

Supplementary information

Does Enzymatic Catalysis lead to more Sustainable Chemicals

Production? A Life Cycle Sustainability Assessment of Isopropyl

Palmitate

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A. Life Cycle Inventory – Ecoinvent inputs

Table S1 - Data used from the ecoinvent 3.9.1 database for modelling the background system

Flow	Ecoinvent data
Isopropyl Alcohol	Isopropanol {RER} market for Cut-off
Nitrogen blanketing reactor	Nitrogen, liquid {RER} market for Cut-off, U
Stripping steam	Steam, in chemical industry {RER} market for steam, in chemical industry Cut-off, U
Stripping nitrogen	Nitrogen, liquid {RER} market for nitrogen, liquid Cut-off, U
Filter aids (Perlite)	Perlite {GLO} market for perlite Cut-off, U
Filter aids (magnesium oxide)	Magnesium oxide {GLO} market for magnesium oxide Cut-off, U
Steam	Heat, central or small-scale, natural gas {Europe without Switzerland} heat and power co-generation, natural gas, 160 kW electrical, ...
Electricity consumption	Electricity, medium voltage {BE} market for Cut-off
Waste treatment	Hazardous waste, for incineration {Europe without Switzerland} treatment of hazardous waste, hazardous waste incineration Cut-off, U
NaOH 50%	Sodium hydroxide, without water, in 50% solution state
Methane Sulfonic Acid	Methane sulfonic acid {RER} production Cut-off, U

B. Life Cycle Inventory – Aggregated LCI

See document titled S2 Aggregated LCI

C. LCA – Uncertainty analysis

Table S2 - Results of the comparative uncertainty assessment between Enzymatic (Route A) and Chemical (Route A) Isopropyl Palmitate production for all environmental impact indicators under study. Confidence interval: 0.95.

Impact category	A >= B (%)	B > A (%)	Mean	Median	SD	CV	2.5%	97.5%	SEM
Acidification	100	0	1.82E-03	1.78E-03	3.18E-04	1.75E+01	1.30E-03	2.52E-03	3.18E-06
Climate change	100	0	7.42E-01	7.30E-01	1.04E-01	1.41E+01	5.67E-01	9.76E-01	1.04E-03
Ecotoxicity, freshwater - part 1	91.12	8.88	5.22E+00	5.14E+00	4.11E+00	7.88E+01	-2.99E+00	1.37E+01	4.11E-02
Eutrophication, freshwater	100	0	4.28E-05	3.63E-05	2.65E-05	6.20E+01	1.70E-05	1.07E-04	2.65E-07
Human toxicity, cancer	53.26	46.74	1.23E-10	1.25E-10	1.75E-09	1.42E+03	-3.38E-09	3.65E-09	1.75E-11
Land use	100	0	7.42E+00	6.91E+00	3.03E+00	4.09E+01	2.91E+00	1.47E+01	3.03E-02
Photochemical ozone formation	100	0	1.65E-03	1.62E-03	2.61E-04	1.59E+01	1.24E-03	2.25E-03	2.61E-06
Water use	54.78	45.22	4.38E-02	6.19E-02	5.43E-01	1.24E+03	-1.08E+00	1.09E+00	5.43E-03
CED	100	0	1.47E+01	1.44E+01	2.69E+00	1.83E+01	1.04E+01	2.09E+01	2.69E-02

D. Social LCA - Questionnaire

See document titled S3 Social LCA - questionnaire.pdf

E. Social LCA – Demographics stakeholder interviews

For the social life cycle assessment, 50 individuals residing at various distances from the industrial site in Ranst were interviewed, ranging from 50 m to 8 km away. The interviews utilised a semi-structured approach, incorporating open-ended questions to elicit specific information while allowing for additional inquiries based on the interviewees' responses (Mashuri et al., 2022)¹. Semi-structured interviews are commonly employed in the social sciences as an exploratory research method, guided by predetermined thematic frameworks (Magaldi and Berler, 2020)².

As illustrated in Figure S1, there was an equal distribution of male and female participants (48% and 52%, respectively). The majority (48%) fell within the age range of 30 to 60 years, with nearly half of the interviewees in the working age range. The highest proportion of interviews was conducted in Oelegem town, situated across the water facing the Oleon site. Other 25% were Oleon's direct neighbours, with some residing just across the street, while 35% lived at varying distances from the Oleon site in Broechem and Ranst.

¹ Mashuri, S., Sarib, M., Rasak, A., Alhabsyi, F., & Syam, H. (2022). Semi-structured Interview: A methodological reflection on the development of a qualitative research instrument in educational studies. *Journal of Research and Method in Education*, 12(1), 22-29.

² Magaldi, D., & Berler, M. (2020). Semi-structured interviews. *Encyclopedia of personality and individual differences*, 4825-4830.

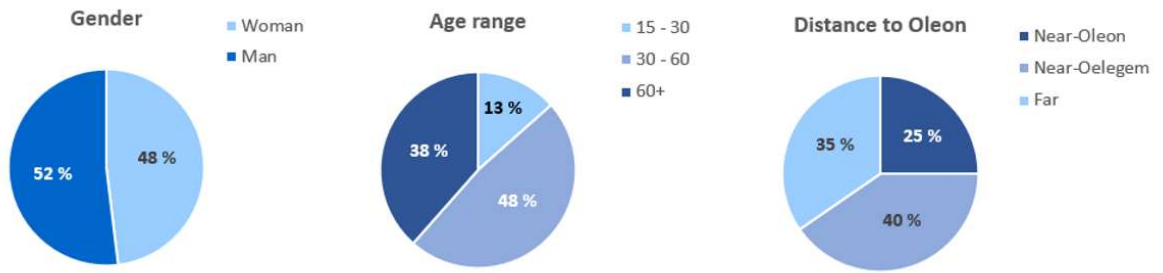


Figure S1 - Different demographic indicators of Interviewed people in Oelegem, Broechem and Ranst for the INCITE project.

F. Social LCA – Full results

Table S3 - Medium risk hours associated with producing 1 kg of IPP via the enzymatic route and the conventional chemical route. For reference, the share of direct and upstream social risks for producing chemicals (general) in Belgium are also listed.

Social impact (med risk hours)		
Impact category	IPP – Enzymatic Route	IPP – Chemical Route
Fair Salary	11.5	9.9
Industrial water depletion	8.2	7.6
Biomass consumption	9.0	8.4
Promoting social responsibility	1.5	1.1
Value added (total)	1.2	0.9
Public sector corruption	7.5	7.3
Trade unionism	7.2	6.9
Trafficking in persons	1.3	1.2
Illiteracy, female	1.2	1.1
Drinking water coverage	0.6	0.5
Child Labour, male	1.4	1.2
Illiteracy, total	0.6	0.5
Illiteracy, male	0.6	0.5
Violations of employment laws and regulations	0.8	0.7
Migration flows	0.3	0.2
Pollution	1.3	1.2
Certified environmental management system	0.4	0.3
Social security expenditures	6.7	6.6
Association and bargaining rights	1.2	1.1
Active involvement of enterprises in corruption and bribery	0.2	0.2
International migrant stock	0.3	0.3
Health expenditure	1.1	1.1
Sanitation coverage	0.3	0.2
Risk of conflicts	0.2	0.2
Youth illiteracy, female	0.1	0.1
Anti-competitive behaviour or violation of anti-trust and monopoly legislation	0.3	0.2
GHG Footprints	0.8	0.8
Women in the sectoral labour force	0.1	0.1
Minerals consumption	0.2	0.2
Child Labour, female	0.8	0.7
Child Labour, total	0.7	0.7
Safety measures	0.2	0.2
Contribution of the sector to economic development	0.1	0.1
Weekly hours of work per employee	0.1	0.1
Gender wage gap	0.7	0.7
Youth illiteracy, total	0.1	0.1
Workers affected by natural disasters	0.7	0.7
Youth illiteracy, male	0.1	0.1
Indigenous rights	0.1	0.1
Life expectancy at birth	0.0	0.0
Non-fatal accidents	0.0	0.0
Unemployment	0.0	0.0
Net migration	0.0	0.0
International migrant workers (in the sector/ site)	0.2	0.1
Embodied biodiversity footprints	0.5	0.5
Expenditures on education	0.0	0.0
DALYs due to indoor and outdoor air and water pollution	0.0	0.0
Goods produced by forced labour	0.1	0.1
Men in the sectoral labour force	0.0	0.0
Fatal accidents	0.0	0.0
Frequency of forced labour	0.0	0.0
Embodied water footprints	0.0	0.0
Fossil fuel consumption	0.0	0.0
Embodied agricultural area footprints	0.1	0.1
Embodied forest area footprints	0.0	0.0
Total	70.6	64.8