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Electronic Supplementary Information (ESI) for:

Life cycle assessment of polyols for polyurethane production using CO_2 as feedstock: insights from an industrial case study

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1 Potential differences in downstream processes

Polyurethane production. The viscosity of polyols increases exponentially with the CO_2 content.[1] An increased viscosity might require extra or stronger pumps in polyurethane processing. However, Langanke *et al.* report that CO_2-based polyols were "readily processed with standard equipment used in industry for the preparation of polyurethane foams."[1]

For production of polyurethanes from polyol blends, an extra storage tank for CO_2-based polyols will become necessary.

Polyurethane use. Polyurethane flexible foams from CO_2-based polyols provide similar properties as flexible foams from conventional polyols according to the same recipe.[1] Some properties of CO_2-based foams are even expected to be superior to conventional foams.[2] The enhanced properties might allow for a reduced material demand or longer product lifetime. However, these expectations still have to be verified.

Polyurethane end-of-life treatment. End-of-life treatment of polyurethanes depends on the polyurethane application. As first application, polyurethane foams for mattresses are projected. Due to sanitary restrictions, mattresses are incinerated and thermal energy is recovered. With increasing CO_2 content, the heat of combustion of polyurethanes decreases. Therefore, CO_2-based mattresses reduce the recovered energy in thermal utilization. For polyols with 20 wt% CO_2, the heat of combustion is lowered by about 12 %.[2] The reduced heat of combustion is also considered as appreciated safety feature for polyurethanes (*cf. polyurethane use*).

2 LCA data sources

The following table contains used datasets from GaBi LCA database.[3]

Process	Name of dataset	Year	Country
CO_2 source / electricity generation			
Lignite	Lignite mix	2010	DE
CO_2 capture solvent	Monoethanolamine*	2010	RER
Water for CO_2 cleaning	Tap water; water purification treatment; production mix, at plant; from surface water	2012	EU-27
CO_2 transport by truck	Truck; diesel driven, Euro 4, cargo; technology mix; 28-32t gross weight/ 22t payload capacity	2012	GLO
Fuel for truck	Diesel mix at refinery; 10 ppm sulphur, 5.75 wt.% bio components	2010	DE
Electricity compensation			
Grid mix	Electricity grid mix; AC, technology mix; consumption mix, at consumer; <1kV	2010	DE
CO_2 utilization / polyol production			
Propylene oxide (CHPO)	Propylene oxide (Chlorohydrin process with Cell Liquor)	2012	DE
Propylene oxide (CHPO)	Propylene oxide (Chlorohydrin process with $Ca(OH)_2$)	2012	DE
Propylene oxide (PO/TBA; PO/MTBE)	Propylene oxide (Oxirane process); by-product *t*-butanol	2012	DE
Ethylene oxide	Ethylene oxide (EO) via O_2/methane	2012	DE
Glycerol	Glycerine (from Epichlorohydrine)	2012	DE
Steam	Process steam from natural gas 90%; 90% efficiency	2010	DE
Compressed air	Compressed air; 7 bar, low efficiency	2010	EU-27
Process water	Process water; ion exchange; production mix, at plant; from groundwater	2012	EU-27
Nitrogen	Nitrogen, via cryogenic air separation	2012	EU-27
Electricity	Electricity grid mix; AC, technology mix; consumption mix, at consumer; <1kV	2010	DE

* LCA data for monoethanolamine as proxy for amine-based solvent were taken from ecoinvent v2.01 database as integrated in GaBi software.

3 Alternative allocation options for cyclic propylene carbonate (cPC)

In the main article, the allocation procedure for cPC is based on different criteria: feedstocks (PO, CO_2 and glycerin) are allocated according to the feedstock masses incorporated in polyols and cPC, respectively. For example, glycerin is only incorporated into polyols and therefore fully assigned to the polyols. The catalyst is also fully assigned to the polyols. Other inputs (utilities such as steam and electricity) are allocated according to polyol and cPC masses.

The effect of alternative allocation options for cPC is assessed (Figure S1):

- Mass allocation
- Economic allocation (assumed prices are 1.90 € / kg polyols and 1.20 € / kg cPC)
- 100 % allocation to polyols (worst-case allocation for polyols)

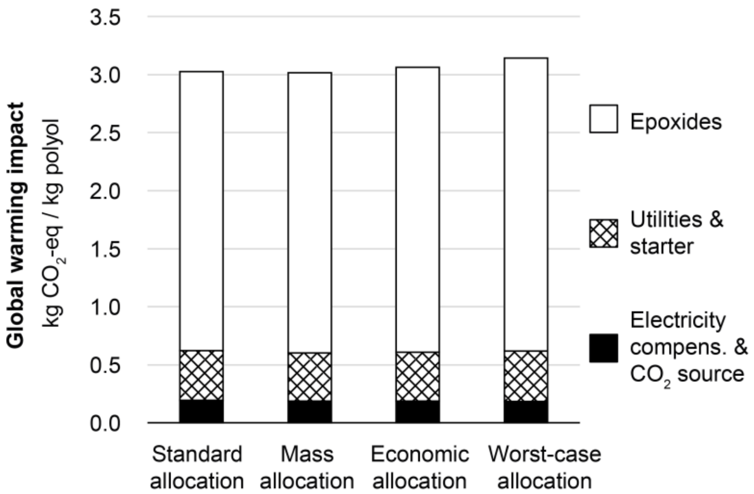

Figure S1 Global warming impact for polyethercarbonate polyols with 20 wt% CO_2 for alternative allocation options for the by-product cPC: left to right: standard allocation, mass allocation, economic allocation and worst-case allocation. The global warming impacts for alternative allocation options change by only −0.3 % (mass allocation) to +3.8 % (worst case allocation) compared to standard allocation.

4 Midpoint LCA results for the benchmark system and the CCU system

In addition to impact on global warming and fossil resource depletion, we analyzed other impact categories. The following figures show midpoint LCA results for (freshwater and marine) eutrophication, ionizing radiation, ozone depletion, particulate matter formation, photochemical oxidant formation, and terrestrial acidification using ReCiPe 1.08 (Hierachist) methodology.[4]

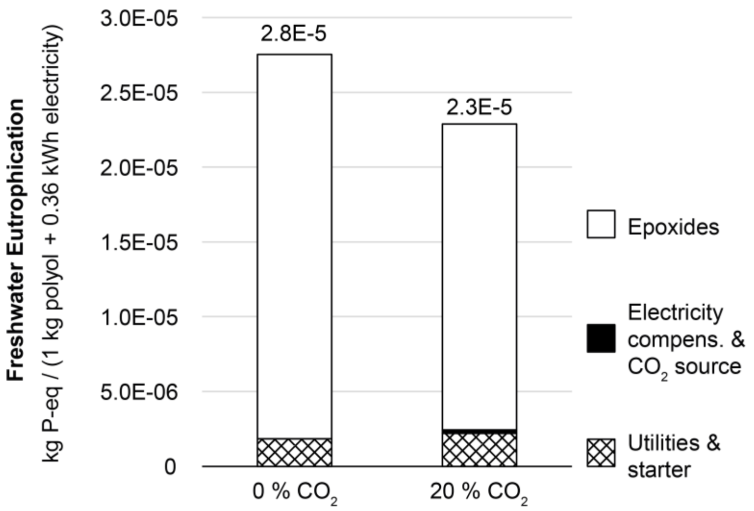

Figure S2 Freshwater eutrophication in kg P-equivalents for product system of conventional polyether polyols (0 % CO_2, left) and CO_2-based polyethercarbonate polyols (20 % CO_2, right).

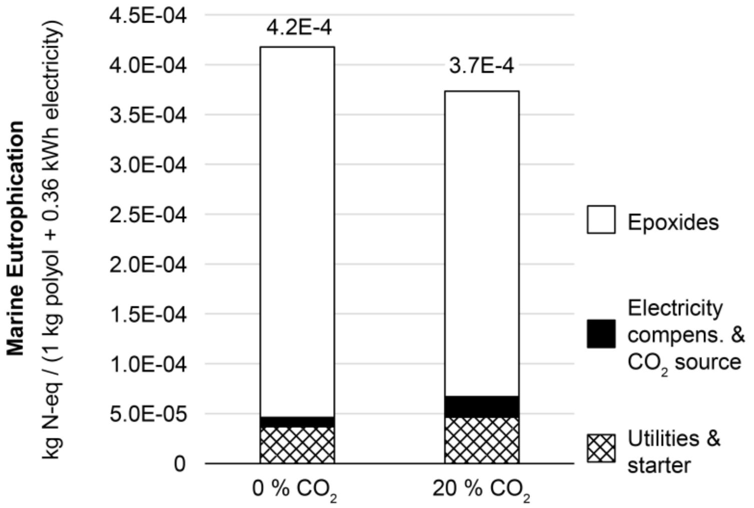

Figure S3 Marine eutrophication in kg N-equivalents for product system of conventional polyether polyols (0 % CO_2, left) and CO_2-based polyethercarbonate polyols (20 % CO_2, right).

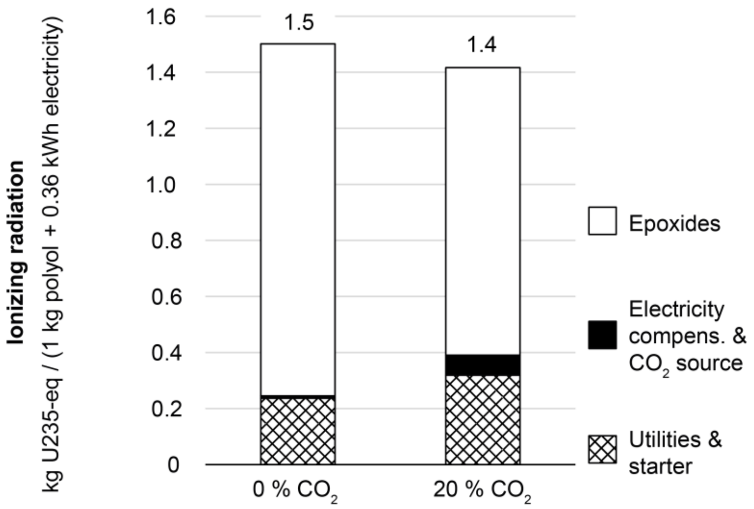

Figure S4 Ionizing radiation in kg U235-equivalents for product system of conventional polyether polyols (0 % CO_2, left) and CO_2-based polyethercarbonate polyols (20 % CO_2, right).

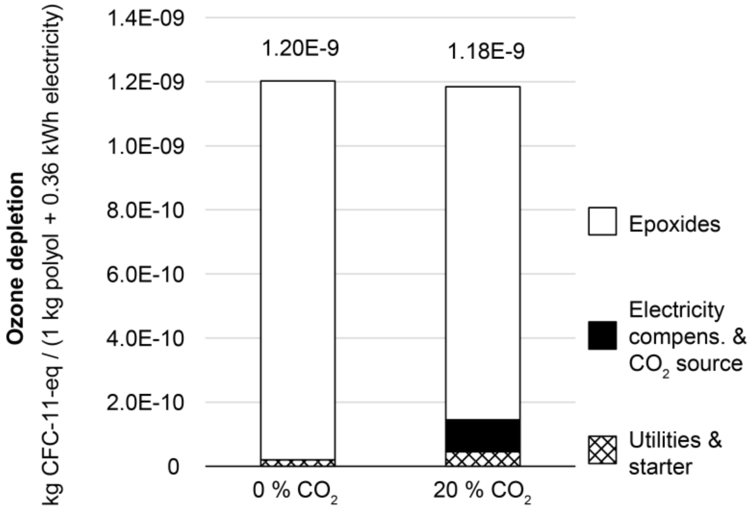

Figure S5 Ozone depletion in kg CFC-11-equivalents for product system of conventional polyether polyols (0 % CO_2, left) and CO_2-based polyethercarbonate polyols (20 % CO_2, right).

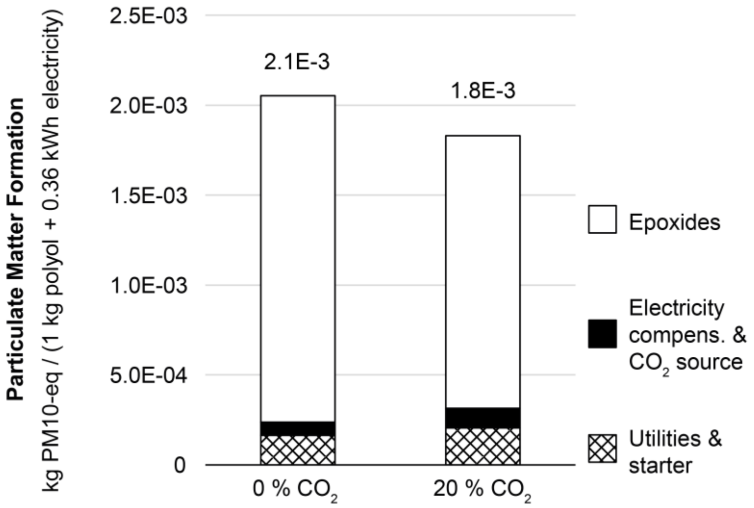

Figure S6 Particulate matter formation in kg PM1011-equivalents for product system of conventional polyether polyols (0 % CO_2, left) and CO_2-based polyethercarbonate polyols (20 % CO_2, right).

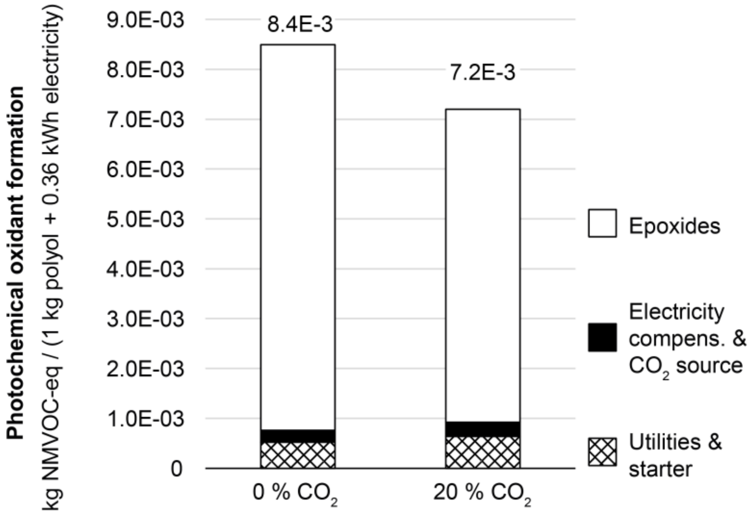

Figure S7 Photochemical oxidant formation ("summer smog") in kg NMVOC-equivalents for product system of conventional polyether polyols (0 % CO_2, left) and CO_2-based polyethercarbonate polyols (20 % CO_2, right).

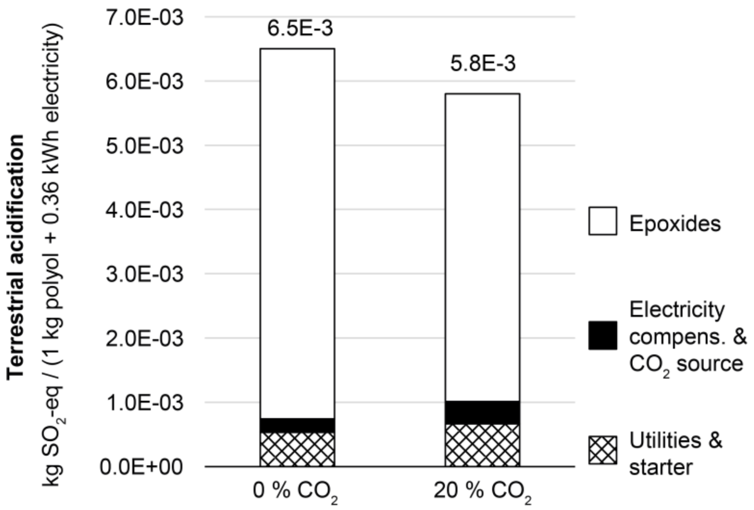

Figure S8 Terrestrial acidification in kg SO_2-equivalents for product system of conventional polyether polyols (0 % CO_2, left) and CO_2-based polyethercarbonate polyols (20 % CO_2, right).

Figures 3 and 5 in the main article and Figures S2 – S8 in this document show how the benchmark system (polyols with 0 wt% CO_2) and the CCU system (polyols with 20 wt% CO_2) perform in different environmental impact categories.

To compare these different categories, one approach is normalization. Normalization can be achieved by dividing the environmental impacts (e.g. in kg CO_2-eq, kg oil-eq etc. per functional unit) by average per-capita emissions (e.g. in kg CO_2-eq/(person-eq · year)) to obtain impact results in a common unit ((person-eq · year) per functional unit). Figure S9 shows normalized midpoint impact category results for the benchmark and the CCU system using average per-capita emissions in Europe.

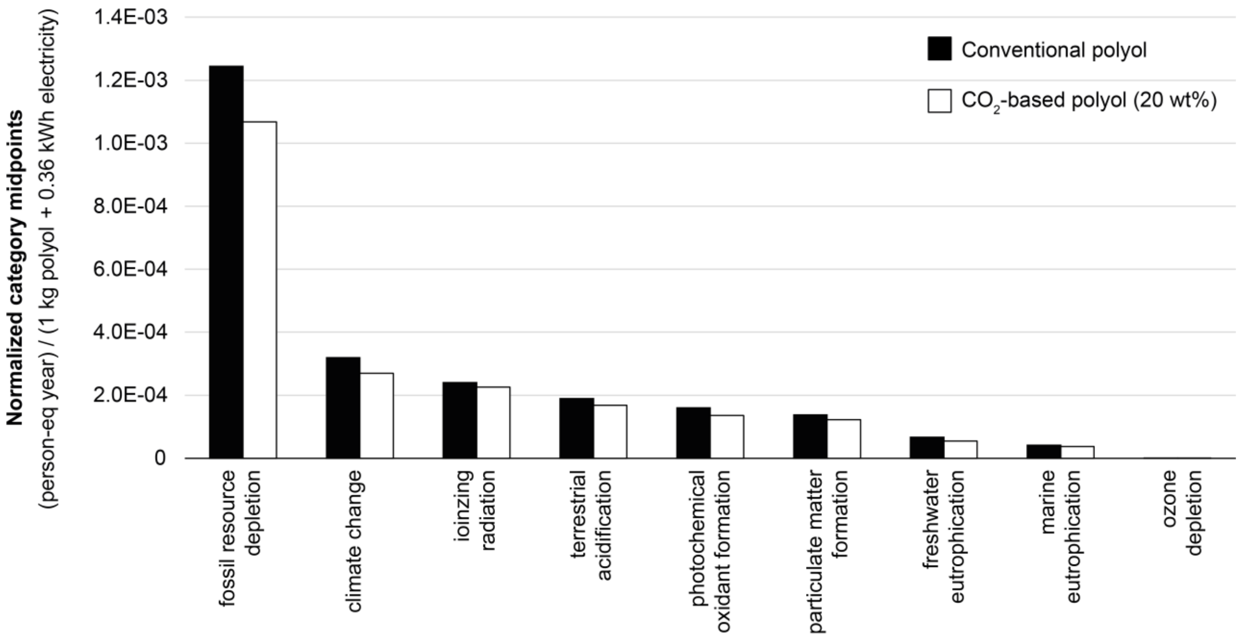

Figure S9 Normalized midpoint impact categories for product system of conventional polyether polyols (0 % CO_2, left) and CO_2-based polyethercarbonate polyols (20 % CO_2, right) using ReCiPe 1.08 normalization data for Europe. In normalization, initial midpoint results are divided by average European emissions per capita. According to this normalization procedure, fossil resource depletion can be considered as most important environmental impact category for polyol production.

ESI References

1 J. Langanke, A. Wolf, J. Hofmann, K. Böhm, M. A. Subhani, T. E. Müller, W. Leitner and C. Gürtler, *Green Chem.*, 2014, **16**, 1865–1870.

2 Bayer Material Science, *Personal communication*, 2014.

3 PE International, *GaBi LCA Software and LCA Databases*, 2012, http://www.gabi-software.com/databases/gabi-databases/.

4 M. Goedkoop, R. Heijungs, M. Huijbregts, A. D. Schryver, J. Struijs and R. V. Zelm, *ReCiPe 2008, A life cycle impact assessment method which comprises harmonised category indicators at the midpoint and the endpoint level; First edition (version 1.08) Report I: Characterisation*, 2013, http://www.lcia-recipe.net.