Maastricht University

AMI Biobased Materials

ROBOX

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Faculty of Science and Engineering, Department of Biobased Materials

A prospective life-cycle assessment (LCA) of monomer synthesis: comparison of biocatalytic and oxidative chemistry

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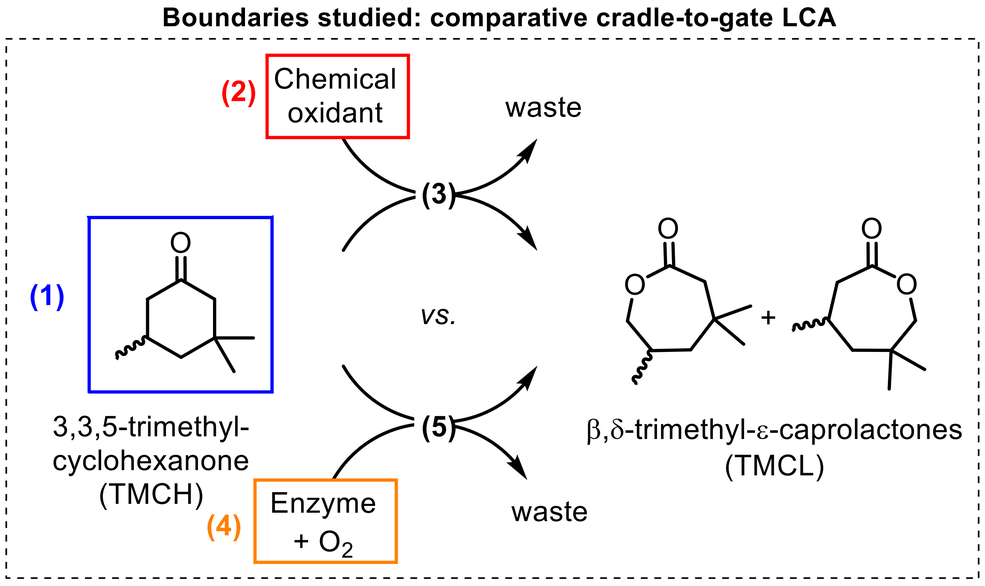
1 Introduction

Biotechnological proccesses are typically perceived as being greener than chemical processes. But is it really the case?

- A comparative life-cycle assessment (LCA) was performed to provide a **quantitative answer**.
- This LCA is **prospective** since the process is at an early stage, and is based on laboratory scale data.[1,2]
- This LCA compares two oxidative synthesis routes to lactones: a biocatalyzed route using a Baeyer-Villiger monooxygenase and a chemical route using an organic peracid.

Boundaries studied: comparative cradle-to-gate LCA

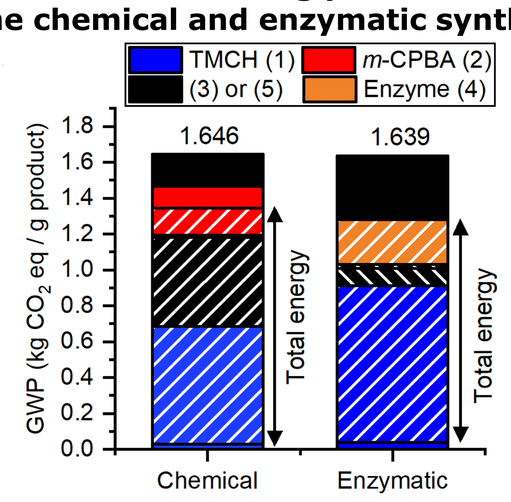


2 LCA methodology

- Function: **synthesize and purify 1 g of TMCL product**
- Boundaries: **cradle-to-gate**, comprising the synthesis of the substrate TMCH (1), the preparation of the chemical oxidant *m*-CPBA (2), the preparation of the enzymes (4), the chemical oxidation (3), and the enzymatic oxidation (5)
- Endpoint category: carbon emissions (climate change) converted in CO_2 equivalents with the global warming potential factor (GWP).

3 Results of the main scenario

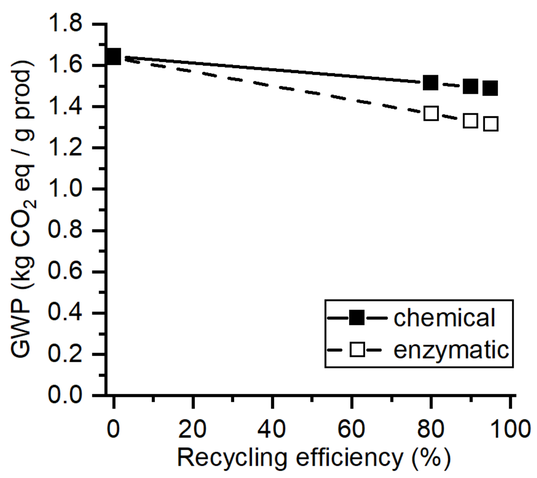
Global warming potential of the chemical and enzymatic syntheses



No significant differences between biocatalysis and chemical oxidation with *m*-CPBA. The energy consumption is the largest contributor: this is typical of laboratory scale LCA.

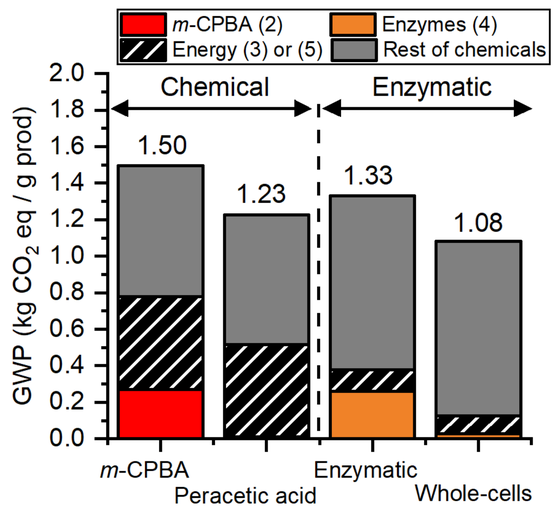
4 Sensitivity analysis: what-if scenarios?

Recycling of solvent streams



Solvents are used as reaction medium (dichlomethane in the chemical synthesis) and in the downstream processing (ethyl acetate for the enzymatic synthesis)

Recycling of enzymes & replacement of chemical oxidant

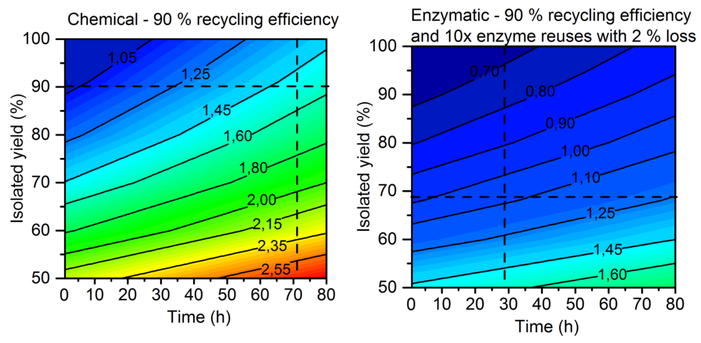


Hypothesis for enzyme recycling: 10 re-uses with 2% enzymatic activity loss.[3]

Enzymes as re-used as whole-cells
→ simplified enzyme preparation procedure

Key process performance metrics

GWP as a function of the isolated yield and the reaction time



Isolated yield → amount of substrate needed
Reaction time → electricity consumption

The environmental impact of the chemical reaction is mostly dependent on the reaction time while recycling of solvents and enzyme is crucial for the enzymatic reaction

5 Conclusions

- ✓ At laboratory scale, the enzymatic and chemical synthesis of TMCL have very similar environmental impacts. The enzymatic reaction is however greener if recycling of solvents and enzymes is implemented.
- ✓ Prospective LCAs based on laboratory scale data can be used as a tool for the improvement of enzymatic reactions.
- ✓ LCA can support the development of greener processes by targeting key process metrics influencing their environmental impact.

References

[1] M. A. F. Delgove, J. Luchies, I. Wauters, G. G. P. Deroover, S. M. A. De Wildeman, K. V. Bernaerts, *Polym. Chem.* **2017**, *8*, 4696-4706
[2] M. A.F. Delgove, M. Elford, K. V. Bernaerts, S.M.A. De Wildeman, *OPRD* **2018**, *22*, 803-812
[3] M. A. F Delgove, D. Valencia, J. Solé, K.V. Bernaerts, S.M.A. De Wildeman, M. Guillén, G. Álvaro, *Applied Catalysis A: General* **2019,** *572*, 134-141

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