CHEMISTRY & SUSTAINABILITY
CHEMSUSCHEM
ENERGY & MATERIALS

Supporting Information

A Prospective Life Cycle Assessment (LCA) of Monomer Synthesis: Comparison of Biocatalytic and Oxidative Chemistry

Marie A. F. Delgove,[a] Achille-B. Laurent,[a] John M. Woodley,[b] Stefaan M. A. De Wildeman,*[a] Katrien V. Bernaerts,[a] and Yvonne van der Meer[a]

cssc_201900007_sm_miscellaneous_information.pdf

Content of the supplementary information:

Table S1. Details of the electricity consumption for each synthesis step.

Synthesis	Operation	Electricity consumption
(1) Synthesis of TMCH	Stirring of the reaction	2.002 kWh
	Reaction under pressure in autoclave	0.002 kWh
(2) Synthesis of *m*-CPBA	Stirring and heating	0.606 kWh
	Removal of solvent by rotary evaporation	0.018 kWh
(3) Chemical synthesis of TMCL	Stirring of the reaction	E_1 = 17.150 kWh
	Filtration of side-product with a vacuum pump	E_2 = 0.017 kWh
	Removal of solvent by rotary evaporation	E_3 = 0.399 kWh
(4) Preparation of enzymes	Pre-incubation	E_1'' = 3.154 kWh
	Incubation	E_2'' = 2.456 kWh
	Cell separation by centrifugation	E_3'' = 0.277 kWh
	Cell sonication	E_4''= 0.007 kWh
	Enzyme separation by centrifugation	E_5''= 0.832 kWh
(5) Enzymatic synthesis of TMCL	Temperature and pH control, stirring of the reaction, continuous addition of substrate	E_1' = 2.575 kWh
	Removal of solvent by rotary evaporation	E_2' = 0.083 kWh
	Removal of protein by centrifugation	E_3' = 0.443 kWh
	Removal of solvent by rotary evaporation	E_4' = 0.083 kWh E_5' = 0.018 kWh
	Enzyme separation by ultrafiltration[1]	E_6' = 0.011 kWh

Table S2. Pedigree matrix.

For all chemicals, the following pedigree matrix was applied (basic uncertainty of 1.07):

Category	**Description**
Reliability	Qualified estimate
Completeness	Representative data from only one site relevant to the market considered
Temporal correlation	Age of data unknown or more than 15 years of difference to the time period of the dataset
Geographical correlation	Average data from larger area in which area under study is included
Further technological correlation	Data on related processes on laboratory scale or from different technology
Sample size	Unknown

For the enzyme production from potato starch which is from the *Ecoinvent* database, the following pedigree matrix was applied (basic uncertainty of 1.5):

Category	**Description**
Reliability	Verified data based on measurements
Completeness	Representativeness unknown or data from a small number of sites and from shorter periods
Temporal correlation	Age of data unknown or more than 15 years of difference to the time period of the dataset
Geographical correlation	Average data from larger area in which area under study is included
Further technological correlation	Data on related processes on laboratory scale or from different technology
Sample size	Unknown

Table S3. Impact category values and uncertainty values for the chemical and enzymatic syntheses.

		Chemical synthesis				Enzymatic synthesis			
		Impact	SD	2.5th percentile	97.5th percentile	Impact	SD	2.5th percentile	97.5th percentile
Ecosystem quality	$PDF.m^{-2}.yr^{-1}$	0.28	0.12	0.13	0.58	0.30	0.15	0.13	0.65
Human health	DALY	$1.20.10^{-6}$	$3.91.10^{-7}$	$6.42.10^{-7}$	$2.30.10^{-6}$	$1.17.10^{-6}$	$5.00.10^{-7}$	$5.47.10^{-7}$	$2.25.10^{-6}$
Resources	MJ primary	32.47	12.69	15.73	66.99	36.35	16.68	16.63	76.71
Global warming	kg CO_2 eq	1.646	0.59	0.83	3.30	1.639	0.67	0.78	3.34

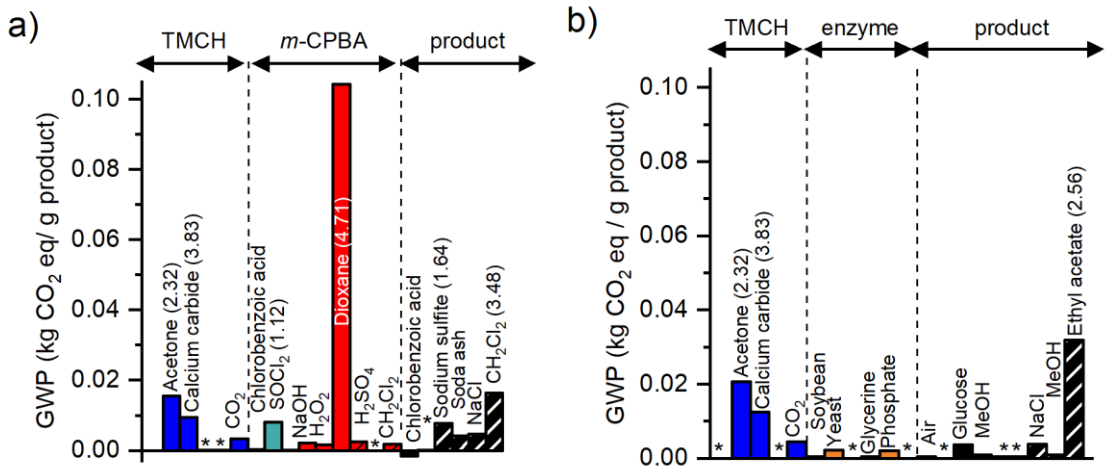

Figure S1. Contribution of chemicals to the GWP of the synthesis of the product when no recycling of chemicals is considered with a) chemical synthesis, and b) the enzymatic synthesis. Stripes indicate chemicals used for downstream processing. Stars indicate chemicals with negligible contributions. The values in parentheses indicate the global warming potential of the synthesis of 1 kg of the chemicals with the largest contributions (as expressed in kg CO_2 eq / kg product).

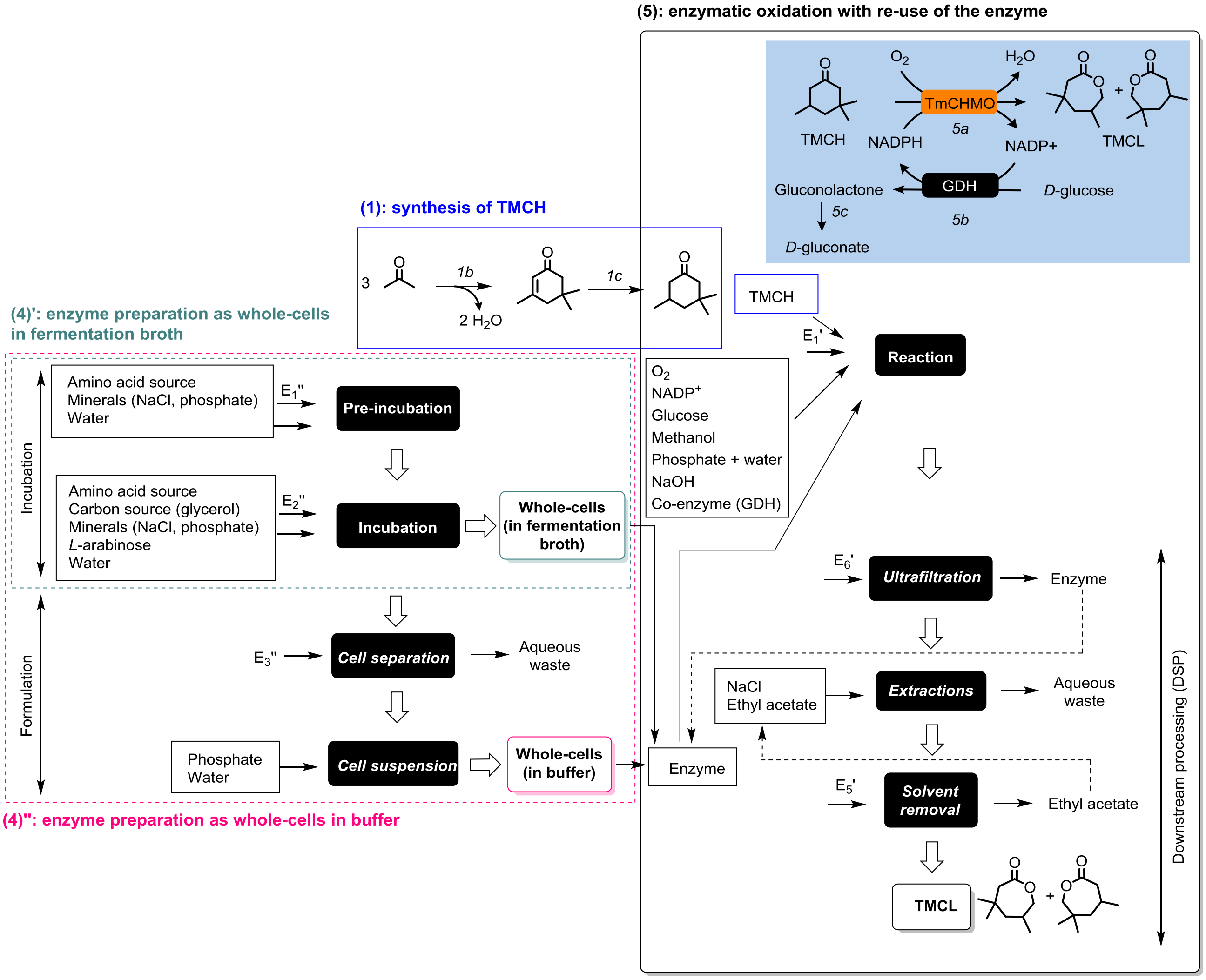

Figure S2. Alternative process flowsheet for the enzymatic synthesis of the product TMCL with recycling of the enzyme with (4)’ whole-cells in fermentation broth (in green), and (4)’’ whole-cells in buffer (in pink). See Table 2 for the details of the electricity consumptions. Dotted arrows indicate recycling streams.

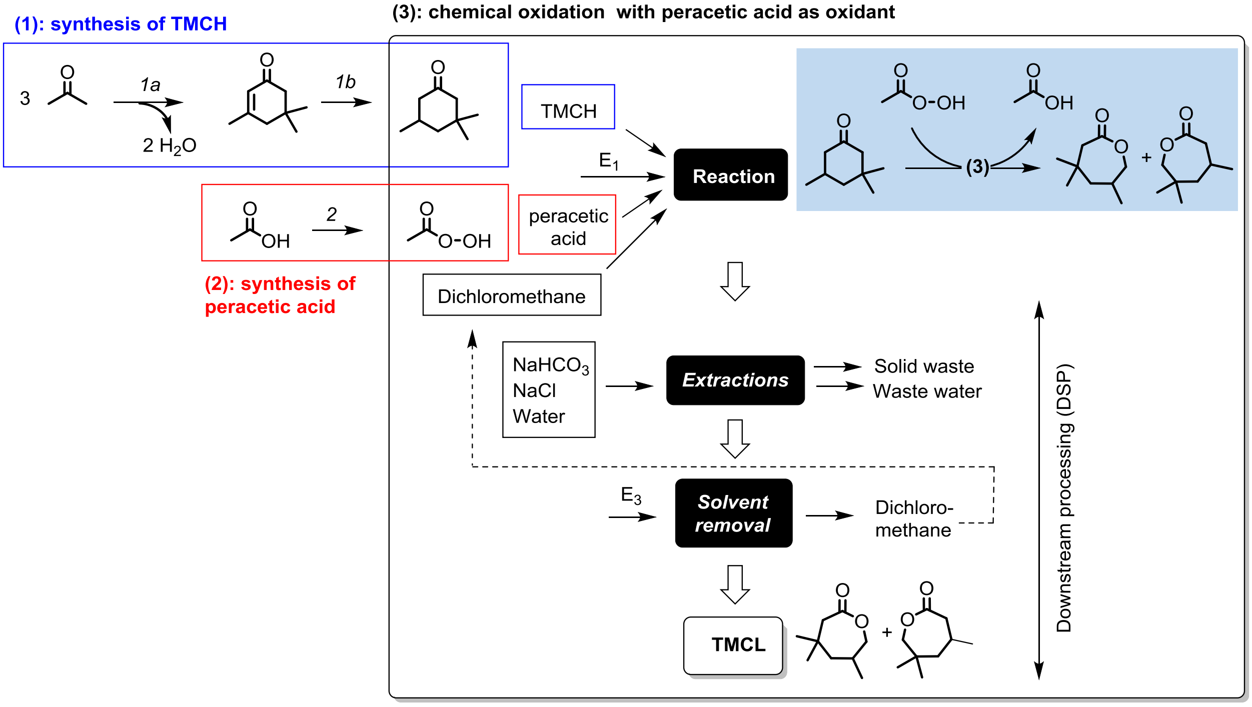

Figure S3. Alternative process flowsheet for the chemical synthesis of the product TMCL using peracetic acid as oxidant. See Table S1 for the details of the electricity consumptions. Dotted arrows indicate recycling streams.

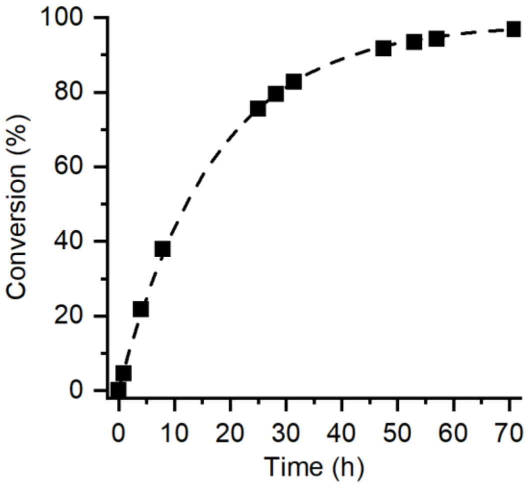

Figure S4. Conversion of the enzymatic reaction followed by GC-FID (the measurements were performed as described in reference [2]). Reaction conditions: 2 equivalents *m*-CPBA, [substrate] = 0.2 M in dichloromethane, room temperature.

References

[1] A. Bahnasawy, M. Shenana, *Australian Journal of Agricultural Engineering* **2010**, *1*, 54.

[2] M. Delgove, M. Elford, K. Bernaerts, S. De Wildeman, *Organic Process Research & Development* **2018**, *22*, 803-812.