9.19	S.I. Eq. S15
Membrane cleaning	kg	-	3.01	S.I. Eq. S16

solvent				
Activated carbon	kg	15.40	-	S.I. Eq. S17
Waste water	kg	60.47	108.43	S.I. Eq. S18, S19
Solid waste	kg	42.29	0.32	S.I. Eq. S20
Energy consumption	MWh	0.27	0.24	S.I. Eq. S2, S3, S6, S9, S10

Table 4. Summary of the dimensions and CapEx of all equipment used in the two processes.

Item	Unit	IPP-activated carbon	IPP-membrane	Resource
Reactor	Volume (m^3)	25	25	-
	Cost (k€)	1,489	1,489	S.I. Eq. S1
Rectification tower	Area (m^2)	0.36	0.36	S.I. Eq. S5
	Cost (k€)	125	125	S.I. Eq. S4
Product distillation tower	Area (m^2)	0.55	0.55	S.I. Eq. S5
	Cost (k€)	209	209	S.I. Eq. S4
PA filter	Area (m^2)	4	-	S.I. Eq. S8
	Cost (k€)	702	-	S.I. Eq. S7
Membrane contactor	Area (m^2)	-	55	Eq. 5
	Cost (k€)	-	274	Eq. 4

3.2 NPVs and production costs

Both processes yield positive and comparable NPVs over a 20-year project lifetime: M€283.6 for the activated carbon process and M€284.8 for the membrane process. On a per-ton product basis, the NPVs are €8,318/ton IPP for the activated carbon process and €8,353/ton IPP for the membrane process. Positive NPVs indicate that the present value of the revenues generated from selling the IPP product is greater than the present value of its production costs. The production costs of the two processes are calculated based on the mass and energy balance for the operating cost, and the equipment size for the capital cost. The breakdown of the two processes' costs is shown in Figure 4. The esterification step has the same cost of €1,831/ton IPP for the two processes, which has the biggest contribution of the whole production process. This big cost share results from the PA cost of €1,016/ton IPP. Therefore, it is necessary to keep a high conversion rate of PA. IPA cost is €178/ton IPP with a recovery rate of 98%. Lipase also has a big cost of €461/ton IPP, due to the high price of €2,500/kg for Novozym 435. The costs of rectification and distillation steps are the same for the two processes as well, which are €6/ton IPP and €11/ton IPP, respectively. The difference of the two processes is from the last step of PA removal, as shown in Figure 5. The membrane process has a lower cost of €31/ton IPP than the activated carbon process (€81/ton IPP). The PA removal cost of the membrane process include the membrane contactor capital cost of

€14/ton IPP (€274,203 for the project lifetime), the extractant and washing solvents cost of €11/ton IPP and other operating costs of €6/ton IPP. For the activated carbon process, the filter combined with the activated carbon are €58/ton IPP. The remaining operating costs are €22 per ton of IPP. The waste disposal cost for the membrane process is lower than that of the activated carbon process. Specifically, disposing of the membrane extractant and washing solvents costs €0.4 per ton of wastewater, compared to €7.2 per ton of solid waste for the disposal of used activated carbon.

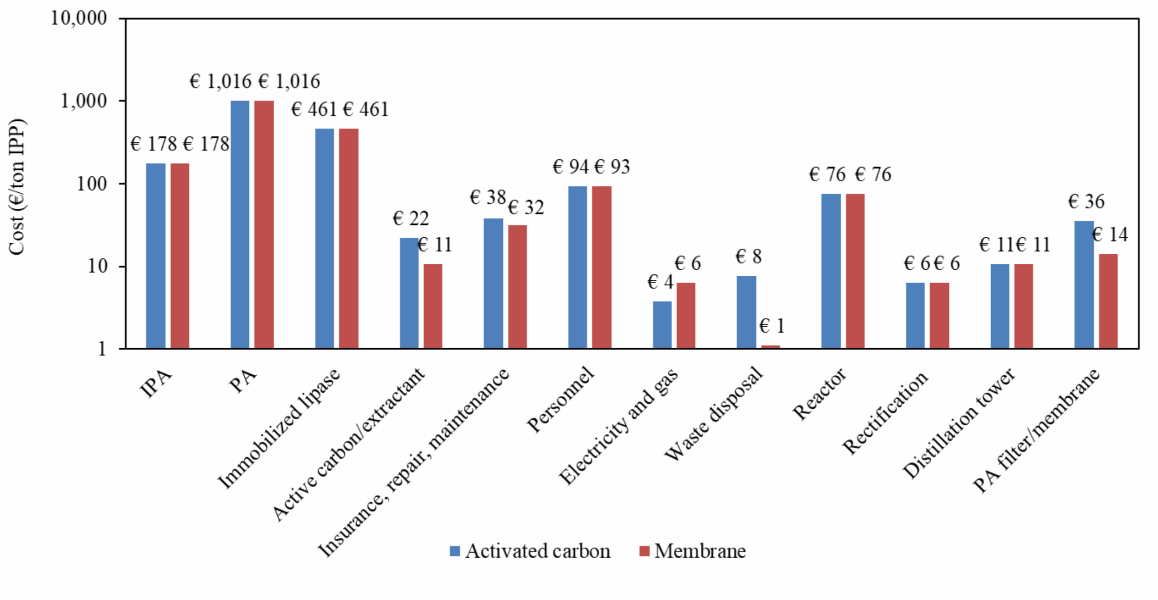


Figure 4. Breakdown of production costs (CapEx and OpEx) for the two processes.

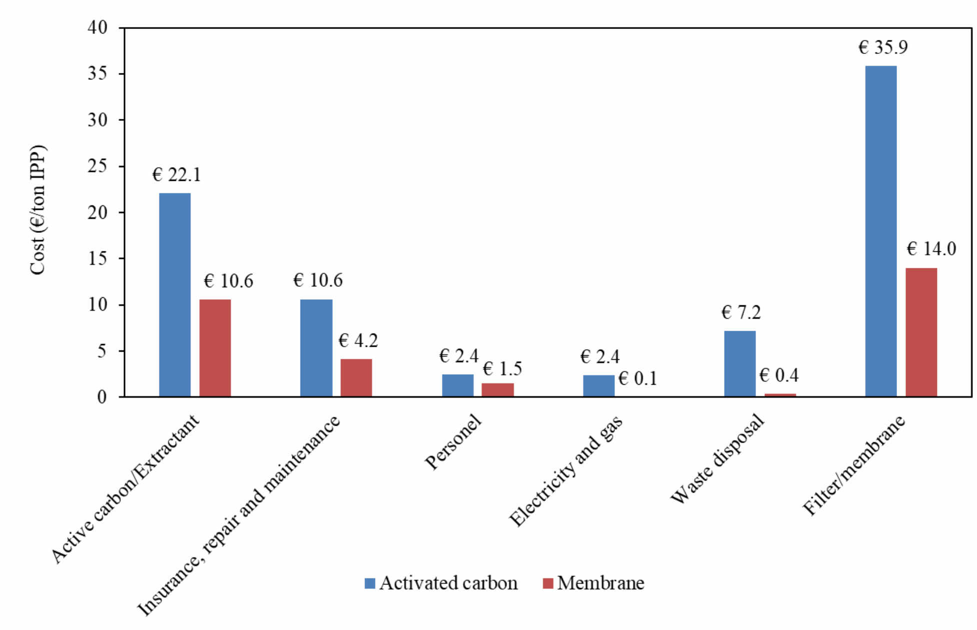


Figure 5. Breakdown of PA removal costs (CapEx and OpEx) for the two processes.

3.3 Global and local sensitivity analyses of the PA removal cost

A Monte Carlo simulation is performed for membrane separation to identify the membrane parameters' impact on the PA removal cost with a membrane contactor, as shown in Figure 6. The PA flux, membrane price, operating time per batch have a major impact, due to the high cost of membrane contactors and the related maintenance, repair and insurance cost (see Figure 5). The membrane contactor's cost is computed by the membrane price and the area needed. The required membrane area is determined by the PA flux and the membrane operating time (see Eq. 5). In addition, the extractant amount also has a big impact of 12%, because the extractant has a big contribution to the PA removal cost, as shown in Figure 6. Membrane lifetime has a minor impact. Note that the parameters, such as purchase prices and extractant amount have positive impacts because the separation cost increases when these parameters go up from the default values, whereas the opposite applies to the other three parameters.

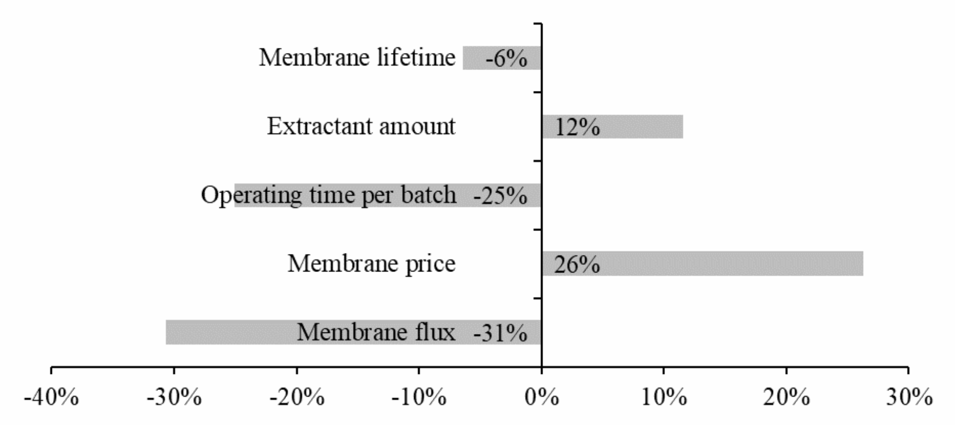


Figure 6. Monte Carlo analysis of parameter contributions to variation of the membrane cost for PA removal.

The PA removal cost with membranes includes the cost of membrane contact and its insurance, repair and maintenance, extractant and washing solvents, personnel, energy and waste disposal. The membrane flux significantly impacts the cost of the membrane contactor, as it determines the required membrane area. As illustrated in Figure 7, the PA removal cost drops sharply from €1,285 to €76 per ton of IPP as the membrane flux increases from 10 g/hm^2 to 200 $g/h{\cdot}m^2$. Beyond 200 $g/h{\cdot}m^2$, the cost of PA removal shows slight reduction with further increases in membrane flux. The cost of the membrane contactor is inversely proportional to the membrane flux, as explained by Eqs. 4 and 5. Specifically, when the membrane flux increases from 10 to 200 $g/h{\cdot}m^2$, the membrane contactor cost decreases significantly, from €981 to €49 per ton of IPP. When the membrane flux continues increasing to 1,000 g/hm^2, the membrane contactor cost is further reduced to €10/ton IPP. Meanwhile, the costs of the extractant and washing solvents, as well as personnel costs, remain constant at €11 and €2 per ton of IPP, respectively. The default value of the membrane flux is 700 g/hm^2 in this study, as marked in Figure 7.

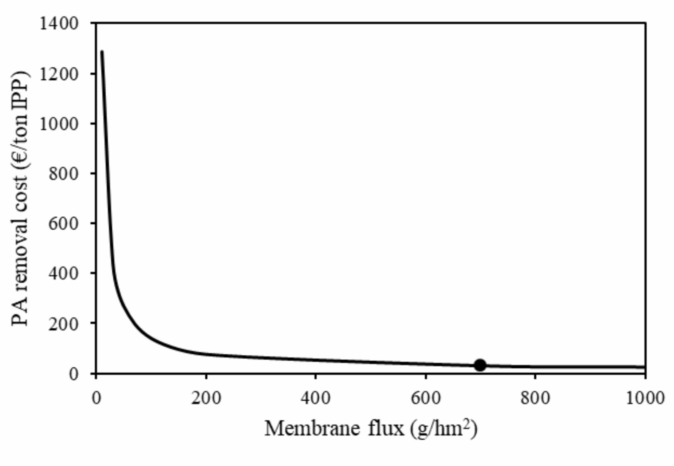


Figure 7. PA removal cost with membranes as a function of membrane flux. The dot is the default value in ETEA.

The membrane operating time is a crucial factor in membrane separation as well. A longer operating time results in a higher personnel cost but simultaneously requires a smaller membrane area, leading to a decrease in membrane contactor cost, as described by Eqs. 4 and 5. In this study, the cost of membrane separation for PA removal decreases from €102 to €21 per ton of IPP as the operating time per batch increases from 2 hours to 40 hours. Beyond this point, the PA removal cost begins to rise gradually with further increases in operating time, as shown in Figure 8. This is because the increase in personnel cost outweighs the reduction in membrane contactor cost. Thus, when the operating time is between 30 to 40 h/batch, the membrane separation cost has the lowest value.

Given that the membrane price is as high as €1,000/m^2, the membrane lifetime is important for membrane application. The capital costs, including membrane contactor, are annualized. As shown in Figure 9, the PA removal cost decreases from €104/ton IPP to €31/ton IPP, when the membrane lifetime is extended from 2 years to 20 years. The default value of the membrane lifetime is 20 years, given that the strong ceramic membrane is used in this study.

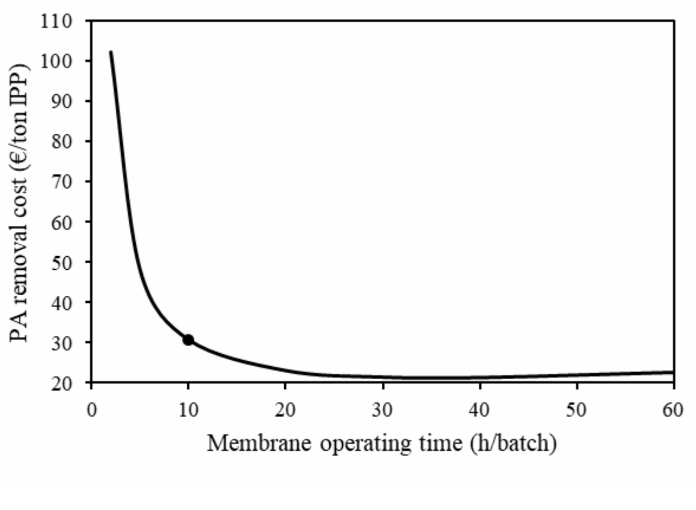


Figure 8. PA removal cost with membranes as a function of membrane operating time. The dot is the default value in ETEA.

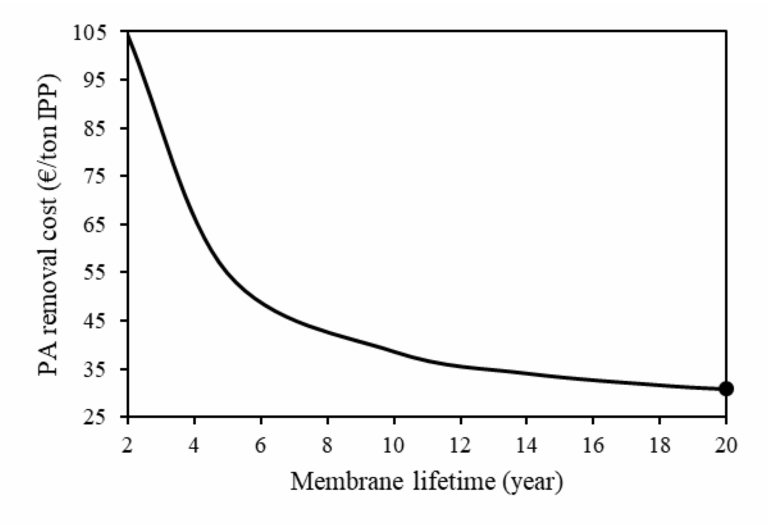


Figure 9. PA removal cost with membranes as a function of membrane lifetime. The dot is the default value in ETEA.

3.4 Environmental impacts

Comparison of environmental impacts of the two production processes and the PA removal steps across categories, interpreted by 13 midpoint categories, is illustrated in Figure 10. In Figure 10 A, the two processes have the same steps for product synthesis and IPA removal. Only the last step of PA removal is different. Among all process steps, the reactor stage contributes the most to most impact categories, with values approximately ten times higher than other steps, especially water consumption, fossil resource scarcity, land use, human non-carcinogenic toxicity, terrestrial ecotoxicity and global warming. It mainly results from the feed materials IPA and PA to produce IPP. The reactor itself and the energy consumption have a much smaller share than the IPA and PA. The rectification and product distillation steps have the smallest impacts for most categories. Within the PA removal step, the environmental impact of the filter with activated carbon is approximately ten times lower than that of the membrane contactor with the amine extractant in most categories. Figure 10 B shows the membrane contactor itself is the primary contributor, particularly in human carcinogenic toxicity (43.4 kg 1,4-DCB). This is largely due to the materials used in the membrane contactor, including titanium dioxide for the membrane, stainless steel for the housing, and O-ring rubber for sealing. Additionally, the extractant amine significantly contributes to fossil resource scarcity (24.8 kg oil eq). For the activated carbon step, the primary contributions are the filter and the wasted PA, as shown in Figure 10 C. The filter is a tank of stainless steel with activated carbon to remove PA, contributing to the overall impact.

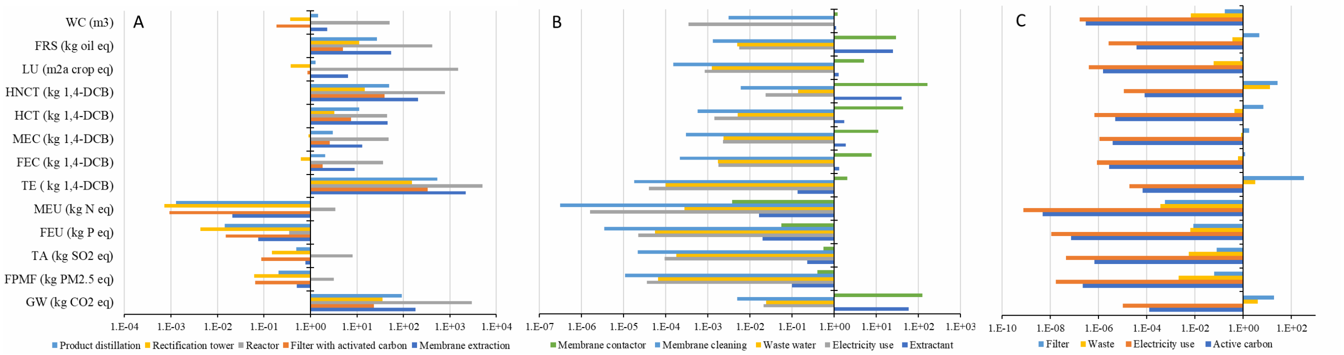


Figure 10. Comparison of environmental impacts across categories of producing 1 ton IPP: (A) Contribution by process stages; (B) Contribution by input sources of membrane extraction step; (C) Contribution by input sources of filtration step with activated carbon, global warming (GW); fine particulate matter formation (FPMF); terrestrial acidification (TA) freshwater eutrophication (FEU); marine eutrophication (MEU); terrestrial ecotoxicity (TE); freshwater ecotoxicity (FEC); marine ecotoxicity (MEC) human carcinogenic toxicity (HCT); human non-carcinogenic toxicity (HNCT); land use (LU); fossil resource scarcity (FRS); water consumption (WC).

4. Conclusion

This study introduces a novel membrane contactor-based extraction system employing a ceramic TiO membrane that enables selective removal of free fatty acids without any oil loss, even under low-pressure conditions. Furthermore, we integrate a full ETEA to evaluate the feasibility of this process in an industrial context. By benchmarking this approach against activated carbon filtration, we provide a comparative analysis not only in terms of technical performance but also economic cost and environmental footprint. This multi-dimension evaluation presents new insights into sustainable process design for green oleochemical production.

We evaluate the technical feasibility, economic performance, and environmental impact of fatty acid removal in the production of 2,000 m^3 of IPP annually over a 20-year project lifetime. Experimental membrane separation was conducted to obtain a PA flux of 700 g/m^{2}h, using a ceramic membrane contactor to extract PA from an IPP esterification solution. The cost of fatty acid removal using the membrane contactor was estimated at €31/ton IPP, significantly lower than €81/ton IPP for the activated carbon process. The cost advantage primarily stems from reduced capital expenditure (€14/ton IPP for membrane and €58/ton IPP for activated carbon filter) and waste disposal costs (€1/ton IPP for solvent and €7/ton IPP for spent activated carbon).

Sensitivity analysis identified membrane flux, membrane price, and operational time as the most influential parameters affecting cost. However, gate-to-gate environmental analysis indicated that the membrane process exhibits higher impacts in categories such as human non-carcinogenic toxicity, terrestrial ecotoxicity, and global warming potential. These are largely attributed to the use of titanium dioxide in the membrane and stainless steel in the contactor housing. The extractant amine also contributed notably to fossil resource depletion.

In comparison, the activated carbon process is primarily impacted by the steel filter housing and fatty acid losses during disposal.

From an investor perspective, the membrane contactor process offers long term economic advantages, process selectivity, and operational simplicity, especially in high-purity applications. Despite its current environmental footprint, material innovations and solvent recovery strategies could significantly reduce its impact in future implementations.

These findings fundamentally advances the field of green separation by combining a high selectivity membrane process with a quantitative ETEA framework. In doing so, it bridges the gap between laboratory-scale innovation and sustainable industrial application, providing a model for future integrated bioprocess design. Future work should focus on scaling up the membrane system, optimizing solvent recovery, and exploring membrane surface modifications to enhance fouling resistance and further improve selectivity. Additionally, combining this process with in-situ enzymatic reactions could pave the way for fully integrated biorefinery systems.

Supporting Information

Formulas of the dimensions, purchase costs, and energy consumptions of process equipment; Formulas of mass inputs and outputs

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Nomenclature

A	membrane area (m^2)
C	cost (€)
f	component flux through the membrane (g/m^2h)
i	discount rate (%)
I_0	the initial investment in year 0 (€)
m	component amount removed per year (g/y)
n	number of years
p	purchase price of membrane in module per square meter (€/m^2)
R_n	the difference between revenues and costs in year n (€)
t	operational time per year (h/y)

T life span of the investment, (y)

Abbreviations

CapEx	capital expenditure
CEPCI	chemical engineering plant cost index
ETEA	environmental techno-economic assessment
FAE	fatty acid esters
FEC	freshwater ecotoxicity
FEU	freshwater eutrophication
FPMF	fine particulate matter formation
FRS	fossil resource scarcity
GW	global warming
HCT	human carcinogenic toxicity
HNCT	human non-carcinogenic toxicity
IPA	isopropyl alcohol
IPP	isopropyl palmitate
LU	land use
MEC	marine ecotoxicity
MEU	marine eutrophication
NPV	net present value
OpEx	operational expenditure
PA	palmitic acid
TA	terrestrial acidification
TE	terrestrial ecotoxicity
WBCSD	World Business Council for Sustainable Development
WC	water consumption

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