

Supporting Information (SI)

Production of Caproic Acid from Mixed Organic Waste- An Environmental Life Cycle Perspective

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This SI contains 22 pages (S1-S15), including a summary (S1), 2 supporting sections (S2 and S3), 6 supporting Tables (Table S1-S6) and the references.

S1. Summary for SI

In this supporting information (SI), firstly, information used for performing the Life Cycle Assessment (LCA) in the present study is documented in section S2 and Table S1 – S4 . In section S2, the exclusion of emissions and environmental impacts associated with the feedstock production during calculating the life-cycle impact of caproic acid is explained. The detailed description for the caproic acid production system based on chain elongation was provided. In Table S1, information used for formulating the Life Cycle Inventory (LCI) of 1 kg caproic acid production from organic waste via chain elongation, which includes the process parameters, data sources and additional remarks/assumptions for each process involved in the life cycle. In Table S2, the information required for calculating the Life Cycle Impact Assessment (LCIA) of 1 kg caproic acid production from organic waste via chain elongation is documented. Note that the LCIA data derived from Ecoinvent 3.1 database was altered in some cases to fit the actual condition of the assessed system. An example is the CO₂ emission in the solid waste incineration in the Netherlands; in Ecoinvent 3.1, 65% of CO₂ emission from the incineration of solid waste is biogenic, and the rest 35% is non-biogenic by default. Considering the waste generated during the chain elongation process mostly resulted from the household kitchen, gardening waste and supermarket food waste, the CO₂ emission from the incineration of solid waste is modified into 100% biogenic. An additional note is that four internal reports (IR1 - 4) were used for completing the LCI. These are: IR1, 2014- Venegas- Chain elongation of propionic acid ; IR2, 2015- De Jong- Granulation in chain elongation; IR3, 2010- Kuiper- MCFA recovery from fermentation broth; IR4, 2014- Vermeer- Selective Extraction of MCFA. These IRs are not provided along with this paper. For accessing these IRs, please contact the corresponding author

for further information. Table S3 presents the overview of the comparison among the assessed cases, i.e. Case LO, Case LS and Case PS. Table S4 shows the cases and parameters used for sensitivity analysis.

Secondly, the SI for the results and discussion is provided in the section S3, Table S5 and Table S6 in this SI. In section S3, the discussion on the SA for the alternatives to extraction solvents and NaOH was elaborated. In Table S5, the SA result was documented in terms of life-cycle impact changes (in percentage) compared with the baseline cases. In Table S6, the data used for the discussion on the comparison of chain elongation to other bio-based waste management strategies, as well as the sources for this data, were provided.

S2. SI for methodology

S2.1 The exclusion of the feedstock emission and life-cycle impacts. The emissions and environmental impacts associated with the generation of mixed organic waste, which is used as feedstock, are not considered. The organic waste used in the present study is a low-grade mixed organic waste, and it exists regardless of whether the caproic acid would have been produced or not. The environmental impacts associated with the generation of the organic waste should, therefore, be allocated to the processes or products from which the waste is generated. In some cases, the environmental impacts are allocated to the waste if the waste is considered as a by-product; for example, glycerol as a by-product from biodiesel production¹. This study differs from these by-product cases as the organic waste used in the present study is low-grade waste with a mixed and complex composition that can hardly be considered as a by-product. However, in the future, when more and more waste-to-resource technologies are implemented specifically for mixed organic waste, mixed organic waste may have to be considered as a by-product, and part of the environmental impacts of the generation of mixed organic waste need to be allocated to these low-grade by-products.

S2.2 Detailed description for the caproic acid production system based on chain elongation. The assessed system consists of six main processes (see Figure 1 in the manuscript), which starts at the mixed organic waste and ends at the production of caproic acid. Two types of mixed organic waste were used for caproic acid production via chain elongation² including the organic fraction of municipal solid waste (OFMSW)³⁻⁵ and the supermarket food waste (SFW) from the food residue processing industry (unpublished data).

The mixed organic waste, i.e. OFMSW or SFW, firstly enters the biological acidification (BAc) process without any pretreatment. In BAc, an undefined mixed culture microbiome hydrolyses the organic solids into soluble organic matters and further degrades the soluble organic matters into basic building blocks like SCFAs, CO₂ and H₂. These basic building blocks are the essential substrates for the next process, chain elongation (CE). Two types of BAc were used in different cases depending on the water content of the organic waste. A dry anaerobic acidification was applied to OFMSW³, and a wet anaerobic acidification was applied to SFW. The effluent of BAc consists of the broth that enters CE and the solid residues that are disposed of. The disposed pellets together with other solid waste generated in Case LO and LS are assumed to be incinerated. In Case PS, according to ChainCraft B.V., anaerobic digestion was applied to recover energy from all solid residue generated during the life cycle of caproic acid production.

In CE, another undefined mixed culture microbiome elongates the SCFAs with the externally added ethanol into caproate. Corn-based bioethanol was used in CE, and the amount of ethanol dose required was derived from the existing literature⁶ (for Case LO) or the internal experimental data (for Case LS and PS). CO₂ was continuously supplied during the entire CE process to provide sufficient CO₂ that is required to sustain the microbial growth^{6, 7}. NaOH was continuously added to maintain an optimal pH for caproate production using an automated pH controller, as the lower pH could lead to product toxicity. The amount of NaOH required was estimated based on the amount needed to neutralise the pH of BAc effluent (from 5.3 to 7) and on the amount of proton formation during the caproate production and the microbial metabolism of *Clostridium kluyveri*, a known chain-elongating bacterium^{7, 8}. The effluent of CE contains about 12.6 g/L caproate, and the caproate yield is about 0.5g COD/gCOD_{waste+ethanol}⁶. Biogas is

produced during both BAc and CE, and currently the produced biogas is not collected for any application. Considering the origin of the feedstock, the CO₂ emission in the biogas during BAc and CE could be attributed to biogenic carbon emission that does not contribute to global warming. CH₄ emission during BAc and CE, on the other hand, is accounted as a Greenhouse Gas (GHG) emission.

The effluent of CE goes through downstream processes including the liquid-solid separation (LSS), the chemical acidification (CAc), the liquid-liquid extraction (LLEx) and the distillation (Ds). LSS is carried out using a centrifuge. The pellet is disposed as a solid waste, which enters the solid waste management (anaerobic digestion in Case PS and incineration in Case LO & LS). The supernatant enters CAc in which hydrochloric acid is added to lower the pH of the supernatant to 4.9, which was the pH used in previous study where LLEx was performed⁹. Low pH enhances the protonation of caproate into caproic acid which can be extracted. The extraction takes place by mixing the solvent with the effluent from CAc. During the mixing, part of the caproic acid transfers from the aqueous phase to the solvent phase. The fraction of the caproic acid entering the solvent phase is based on the distribution coefficient. Several extraction solvents were examined for their distribution coefficients in the literature, e.g. ethyl caproate⁹ and petroleum ether⁹. To our best knowledge, the life-cycle impact of both ethyl caproate and petroleum ether have not been reported so far. The life-cycle impact of ethyl acetate is used for simulating the life-cycle impact of ethyl caproate. Ethyl acetate itself was also used for extraction of propionic acid in a biorefinery system that is similar to the present study¹. After LLEx, the solvent phase is distilled to recover both the caproic acid in high purity and the reusable solvent, while the distillate enters the wastewater treatment system.

S3. SI for results and discussion

S3.1. Sensitivity analysis for the extraction solvent and the base. The use of mineral oil as the extraction solvent was investigated in internal experiments, which had a similar extraction performance as the ethyl caproate (data not shown). In SA, the use of mineral oil decreases all life-cycle impacts in all cases, except for the life-cycle AP in Case PS. Mineral oil is a by-product from oil refinery with a low economic value. Due to its low economic value, the life-cycle impacts allocated to mineral oil is low compared with other products produced from the oil refinery. This may be the reason why the use of mineral oil in chain elongation leads to a lower life-cycle impact. However, it should be kept in mind that mineral oil is still a fossil-based material which is considered as a non-renewable resource. Moreover, even in the case that mineral oil is used as the recovery solvent, the contribution of solvent use to the life-cycle impacts in Case LO and LS is still considerably high. The solvent recovery efficiency still has a higher influence on the environmental impact associated with the use of extraction solvent. The use of alternative data for NaOH reduced the overall life-cycle impacts in all cases and impact categories. Although it is difficult to identify the main cause for the lower life-cycle impacts of the alternative NaOH data¹⁰ compared with that from Ecoinvent 3.1¹⁰, the SA result implies that the baseline scenario in this study represents the worst-case scenario and the environmental impact from NaOH may be reduced.

Table S1. Overview of the parameters used in each process of the assessed system, i.e. gate-to-gate life cycle of caproic acid production from organic waste via chain elongation.

Process	Process parameters	Source
Biological Acidification (BAc)	Hydraulic Retention Time (HRT) = 7 days ^a	⁶ for Organic Fraction of Municipal Solid Waste (OFMSW) Internal experiment data for supermarket food waste (SFW; information from IR1 and IR2, which are available upon requests).
	Dilution factor = 0.6 L water/kg OFMSW or 0.8 L water/kg SFW ^b .	
	Yield (OFMSW) ^c = 0.04 gCOD _{SCFA} /gCOD _{Waste}	
	Yield (SFW) ^c = 0.2 gCOD _{SCFA} /gCOD _{waste}	
	CO ₂ produced = 5% of COD _{SCFA} ^d	
Chain Elongation (CE)	HRT = 11 hours	⁶ for OFMSW
	Yield(OFMSW) ^e = $\frac{\text{gCOD}_{\text{Caproate}}}{(\text{gCOD}_{\text{SCFA}} + \text{gCOD}_{\text{Ethanol}})}$	0.5
	Yield(SFW) ^e = $\frac{\text{gCOD}_{\text{Caproate}}}{(\text{gCOD}_{\text{SCFA}} + \text{gCOD}_{\text{Ethanol}})}$	0.5
	Require CO ₂ ^f = 4.60 ml per g COD _{Caproate}	
	Require NaOH ^g = 0.36 g per g COD _{Caproate}	
	CH ₄ produced = 2% of the total COD ^d	
Liquid-Solid Separation (LSS)	Total solids = 5 wt% of CE effluent, disposed.	Assumption.
Chemical Acidification (CAc)	HCl addition ^h = 0.75 ml HCl (37%; 12M) per g COD _{Caproate}	Based on calculation and assumption.
Liquid-Liquid Extraction (LLEx)	The caproic acid extraction efficiency ^l is defined as the ratio between the amount of caproic acid entering the solvent phase and the amount of caproic acid available in the aqueous phase before extraction, i.e. the fermentation broth, this is described as the formula	Steinbusch et al. 2010 ⁹ Internal experimental data (IR3 and IR4)

below:

$$\text{Extraction efficiency} = \text{HC}_{\text{Sol},f} / \text{HC}_{\text{ag},i}$$

where HC = the amount of caproic acid, Sol= solvent phase, aq = aqueous phase, f = final (after extraction), i = initial (before extraction).

The amount of solvent (V_{sol}) required for reaching a specific caproate extraction efficiency^h can be calculated as described below:

$$[\text{HC}]_{\text{Sol}} = D * [\text{HC}]_{\text{aq}}$$

where [HC] = Concentration of caproic acid, D = the distribution coefficient of a compound between two liquid phases. Assuming that no chemical reaction occurs during the extraction, and the total amount of caproic acid is a constant, the formula above can be further expanded as below:

$$\text{HC}_{\text{Sol},f} / V_{\text{sol}} = D * \text{HC}_{\text{aq},f} / V_{\text{aq}} = D * (\text{HC}_{\text{aq},i} - \text{HC}_{\text{Sol},f}) / V_{\text{aq}}$$

By reorganising this formula, the extraction efficiency can be expressed as below:

$$\text{Extraction efficiency} = \text{HC}_{\text{Sol},f} / \text{HC}_{\text{ag},i} = 1 / (1 + V_{\text{aq}} / V_{\text{sol}} / D)$$

As V_{aq} and D are known, the amount of solvent required for achieving a specific extraction efficiency can be calculated. Subsequently, the amount of caproic acid extracted into the solvent can also be calculated.

Diffusion coefficient of caproate between acidified CE broth (pH=5) and ethyl caproate is around 22, based on the previous study⁹.

Lab-scale process: 95 wt% solvent is reused; 5 wt% solvent is lost during extraction. Assumption.

Pilot-scale process: 99.5 wt% solvent is reused; 0.5 wt% solvent is lost during extraction.

Calculated based on the solubility of ethyl caproate (i.e. 0.629 g/L; <http://www.ymdb.ca/compounds/YMDB01381>, accessed on 22nd Sep 2016). In the pilot-scale system, all ethyl caproate is assumed to be recovered except for those dissolved, which is about 0.5 v/v% of the total solvent added. In the lab-scale system, the solvent loss is assumed to be 10 times higher than in the pilot-scale system, which is about 5 v/v% of the total solvent used.

Distillation (Ds)	Assume the caproic acid in the solvent phase was fully recovered.	Assumption
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Lab-scale process: 95 wt% solvent is reused; 5 wt% solvent is lost during distillation. Assumption

Pilot-scale process: 99.5 wt% solvent is reused; 0.5 wt% solvent is lost during distillation.

a. Longer HRT (21 days) was tried and resulted in 3 times higher VFA concentrations⁶. But considering the process feasibility, an HRT of 7 days is used in this LCA.

b. Dilution factors taken from the literature⁶ and the internal experiments. The former used dry anaerobic digestion and the later used wet anaerobic digestion. Moreover, the solid contents of OFMSW and SFW were different. The amounts of water addition for dilution is therefore subject to the feedstock used.

c. SCFAs include mainly acetate and butyrate. The yield was calculated from the experimental data from the literature⁶ and from the internal experiment.

d. The biogas composition was not specified in the literature where we took the process data from. In our internal data, the compositions of biogas produced during BAc and CE processes vary depending on the fermentation conditions applied. In this study, we assumed that around 5% of the total chemical oxidation demand (COD) of the short chain fatty acids (SCFAs) produced during BAc are converted into CH₄ eventually. We also assumed that the CH₄ formation during BAc is negligible due to the inhibition caused by the low pH. For the biogas produced during CE, there is hardly any CO₂ in the biogas, as the CO₂ supply was controlled at a minimal level and chain-elongating microorganisms consume CO₂ rapidly. For the CH₄ produced during CE, it was reported that, in a chain elongation bioreactor without applying a chemical inhibitor, the CH₄ production was only 2% of the total COD¹¹. Suppressing methanogens can be further enhanced by, for example, controlling the CO₂ feeding rate in CE.

Thus, we assumed that 1% of total COD was converted into CH₄.

e. $\text{COD}_{\text{Ethanol}} = [\text{Ethanol}] (19.3 \text{ g/L}) * 2.1 \text{ gCOD/gEthanol} = 40.5 \text{ gCOD/gEthanol.L}$. $\text{COD}_{\text{Caproate}} = [\text{Caproate}] (12.6 \text{ g/L}) * 1.9 \text{ gCOD/gCaproate} = 23.9 \text{ gCOD/gCaproate.L}$.

f. 240 ml gaseous CO₂ was fed into chain elongation bioreactor every day, and regarding the HRT for the chain elongation bioreactor (11 hours) around 52.23 gCOD caproate was produced per day⁶.

g. Based on the metabolism, 2 moles of protons are produced with the production of 220.4 gCOD caproate (1 mole)^{7, 8}. NaOH for neutralising the BAc effluent from pH 5.3 to 7 is also included, which is around 0.2 g/L BAc effluent without considering the buffer capacity of BAc effluent. NaOH required for stable the pH of the whole reactor is not included as we assume the reactor has certain pH-buffer capacity.

h. 1 mole of caproate requires 1 mole of HCl to be acidified into caproic acid, which means 4.5 ml HCl (1M) per g COD_{Caproate} is required for CAc. This number is multiplied by 2 to give sufficient protons to lower the pH of the solution (i.e. for other MCFAs but preferably not SCFAs) and to overcome the buffer capacity of the solution.

i. Extraction efficiency is limited by the distribution coefficient of the solvent used (concentration in solvent phase v.s. concentration in aqueous phase). For ethyl caproate this is assumed to be 22 when pH of the solution is around 4.9⁹.

Table S2. The overview of the activity, material and energy used as well as their purpose of use and data sources for calculating the LCIA in this study.

Activity/Material/Energy	Unit	Purpose of use	Comment/Data source (in Ecoinvent 3.1 or otherwise specified)
Solid waste management	per kg	Treat the solid residue from BAc, CE, LSS & Ds in Case LO and LS.	Municipal solid waste {NL} treatment of, incineration Alloc Def, U. The biogenic CO ₂ content in the total CO ₂ emission is set as 100% instead of 65% (the default value in Ecoinvent 3.1)
	per kg	Treat the solid residue from BAc, CE, LSS & Ds in Case PS, as ChainCraft advised.	Biowaste {RoW} market for Alloc Def, U
Wastewater treatment	per L	Treat the wastewater from LLEx & Ds.	Wastewater, from residence {RoW} treatment of, capacity 1.1E10l/year Alloc Def, U
Heat from natural gas	per MJ	Heat up bioreactors.	Heat, in chemical industry {RER} market for Alloc Def, U
Electricity	per MJ	For operation of apparatus and bioreactors.	Electricity, low voltage {NL} market for Alloc Def, U
Ethyl caproate	per kg	Extraction solvent in LLEx in all baseline cases.	Ethyl acetate {GLO} market for Alloc Def, U Use the data for ethyl acetate as a simulation due to the lack of data for ethyl caproate.
	per kg	For sensitivity analysis.	White mineral oil, at plant/RNA
Hydrochloric acid	per kg	Protonation of caproate into caproic acid.	Hydrochloric acid, without water, in 30% solution state {RER} market for Alloc Def, U
Carbon dioxide (Liquefied)	per kg	Essential substrate for supporting microbial growth	Carbon dioxide, liquid {RER} market for Alloc Def, U

		in CE.	
Sodium hydroxide (NaOH)	per kg	Base for neutralisation of pH in BAc and CE.	Neutralising agent, sodium hydroxide-equivalent {GLO} market for Alloc Def, U
	per kg	A more recent LCA study on NaOH (2013) for sensitivity analysis. The data from Ecoinvent 3.1 is published in 2007 with the process data collection before 2007.	Literature ¹⁰
Ethanol	per kg	Essential substrate for CE in all baseline cases.	Ethanol, without water, in 95% solution state, from fermentation {RoW} ethanol production from maize Alloc Def, U
	per kg	Sugarcane bioethanol for sensitivity analysis.	Ethanol, without water, in 95% solution state, from fermentation {BR} ethanol production from sugar cane Alloc Def, U
	per kg	Fossil-based ethanol for sensitivity analysis.	Ethanol, without water, in 99.7% solution state, from ethylene {RER} ethylene hydration Alloc Def, U
	per kg	Lignocellulosic bioethanol produced from grass via saccharification and simultaneous fermentation (SSF) for sensitivity analysis.	Ethanol, without water, in 95% solution state, from fermentation {CH} ethanol production from grass Alloc Def, U
Water	per kg	Dilution.	Water, deionised, from tap water, at user {GLO} market for Alloc Def, U

Table S3. The setup of the three cases assessed in the present study. L refers to lab-scale and P refers to pilot-scale. O refers to Organic Fraction of Municipal Solid Waste (OFMSW), and S refers to supermarket food waste (SFW).

	Case LO	Case LS	Case PS
Feedstock	OFMSW, 90% gardening waste + 10% kitchen food waste	SFW, 100% food waste from supermarket food processing chain	SFW, 100% food waste from supermarket food processing chain
BAc process	Dry anaerobic digestion	Wet anaerobic digestion	Wet anaerobic digestion
Solvent recovery efficiency	90%	90%	99%
Solid waste management	Incineration with heat recovery	Incineration with heat recovery	Anaerobic digestion with energy recovery

Table S4. Overview of the cases used in sensitivity analysis (SA) in this study and the description of the parameters used.

Cases/parameters	Description	Reference
Baseline case	The life-cycle impacts of the caproic acid production from organic waste in Case LO, LS and PS assessed in this study.	This study
Use of sugarcane bioethanol, Brazil	Alternative source for the bioethanol	Ecoinvent 3.1 (Ethanol, without water, in 95% solution state, from fermentation {BR} ethanol production from sugar cane Alloc Def, U)
Use of fossil-based ethanol, Europe [†]	Alternative source for the bioethanol	Ecoinvent 3.1 (Ethanol, without water, in 99.7% solution state, from ethylene {RER} ethylene hydration Alloc Def, U)
Use of lignocellulosic bioethanol (from grass), Europe	Alternative source for the bioethanol	Ecoinvent 3.1 (Ethanol, without water, in 95% solution state, from fermentation {CH} ethanol production from grass Alloc Def, U)
Precise control of ethanol dose during CE (50% ethanol dose reduction)	Assumption of the minimal ethanol does required for maintaining the same caproate production rate as in the baseline scenarios. The assumption is made based on the microbial reaction stoichiometry of <i>Clostridium kluyveri</i> converting acetate and ethanol to caproate..	Seedorf et al. 2008 ⁷
Mineral oil as the extraction solvent	Mineral oil was used in the internal experiments as an extraction solvent for caproic acid, which has a similar extraction performance to ethyl caproate. The LCI data was derived from Ecoinvent 3.1.	Internal experiments (IR3 and IR4). Ecoinvent 3.1 (White mineral oil, at plant/RNA)

NaOH alternative data	The use of a more recent LCI data for assessing the possible reduction on life-cycle impact of NaOH with the improved production process.	Thannimalay et al. 2013 ¹⁰
Reuse of LLEx effluent in BAc	The LLEx effluent contains trace amount of SCFAs and nutrients, which may be reused in BAc to replace de-ionised water used for diluting the feedstock (OFMSW and SFW). The influence of salt concentration in the LLEx effluent is not considered in this SA.	Assumptions
Use of biogas from BAc as the CO ₂ source to CE	The biogas produced during BAc contains mainly CO ₂ , which is sufficient to supply the CO ₂ required during CE. In this SA, biogas produced is fed back into CE to sustain the microbial growth. The infrastructure needed for carrying out this feeding process is not included in this SA.	Assumptions

[†]Excluding end-of-life emissions (e.g. CO₂ during combustion), which are usually for fossil ethanol considerably higher than for bio-ethanol depending on the applications.

Table S5. Overview of the results of the sensitivity analysis, presented in terms of the absolute values of the life cycle impacts in all cases and impact categories.

	Case LO			Case LS			Case PS		
	GWP	AP	EP	GWP	AP	EP	GWP	AP	EP
Baseline (kg CO ₂ /SO ₂ /PO ₄ ³⁻ eq per f.u.)	14.9	0.09	0.05	12.34	0.07	0.04	8.66	0.04	0.03
Use of sugarcane bioethanol, Brazil	12.97	0.08	0.05	10.89	0.07	0.04	7.21	0.04	0.03
Use of fossil-based ethanol, Europe [†]	14.08	0.07	0.05	11.72	0.06	0.03	8.03	0.03	0.03
Use of lignocellulosic bioethanol (from grass), Europe	13.38	0.09	0.05	11.20	0.07	0.04	7.52	0.05	0.03
Precise control of ethanol dose during CE (50% ethanol dose reduction)	13.18	0.07	0.05	10.73	0.06	0.03	7.05	0.03	0.03
Mineral oil as the extraction solvent	13.36	0.08	0.05	10.72	0.06	0.03	8.49	0.04	0.03
NaOH alternative data ¹⁰	14.20	0.08	0.05	11.81	0.06	0.03	8.13	0.04	0.03
Reuse of LLEx effluent in BA _C for diluting organic waste	14.71	0.08	0.05	12.32	0.07	0.04	8.64	0.04	0.03

Use of biogas produced during BAc as an alternative CO ₂ supply to CE	14.89	0.09	0.05	12.32	0.07	0.04	8.64	0.04	0.03
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[†]Excluding end-of-life emissions (e.g. CO₂ during combustion), which are usually for fossil ethanol considerably higher than for bio-ethanol depending on the applications.

Table S6. The comparison of the outcome of this study (Case PS) with other competing processes, namely the caproic acid from crude palm oil, the polyhydroxyalkanoate (PHA) production from wastewater via a mixed culture fermentation and the use of anaerobic digestion for treating OFMSW.

	GWP (unit)	AP (unit)	EP (unit)
Caproic acid produced via chain elongation (Case PS in this study)	8.7 kg CO ₂ -eq/f.u.	0.04 kg SO ₂ -eq/f.u.	0.03 kg PO ₄ ³⁻ -eq/f.u.
	or	or	or
	2.5 kg CO ₂ -eq/kg COD _{SFW}	0.01 SO ₂ -eq/kg COD _{SFW}	0.007 kg PO ₄ ³⁻ -eq/kg COD _{SFW}
Caproic acid produced via extraction from palm kernal oil ^a	0.23 kg CO ₂ -eq/f.u.	0.001 kg SO ₂ -eq/f.u.	0.001 kg PO ₄ ³⁻ -eq/f.u.
Polyhydroxyalkanoate production from a mixed wastewater via a mixed culture bioprocess ^{12,b}	20.4 kg CO ₂ -eq/kg PHA	-	-
	or		
	3.9 kg CO ₂ -eq/kg COD _{feed}		
Solid waste management via anaerobic digestion ^{13,c}	0.056 kg CO ₂ -eq/kg OFMSW treated	0.0003 kg SO ₂ -eq/kg OFMSW treated	-
	or	or	
	0.1 kg CO ₂ -eq/kg COD _{OFMSW}	0.0005 kg CO ₂ -eq/kg COD _{OFMSW}	

^aThis is the best-case estimation based on the known parameters. The life-cycle impacts of 1 tonne crude palm oil (CPO) production was derived from Stichnothe *et al.*, 2011¹⁴. For every 1 tonne CPO produced, around 100 kg palm kernel oil is produced (PKO)¹⁵. In PKO,

there is around 0.5% caproic acid in crude palm oil^{16, 17}. This means 1 tonne of crude palm oil can produce 0.5 kg of caproic acid, assuming a complete extraction. Using a mass-based allocation, the life-cycle impacts for caproic acid from crude palm oil can, therefore, be estimated. The downstream process was not included, as it is uncertain what process is employed for extraction of caproic acid from crude palm oil. The allocation method should also be further evaluated; for example, in the previous study on the life-cycle energy consumption for CPO production, 29% of energy consumption was allocated to PKO production¹⁸.

^bExclude the environmental benefits of the PHA itself.

^cHere the functional unit is per kilogram of organic waste treated.

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