Electronic Supplementary Information

Towards sustainable Elastomers from CO_2: Life Cycle Assessment of Carbon Capture and Utilization for Rubbers

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S1 Table of used LCA datasets

Table 1: Life cycle inventory data collected from literature.

Process	Data source
CO_2 source	Ecoinvent[1] and Farla et. al (1999)[2]
Polyol production energy and utility demands	Von der Assen et. al (2013)[3]
DMC catalyst production	Von der Assen et. al (2013)[3]
HNBR production	Own calculations based on Happ et al.[4]
Polyol production and chain extension	Pilot plant datasets

Table 2: Datasets used from the GABI database.[5]

Product	Name of dataset	Country
Maleic anhydride	DE: Maleic anhydride ts	DE
Propylene glycol	DE: Propylene glycol ts	DE
Hexamethylene diisocyanate (HDI)	DE: Hexamethylene diisocyanate (HMDI) by-product HCl ts	DE
Process water	EU-27: Process water ts	EU-27
Electricity	DE: Electricity grid mix ts	DE
Compressed air	EU-27: Compressed air ts	EU-27
Nitrogen	EU-27: Nitrogen ts	EU-27
Process steam	EU-27: Process steam from natural gas 90% ts	EU-27
Waste water treatment	EU-27: Waste water treatment	EU-27
NBR	DE: Nitrile butadiene rubber (NBR, 33% acrylonitrile) ts	DE
EPDM	DE: Ethylene Propylene Diene Rubber (EPDM) ts	DE
CR	DE: Chloroprene ts	DE

S2 Elementary composition of CO_2-based and conventional rubbers

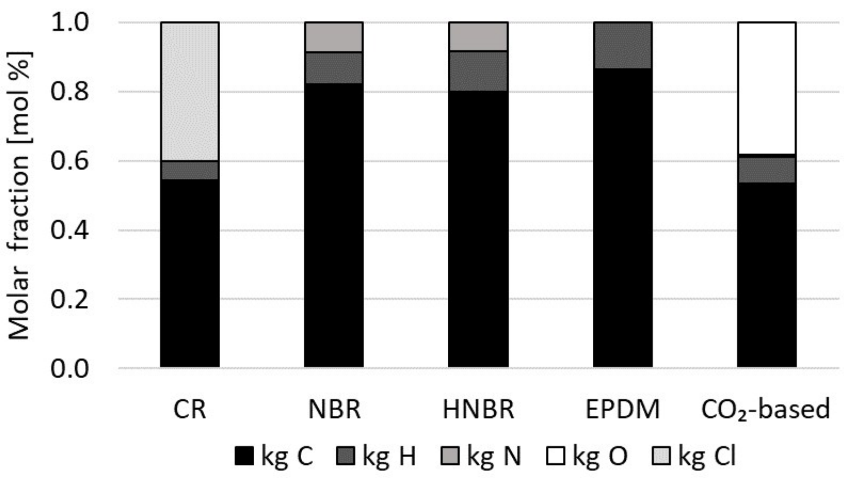

Figure S1: Composition of CO_2-based and 4 conventional rubbers: hydrated nitrile butadiene rubber (HNBR), nitrile butadiene rubber (NBR), ethylene propylene diene rubber (EPDM) and polychloroprene (CR).

S3 Midpoint LCA results for conventional and CO_2-based rubbers

S3.1 Freshwater eutrophication

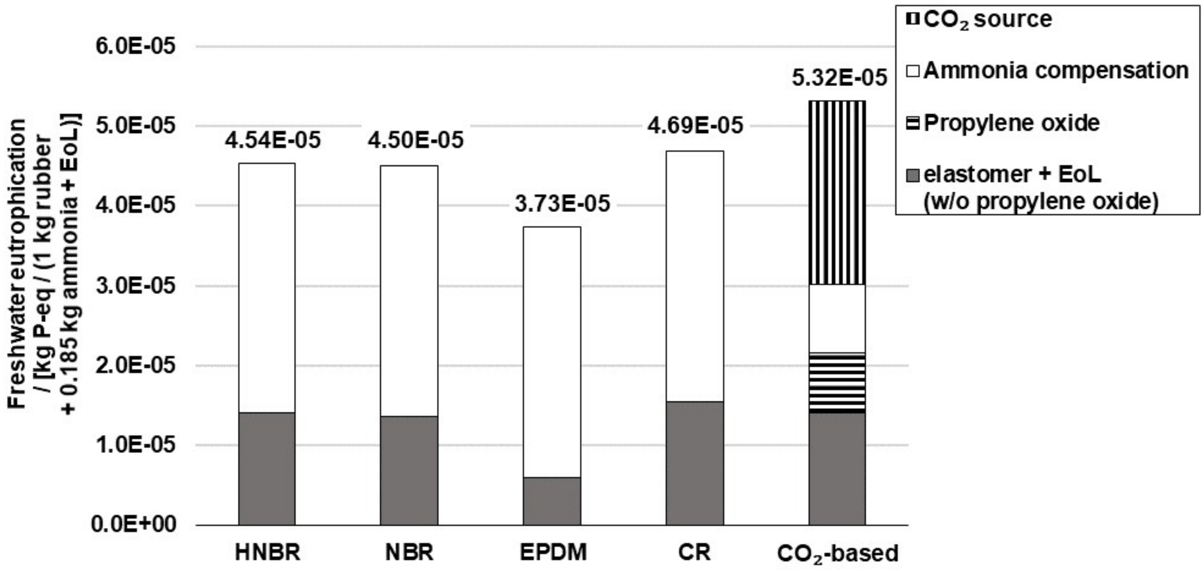

Figure S2: Freshwater eutrophication in kg phosphorous (P) equivalents of product systems for conventional and CO_2-based rubbers. The CO_2 source includes environmental impacts of the ammonia plant including CO_2 capture, CO_2 compression and CO_2 transport.

S3.2 Stratospheric ozone depletion

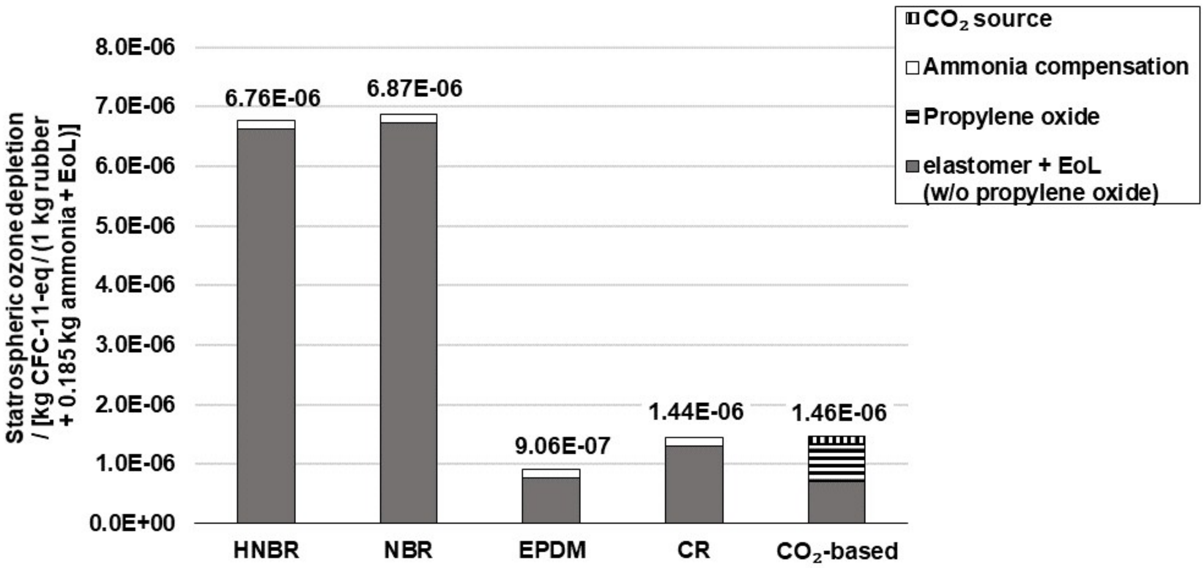

Figure S3: Stratospheric ozone depletion in kg CFC-11-equivalents of product systems for conventional and CO_2-based rubbers. The CO_2 source includes environmental impacts of the ammonia plant including CO_2 capture, CO_2 compression and CO_2 transport.

S3.3 Particulate matter formation

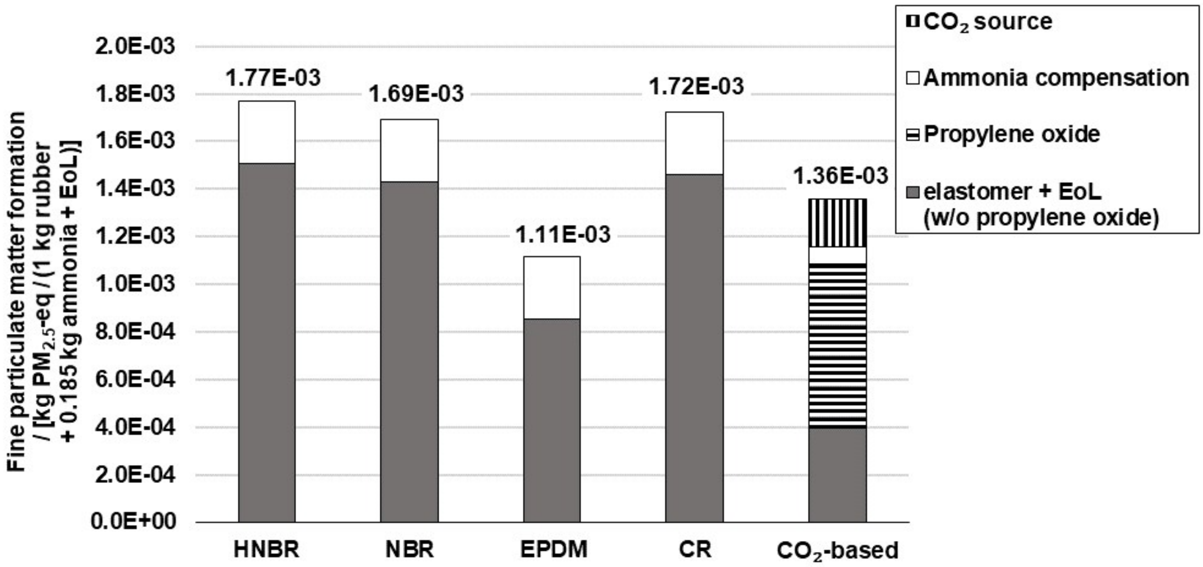

Figure S4: Fine particulate matter formation in kg $PM_{2.5}$-equivalents of product systems for conventional and CO_2-based rubbers. The CO_2 source includes environmental impacts of the ammonia plant including CO_2 capture, CO_2 compression and CO_2 transport.

S3.4 Photochemical ozone formation

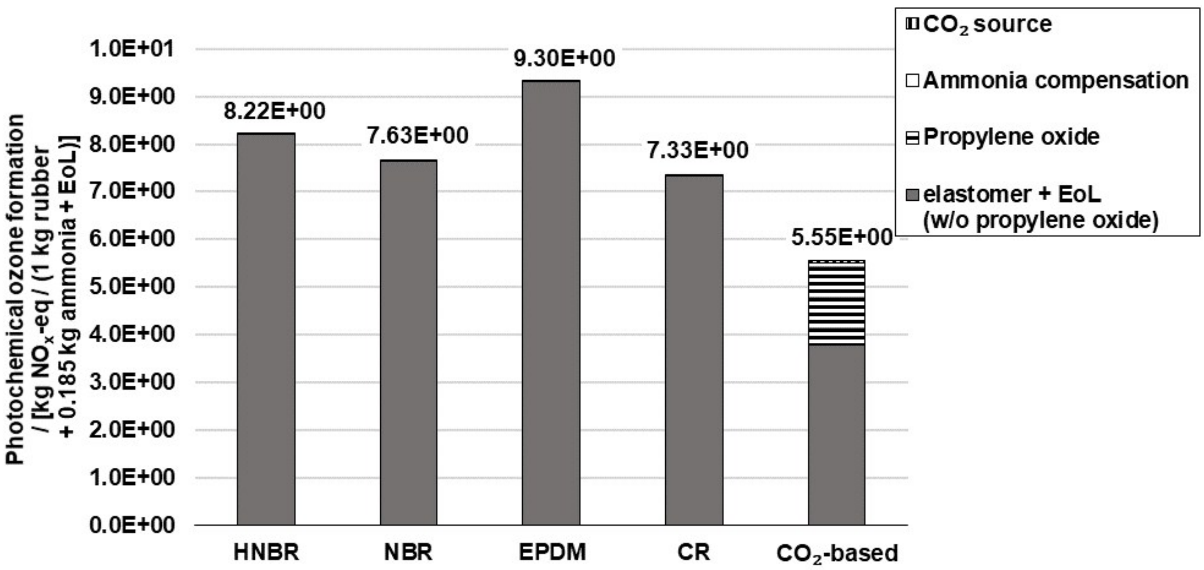

Figure S5: Photochemical ozone formation in kg NO_x-equivalents of product systems for conventional and CO_2-based rubbers. The CO_2 source includes environmental impacts of the ammonia plant including CO_2 capture, CO_2 compression and CO_2 transport.

S3.5 Terrestrial acidification

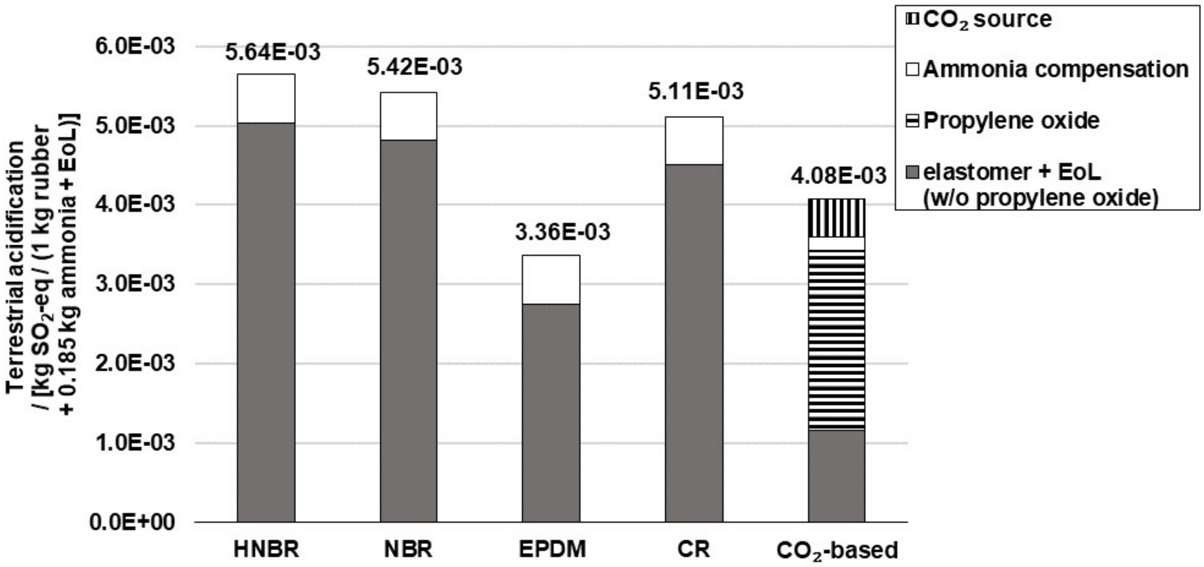

Figure S6: Terrestrial acidification in kg SO_2-equivalents of product systems for conventional and CO_2-based rubbers. The CO_2 source includes environmental impacts of the ammonia plant including CO_2 capture plus CO_2 compression and CO_2 transport.

S3.6 Marine eutrophication

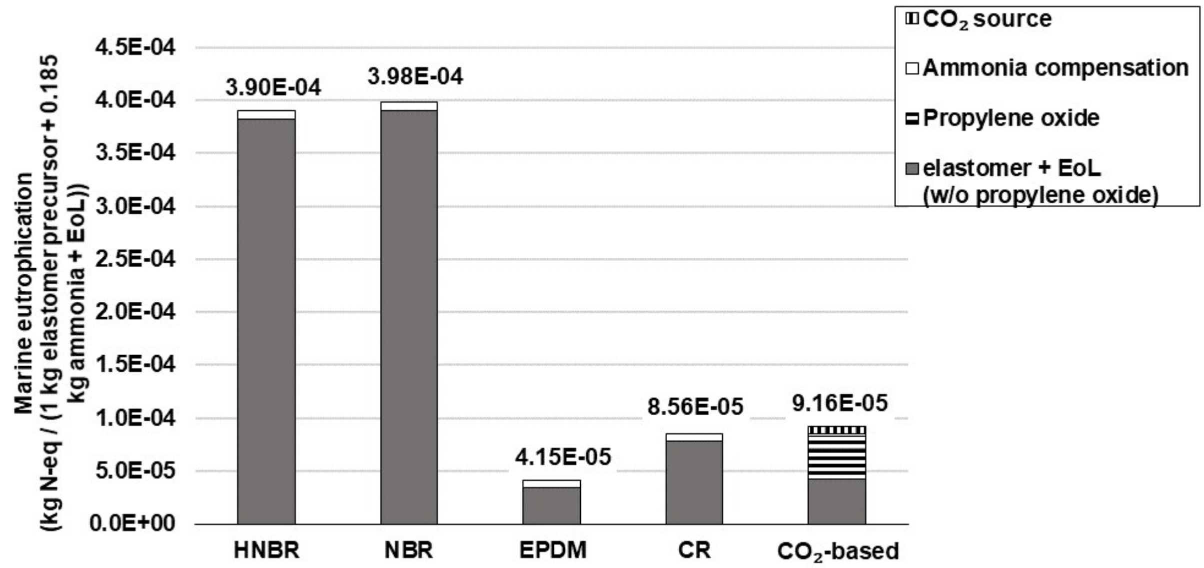

Figure S7: Marine eutrophication in kg nitrogen (N) equivalents of product systems for conventional and CO_2-based rubbers. The CO_2 source includes environmental impacts of the ammonia plant including CO_2 capture plus CO_2 compression and CO_2 transport.

S4 Product-specific global warming impacts

The functional unit of this LCA study includes three services: (i) the production of rubbers, (ii) the production of ammonia as the co-product of the CO_2-source and (iii) the disposal of rubbers, e.g. their incineration. However, in some cases a product-specific environmental impacts can be required[3,6]. To derive such product-specific impacts, all environmental impacts have to be allocated to the rubber or the ammonia production[7]. This allocation includes ambiguity to the results.

To illustrate the effect of allocation procedure, we defined two scenarios for CO_2-based rubbers: (i) a worst-case and (ii) a best-case allocation scenario. The worst-case allocation scenario assumes that all environmental impacts of CO_2 compression and transport are allocated solely to the CO_2-based rubber. In the best-case scenario, a credit is given for the amount of produced ammonia. The credit is based on the environmental impacts of a conventional ammonia plant without utilizing CO_2 for rubber production. Incineration impacts are not affected in both scenarios.

The global warming impacts of CO_2-based rubbers range between 4.83 kg CO_2-eq for the worst-case and 4.57 kg CO_2-eq for the best-case allocation (Figure S8, right side). Conventional rubbers range from 5.67 kg CO_2-eq for CR to 7.07 kg CO_2-eq for HNBR. CO_2-based rubbers reduce global warming impacts between 15 % (worst-case, CR) and 35 % (best-case, HNBR). Thus, CO_2-based rubbers reduce global warming impacts even in the worst-case allocation scenario.

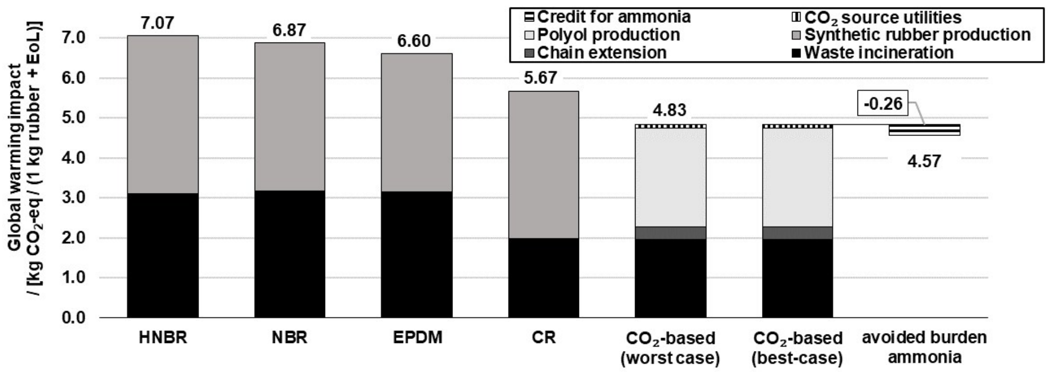

Figure S8: Product specific global warming impacts are shown in kg CO_2-equivalents per 1 kg of rubber and the end-of-life treatment of 1 kg rubber. For CO_2-based rubbers, environmental impacts were obtained by (i) a worst-case scenario (100 % of environmental impacts allocated to the CO_2-based rubbers) and (ii) a best-case scenario (credit for ammonia). The CO_2 source utilities include CO_2 compression and CO_2 transport.

S5 Influence of end-of-life allocation

This LCA study uses the so-called cut-off approach[8] to deal with the multifunctionality of waste treatment. The cut-off approach assumes that no environmental impacts are allocated to products of waste treatment. Thus, this assumption allocates all environmental impacts of waste treatment to the product under study and can be seen as a worst-case allocation from the perspective of rubber products. However, waste incineration has been shown to produce electricity and heat, especially if high calorific wastes like polymers are incinerated[9]. In LCA literature, the by-products of waste treatment are frequently credited by their conventional production technology. This approach is frequently referred to as the avoided-burden approach[7] and can be seen as a best-case scenario for rubber products.

To highlight the effect of allocation procedure for waste treatment products, we calculated the global warming impact and fossil resource depletion of CO_2-based and conventional rubbers for the avoided burden approach. For this purpose, we assumed an overall energy efficiency of 41 % for the energy recovery[9] from polymer incineration. The share of produced heat is assumed 72 % based on data for average municipal solid waste incinerators in Europe[9]. The given credit is based on the average German electricity grid and the supply of thermal energy based on natural gas[5]. To calculate the amount of produced electricity and heat, the lower heating values of CO_2-based and conventional rubbers are required. Unfortunately, no lower heating values could be obtained from scientific literature. To fill the data gap, we chose to estimate higher heating values of CO_2-based and conventional rubbers based on the Vondracek equation and correct the obtained higher heating values with the standard enthalpy of evaporation of formed water (44 kJ/mol[10]). The Vondracek equation has been shown to have the highest accuracy when estimating higher heating values of waste components[11]. The calculated lower heating values range between 21.78 MJ/kg for CO_2-based rubbers to 42.78 MJ/kg for EPDM.

The results for the avoided burden approach with regard to the global warming impact can be found in Figure S9. We used the same recipe for cross-linkable polyether carbonate polyols as in the main paper: approx. 20 % CO_2, approx. 2 % double bond moieties and a molar mass of polyols of approx. 4200 g/mol.

Global warming impacts of CO_2-based rubbers equal 4.08 kg CO_2-eq, if a credit is given for electricity and heat produced from waste incineration. For conventional rubbers, global warming impacts range between 5.06 kg CO_2-eq for CR and 5.90 kg CO_2-eq for HNBR. Credits for electricity and heat production range from 1.67 kg CO_2-eq for EPDM to 0.85 kg CO_2-eq for CO_2-based rubbers. CO_2-based rubbers have smaller lower heating values due to increased oxygen content (cf. Figure S1) and thus, CO_2-based rubbers have lower credits for electricity and heat production. However, CO_2-based rubbers reduce global warming impacts between 19 % for CR and 31 % for HNBR. For fossil resource depletion, reductions range between 15 % for CR and 25 % for HNBR.

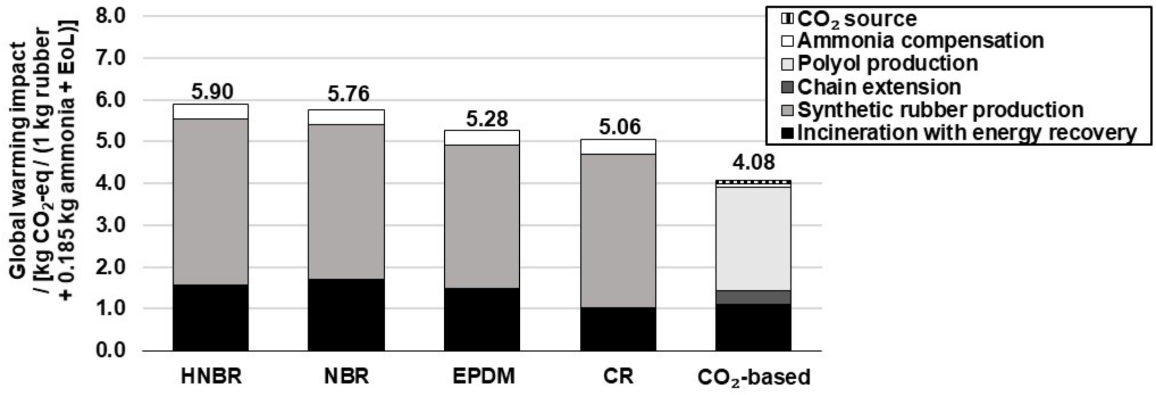

Figure S9: Global warming impacts in kg CO_2-equivalents of product systems for conventional and CO_2-based rubbers. The CO_2 source utilities include CO_2 compression and CO_2 transport. Here, a credit is given for produced electricity and heat from waste incineration and subtracted from waste incineration emissions.

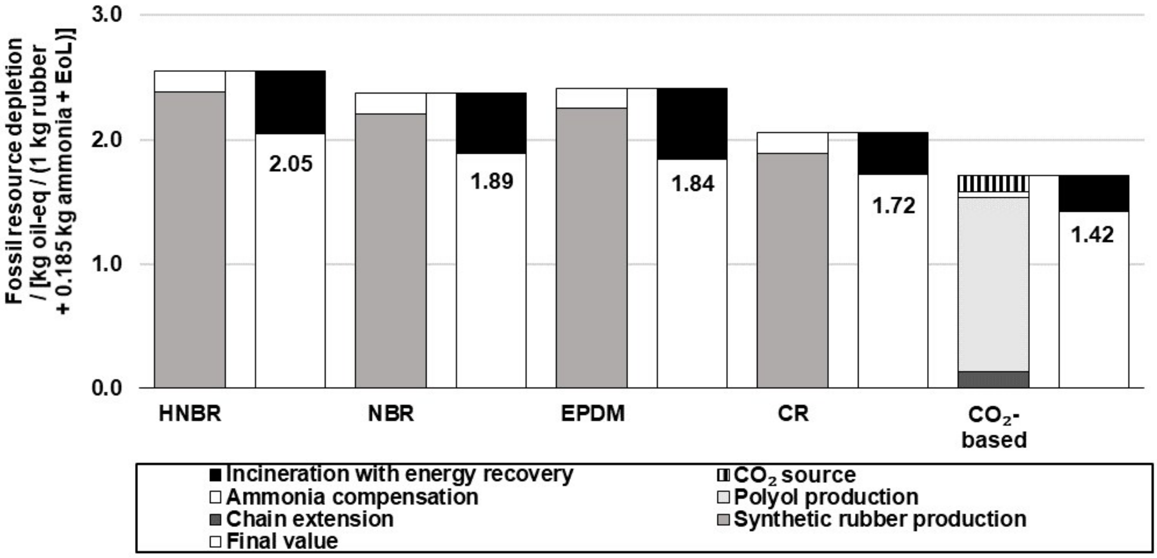

Figure S10: Fossil resource depletion in kg oil-equivalents of product systems for conventional and CO_2-based rubbers. The CO_2 source utilities include CO_2 compression and CO_2 transport. Here, a credit is given for produced electricity and heat from waste incineration (incineration with energy recovery). For conventional rubbers, the final fossil resource depletion is calculated by subtracting the credit for energy recovery from the fossil resource depletion of rubber production and the ammonia compensation. In case of CO_2-based rubbers, the credit is subtracted from the fossil resource depletion of chain extension, polyol production, ammonia compensation and the CO_2 source.

S6 References

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