Title: Comparative life cycle sustainability assessment of chemical and enzymatic production: the case of isopropyl palmitate

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Abstract:

INnovative **C**hemoenzymatic **I**n**TE**grated processes (INCITE) is an EU H2020 project seeking to demonstrate the use of flow chemistry and membrane technology in enzymatic processes. A first demonstration case in INCITE deals with the solvent-free synthesis of natural oleochemical esters utilizing lipase enzymes, which has applications in food/feed, personal care and crop protection. OLEON N.V, a leading oleochemical company, selected the commonly used cosmetic emollient "Isopropyl palmitate" (IPP) for this case. IPP is synthesized by esterifying palmitic acid with isopropyl alcohol. In the current industrial process, this is done at high temperatures using an acid catalyst. The conventional process is characterized by a low alcohol efficiency, as IPA is constantly evaporating out of the reactor vessel. After the reaction, the acid catalyst has to be neutralized and removed and a distillation step is needed to remove any impurities and degradation products caused by the high temperatures, limiting the overall yield. In this study, the sustainability profile of the novel enzymatic IPP production is investigated and compared to conventional chemical IPP production.

For this purpose, a goal and scope guideline for applying life cycle sustainability assessment (LCSA) to enzymatic processes was developed via an extensive bibliographic review. Based on this review, the functional unit was defined as 1 kg of end product, e.g., IPP, produced via chemical or chemo-enzymatic production with the same functionality and specifications. The system boundaries for the case study consist of the production of IPP, where a cradle-to-gate analysis (excluding use and disposal of this product), including enzyme production, was recommended and implemented. As foreground data, mass and energy balances collected at Oleon's production site were used. Background data, e.g., electricity production, was primarily taken from the Ecoinvent database version v3.8.

Following the proposed guidelines from the European Commission, the Environmental Footprint (EF) v 3.0 method was applied for Life Cycle Assessment (LCA). This method provides a default list of 16 different impact categories, from which climate change, photochemical ozone formation, acidification, freshwater eutrophication, ecotoxicity, and human toxicity were chosen according to the recommendations from the Life Cycle Metrics for Chemicals Products. Apart from the emission-based indicators, land use and water use as well as the direct and indirect energy use were analyzed. The Reference Scale Assessment is currently the most feasible and applicable approach for assessing potential social impacts and is also adopted by the Social Life Cycle Metrics for Chemical Products; therefore, this approach was selected and applied for assessing social sustainability. Economic performance was assessed via techno-economic assessment (TEA), however, TEA results are not included due to confidentiality.